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# A microscopic theory of fission dynamics based on the generator coordinate method

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# Preface

The development of a predictive and quantitative theory of fission remains one of the most daunting challenges in nuclear physics. Interest in the theory of fission spans 75 years, starting from the first theoretical approach by Bohr and Wheeler [1], which gave the basic picture of fission as that of a nucleus elongating to its breaking point, to later calculations which include dynamical aspects through the use of time-dependent Hartree-Fock [2], Langevin theory [3, 4, 5], Brownian motion [6, 7], and microscopic descriptions based on the Time-Dependent Generator Coordinate Method [8, 9, 10, 11].

A proper microscopic description of fission (i.e., starting from the nucleon degrees of freedom) brings with it all the known complexities of the quantum many-body problem [12], with the additional difficulties of describing the scission of the parent nucleus into two or more fragments within a quantum-mechanical context [13]. This book presents a quantum-mechanical description of the induced nuclear fission process from an initial compound state to scission, starting from protons, neutrons, and an effective interaction between them. This is an ambitious program that raises a host of fundamental questions such as: what are the relevant degrees of freedom throughout the process? How do the collective and intrinsic degrees couple during the fission process? How does a nucleus divide into two separate daughters in a quantum-mechanical description where its wave function can be non-local? How is the energy of the fissioning nucleus partitioned between the kinetic and excitation energies of its daughters? These and other questions about fission are currently being investigated through a variety of theoretical, computational, and experimental techniques that are generating a growing body of literature.

For a broad overview of various theoretical approaches to nuclear fission, the reader can consult the recent textbook by Krappe and Pomorski [14]. For a more specialized discussion of microscopic methods, we recommend the very thorough review by Schunck and Robledo [15]. In this manuscript we will focus in greater detail on the approach originally developed in the 1980's at the Bruyères-le-Châtel laboratory in France, which uses a collective Schrödinger-like equation derived from the time-dependent generator-coordinate method, with ingredients built from constrained Hartree-Fock-Bogoliubov solutions. The term "microscopic" in the present context refers to an approach that starts from protons, neutrons, and an effective (i.e., in-medium) interaction between them. The form of this interaction is inspired by more fundamental theories of nuclear matter, but still contains parameters that have to be adjusted to data. However these parameters were adjusted once and for all, and not tuned to reproduce the particular fission observables we will be discussing. The appeal of a microscopic approach is that it does not contain any parameters that depend on the mass, charge, configuration etc. of the nucleus. This is especially important in the case of fission studies where the parent nucleus eventually splits into two (or more) very different daughter nuclei. In addition, a microscopic approach allows both single-particle and collective degrees of freedom to be treated in a consistent manner. In this way, while the motion of individual nucleons can be described by a mean field, oscillations of this mean field about an equilibrium solution can provide the collective excitations of the system. Finally, the microscopic approach provides a natural description of the approach to scission as a progressive localization of the individual nucleons on the respective nascent fragments, and mitigates the otherwise jarring jump that would occur if we had to switch abruptly from a one-body to a two-body formalism. To be sure, the microscopic approach presented in this work is far from complete, but we felt that sufficient progress had been made to warrant taking stock of what has been accomplished so far.

The book is divided into two parts. The first part covers the mathematical tools used in our preferred approach to the fission problem. Chapter 1 gives a detailed overview of the formalism for a microscopic approach to the nuclear many body problem. The chapter gives a general introduction to the Hartree-Fock-Bogoliubov theory with multiple constraints. The formalism is specialized to the case of a finite-range interaction in chapter 2. Next, in chapter 3, the generator coordinate method is presented to construct a collective Hamiltonian from the underlying single-particle degrees of freedom, and the technique is extended to include the coupling between collective and intrinsic motion of the nucleus. Finally, the limiting adiabatic case is considered and the time-dependent treatment of the problem is discussed. The tools and techniques presented in this chapter have much wider applicability than to the fission problem alone, and we have strived to present them in a self-contained pedagogical manner. The second part of the book specializes the discussion to the fission problem. In chapter 4, the question of the choice of collective coordinates appropriate for the fission process is explored. The description of scission is then studied within a quantum mechanical context, along with the theory and practical aspects of calculating fission-fragment mass and energy distributions. The particular case of induced fission from $^{240}$Pu is presented in detail in chapter 5 to extract the energies and mass distributions of its primary fragments. Finally in chapter 6 we take a broader view of the microscopic approach to the fission problem and look at potential future directions in this field. In addition to presenting the research, we have sought to make this book more pedagogical by illustrating some of the concepts in part I by applying them to a relatively simple toy model of the nucleus, and by expanding the discussion in a series of appendices at the end of the book.

This book is intended as a reference for advanced graduate students and researchers in fission theory. It is also written for practitioners in the field who find themselves frustrated by the paucity of information which is often unavoidable in page-restricted scholarly articles. Therefore we have included illustrative examples throughout the text to hopefully make it easier for the reader to understand, implement, and verify the formalism that is presented here. Two of the authors, D. Gogny and J.-F. Berger, began this work in the 1980's with W. Younes joining the effort in 2006. All three of us have a longstanding interest in the beautiful complexity of the fission process and in trying to understand it as an emergent phenomenon from the underlying nucleon degrees of motion. Sadly D. Gogny passed away in May 2015, when this book was still in its early stages, but his presence and influence is on every page.

Walid Younes, Livermore, CA, USA, April 2017

Jean-François Berger, Leudeville, France, April 2017

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# Contents

# Part I
# Tools for a Microscopic Theory of the Nucleus

## Chapter 1
# Hartree-Fock-Bogoliubov theory

We review the general theory of the Hartree-Fock-Bogoliubov method in the context of the nuclear many-body problem. We examine the response of the Hartree-Fock-Bogoliubov solutions to a one-body external field and derive the formalism needed to impose multiple constraints on the calculations. Finally, a pedagogical example is given to illustrate the Hartree-Fock-Bogoliubov method using a schematic model of the nucleus.

## 1.1 General formalism

Let us recall here some generalities concerning the Bogoliubov theory (see also, e.g., [1, 2, 3, 4]). This theory is an extension of the mean-field approximation that allows one to take into account, in addition to the mean nuclear field, the pairing correlations between nucleons. This is a self-consistent framework that generalizes both the usual Hartree-Fock and BCS approximations. The approach designed by Bogoliubov is based on a simple linear transformation which mixes creation and destruction operators. This transformation defines quasi-particle (qp) creation and destruction operators in the form:

$$\begin{aligned} \eta_\mu^\dagger &= \sum_n \left( U_{n,\mu} a_n^\dagger + V_{n,\mu} a_n \right) \\ \eta_\mu &= \sum_n \left( U_{n,\mu}^* a_n + V_{n,\mu}^* a_n^\dagger \right) \end{aligned} \tag{1.1}$$

which represent the elementary excitations of a paired many-body system. For convenience we use Greek letters and Latin for quasi-particles and particles, respectively. The requirement that this transformation be unitary guarantees that the quasi-particle operators satisfy the usual anti-commutation rules:

$$\begin{aligned} \left\{ \eta_\mu^\dagger, \eta_\nu^\dagger \right\} &= \left\{ \eta_\mu, \eta_\nu \right\} = 0 \\ \left\{ \eta_\mu^\dagger, \eta_\nu \right\} &= \delta_{\mu\nu} \end{aligned}$$

Using the definition in Eq. (1.1), and the fact that the operators $a^\dagger, a$ satisfy similar rules we obtain the following relations:

$$\begin{aligned} \sum_n \left( U_{n,\mu} U_{n,\nu}^* + V_{n,\mu} V_{n,\nu}^* \right) &= \delta_{\mu,\nu} \\ \sum_n \left( U_{n,\mu} V_{n,\nu} + V_{n,\mu} U_{n,\nu} \right) &= 0 \end{aligned} \tag{1.2}$$

Since the transformation is unitary the inverse of Eq. (1.1) is given by Eq. (1.2)

$$\begin{aligned} a_n^\dagger &= \sum_\mu \left( U_{n,\mu}^* \eta_\mu^\dagger + V_{n,\mu} \eta_\mu \right) \\ a_n &= \sum_\mu \left( U_{n,\mu} \eta_\mu + V_{n,\mu}^* \eta_\mu^\dagger \right) \end{aligned} \tag{1.3}$$

and similar relations to Eq. (1.1) are deduced:

$$\begin{aligned}\sum_\mu \left(U_{m,\mu} U^*_{n,\mu} + V^*_{m,\mu} V^*_{n,\nu}\right) &= \delta_{m,n} \\ \sum_\mu \left(U_{m,\mu} V^*_{n,\mu} + V^*_{m,\mu} U_{n,\mu}\right) &= 0\end{aligned} \tag{1.4}$$

If we denote the transformation by the matrix

$$B_{n,\mu} \equiv \begin{pmatrix} U_{n,\mu} & V^*_{n,\mu} \\ V_{n,\mu} & U^*_{n,\mu} \end{pmatrix}$$

We observe that Eqs. (1.2) and (1.4) can be written as

$$\begin{aligned}\left[BB^\dagger\right]_{n,m} &= \delta_{m,n} \\ \left[B^\dagger B\right]_{\mu,\nu} &= \delta_{\mu,\nu}\end{aligned}$$

At this stage we assume that there exists a vacuum of the destruction operators $\eta_\mu$ and denote it as $\left|\tilde{O}\right\rangle$ . By definition the latter satisfies $\eta_\mu \left|\tilde{O}\right\rangle = 0$ and consequently it depends on the coefficients $U, V$ of the Bogolyubov transformation. In order to define these coefficients one identifies the vacuum as the nucleus ground state and applies a variational principle consisting in the minimization of the energy calculated with $\left|\tilde{O}\right\rangle$ :

$$E\left(U, V\right) = \left\langle \tilde{O} \left| H \right| \tilde{O} \right\rangle$$

In what follows we detail a little more the minimization procedure and derive the so-called Bogoliubov equations.

First one has to express the energy given by the mean value of $H$ in the Bogoliubov vacuum. This calculation is made easy by noticing that we can still apply Wick's theorem due the fact that $\left|\tilde{O}\right\rangle$ is a vacuum and that the Bogoliubov transformation is linear. The procedure is very similar to the one used in the Hartree-Fock case with the difference that we must introduce "abnormal" contractions which are not present in the Hartree-Fock formalism:

$$\left\langle \tilde{O} \left| a_m a_n \right| \tilde{O} \right\rangle, \quad \left\langle \tilde{O} \left| a^\dagger_m a^\dagger_n \right| \tilde{O} \right\rangle$$

Let us recall the expression of Wick's theorem in the following case:

$$\begin{aligned}\left\langle \tilde{O} \left| a^\dagger_m a^\dagger_n a_p a_q \right| \tilde{O} \right\rangle = &\left\langle \tilde{O} \left| a^\dagger_m a_q \right| \tilde{O} \right\rangle \left\langle \tilde{O} \left| a^\dagger_n a_p \right| \tilde{O} \right\rangle \\ &- \left\langle \tilde{O} \left| a^\dagger_m a_p \right| \tilde{O} \right\rangle \left\langle \tilde{O} \left| a^\dagger_n a_q \right| \tilde{O} \right\rangle \\ &+ \left\langle \tilde{O} \left| a^\dagger_m a^\dagger_n \right| \tilde{O} \right\rangle \left\langle \tilde{O} \left| a_p a_q \right| \tilde{O} \right\rangle\end{aligned} \tag{1.5}$$

Abnormal contractions occur here because the Bogoliubov vacuum is a superposition of states with different number of particles. We are content to give the final expression of the energy in the form:

$$\begin{aligned} E\left(U,V\right) = &\sum_{m,n} T_{m,n}\rho_{n,m} + \frac{1}{2}\sum_{m,n,p,q}\left\langle m,n\left|V\right|\widetilde{p,q}\right\rangle \rho_{q,n}\rho_{p,m} \\ &+\frac{1}{4}\sum_{m,n,p,q}\left\langle m,n\left|V\right|\widetilde{p,q}\right\rangle \kappa_{q,p}\kappa^*_{n,m} \end{aligned} \tag{1.6}$$

where we have used the notations $|\widetilde{p,q}\rangle = |p,q\rangle - |q,p\rangle$ and

$$\kappa_{m,n} = \left\langle \tilde{O}\left|a_m a_n\right|\tilde{O}\right\rangle, \quad \rho_{m,n} = \left\langle \tilde{O}\left|a^\dagger_n a_m\right|\tilde{O}\right\rangle$$

are the pairing tensor and the one-body density matrix, respectively. It is obvious that the pairing tensor is antisymmetric and the density matrix hermitian,

$$\kappa_{m,n} = -\kappa_{n,m}, \quad \rho_{m,n} = \rho^*_{n,m}$$

Notice also that we use quantities and their complex conjugate which is the convenient form to express the variational equations as will be seen later.

At this stage it is interesting to derive the expressions of the density matrix and pairing tensor in terms of the coefficients of the Bogoliubov transformation. This is achieved simply by using Eq. (1.3) and taking into account the property of the ground state to be the vacuum of the quasi-particles's. We find:

$$\kappa_{m,n} = \sum_\mu U_{m,\mu}V^*_{n,\mu}, \quad \rho_{m,n} = \sum_\mu V_{n,\mu}V^*_{m,\mu} \tag{1.7}$$

Since the total energy involves only these quantities we will perform the variation with respect to the matrix elements of $\rho$ and $\kappa$ instead of the variables $U, V$. The question however is to perform variations which satisfy Eqs. (1.2) and (1.4). A very elegant way to express these relations in terms of $\rho$ and $\kappa$ is given by introducing the generalized density matrix defined as:

$$R \equiv \begin{pmatrix} R^{1,1} & R^{1,2} \\ R^{2,1} & R^{2,2} \end{pmatrix} = \begin{pmatrix} \rho & -\kappa \\ \kappa^* & I-\rho^* \end{pmatrix} \tag{1.8}$$

where $I$is the identity matrix. In fact it can be shown that the unitary conditions (1.2) and (1.4) are equivalent to

$$R^2 = R \tag{1.9}$$

and conversely Eq. (1.9) guarantees the unitarity of the Bogoliubov transformation.

Consequently we will perform variations by adding the subsidiary condition (1.9) and also the constraint that the average number of protons and neutrons correspond to the nucleus under consideration. For this we introduce Lagrange parameters $\lambda_p, \lambda_n, \Lambda_{m,n}$ and write the quantity to be minimized in the form

$$\begin{aligned} E(\rho, \kappa, \lambda_p, \lambda_n, \Lambda) &= E(\rho, \kappa) - \lambda_p \left\langle \tilde{O} \left| \hat{N}_p \right| \tilde{O} \right\rangle - \lambda_n \left\langle \tilde{O} \left| \hat{N}_n \right| \tilde{O} \right\rangle \\ &\quad - \mathrm{Tr}\left[\Lambda \left(R^2 - R\right)\right] \\ &\equiv E(\rho, \kappa, \lambda_p, \lambda_n) - \mathrm{Tr}\left[\Lambda \left(R^2 - R\right)\right] \end{aligned}$$

This long but necessary introduction simplifies considerably the derivation of the variational equations. In effect, by taking the first order variation with respect to the matrix elements of the generalized density matrix which is equivalent to performing the variations with respect to $\rho$ and $\kappa$, we obtain

$$\delta E(\rho, \kappa, \lambda_p, \lambda_n) = \sum_{i,j,m,n} \frac{\delta}{\delta R^{i,j}_{m,n}} E(\rho, \kappa, \lambda_p, \lambda_n) \delta R^{i,j}_{m,n}$$

which in turn takes the form of a trace,

$$\delta E(\rho, \kappa, \lambda_p, \lambda_n) = \mathrm{Tr}\,(H \delta R)$$

with $H$, the Bogoliubov Hamiltonian, defined as[1]

$$H^{i,j}_{m,n} = \frac{\delta E(\rho, \kappa, \lambda_p, \lambda_n, \Lambda)}{\delta R^{j,i}_{n,m}} \tag{1.10}$$

Consequently, thanks to the properties of the trace we can reorder the operators and obtain the compact form

$$\delta E(\rho, \kappa, \lambda_p, \lambda_n, \Lambda) = \mathrm{Tr}\left\{\left[H - (\Lambda R + R\Lambda - \Lambda)\right] \delta R\right\}$$

The condition that the energy be stationary i.e., an extremum or a minimum reads

$$\delta E(\rho, \kappa, \lambda_p, \lambda_n, \Lambda) = \mathrm{Tr}\left\{\left[H - (\Lambda R + R\Lambda - \Lambda)\right] \delta R\right\} = 0, \quad \forall\, \delta R$$

which implies

$$H - (\Lambda R + R\Lambda - \Lambda) = 0$$

at the stationary point.

It remains to eliminate the matrix of Lagrange parameters. This is easily achieved in the following manner. In effect by multiplying the equation above

[1] In an alternate formulation, Eq. (1.6) can be symmetrized so that it depends explicitly on both $\rho$ and $\rho^*$, as in [5]. In that case, the density and its complex conjugate are treated as independent variables when minimizing the energy, and Eq. (1.10) must be modified by a factor of 2 on the right-hand side, as in Eq. (2) of [5].

to the right by $R$ and taking into account the condition $R^2 = R$, we obtain

$$HR - \Lambda R \Lambda = 0$$

Performing the same calculation by multiplying to the left the result is

$$RH - \Lambda R \Lambda = 0$$

These two equations lead to the conclusion that the stationary solutions satisfy the condition

$$[H(R), R] = 0 \tag{1.11}$$

In this notation we make explicit the fact that the Bogoliubov Hamiltonian is a functional of the generalized density matrix. The matrix elements of $H$ are given by

$$\begin{aligned}
H^{1,1}_{i,j} &= \frac{\delta E}{\delta R^{1,1}_{j,i}} = \frac{\delta E}{\delta \rho_{j,i}} = h_{i,j} - \lambda_{qi}\delta_{i,j} \equiv e_{i,j} \\
H^{2,2}_{i,j} &= \frac{\delta E}{\delta R^{2,2}_{j,i}} = \frac{\delta E}{\delta (1 - \rho^*_{j,i})} = -\frac{\delta E}{\delta \rho^*_{j,i}} \equiv -e^*_{i,j} \\
H^{1,2}_{i,j} &= \frac{\delta E}{\delta R^{2,1}_{j,i}} = \frac{\delta E}{\delta \kappa^*_{j,i}} \equiv \Delta_{i,j} \\
H^{2,1}_{i,j} &= \frac{\delta E}{\delta R^{1,2}_{j,i}} = -\frac{\delta E}{\delta \kappa_{j,i}} = -\Delta^*_{i,j}
\end{aligned} \tag{1.12}$$

We thus recognize the well-known form of the Bogoliubov Hamiltonian [1]

$$H = \begin{pmatrix} e & \Delta \\ -\Delta^* & -e^* \end{pmatrix} \tag{1.13}$$

The quantities entering in its definition are given explicitly below

$$\begin{aligned}
e_{i,j} &= T_{i,j} - \lambda_q \delta_{i,j}\delta_{q,q_i} + \sum_{kl} \langle i,k| V \left|\widetilde{j,l}\right\rangle \rho_{l,k} \\
\Delta_{i,j} &= \frac{1}{2}\sum_{kl} \langle i,j| V \left|\widetilde{k,l}\right\rangle \kappa_{l,k}
\end{aligned}$$

Equation (1.11) and the definitions just given above define completely the problem to be solved and show clearly that it involves quite complicated non-linear equations. Equation (1.11) tells us that $H$ and $R$ can be made diagonal in the same representation. The question is then to find a procedure that achieves a simultaneous diagonalization of both matrices.

Let us then perform the diagonalization of the Bogoliubov Hamiltonian and denote its eigenvectors $v$ as

$$Hv = \begin{pmatrix} e & \Delta \\ -\Delta^* & -e^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \varepsilon \begin{pmatrix} U \\ V \end{pmatrix}$$

Since $H$ is hermitian, the eigenvalues $\varepsilon$ are real. It can be shown that the eigenvectors are associated by pairs, which means that if we find a solution

$$Hv = \begin{pmatrix} e & \Delta \\ -\Delta^* & -e^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \varepsilon \begin{pmatrix} U \\ V \end{pmatrix}, \quad \varepsilon > 0$$

then the vector

$$\begin{pmatrix} V^* \\ U^* \end{pmatrix}$$

is also solution but with $\varepsilon < 0$. Accordingly if the dimension of the Hamiltonian is $2N$, then there are $N$ "positive" and $N$ "negative" eigenvectors. Therefore the matrix $B$ which diagonalizes $H$ can be written as the block matrix

$$B \equiv \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \tag{1.14}$$

The first $N$ columns correspond to the positive eigenvalues and the other $N$ columns correspond to the negative ones. Notice that this matrix satisfies the identity

$$HB = B \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix} \tag{1.15}$$

It now remains to show that the same transformation $B$ diagonalizes the generalized density matrix. For this purpose it is convenient to rewrite equation (1.8) in the form

$$\begin{aligned} R &= I - \left\langle \tilde{O} \middle| \begin{pmatrix} A \\ A^\dagger \end{pmatrix} \begin{pmatrix} A^\dagger & A \end{pmatrix} \middle| \tilde{O} \right\rangle \\ &= \begin{pmatrix} I - \left\langle \tilde{O} \middle| AA^\dagger \middle| \tilde{O} \right\rangle & -\left\langle \tilde{O} \middle| AA \middle| \tilde{O} \right\rangle \\ -\left\langle \tilde{O} \middle| A^\dagger A^\dagger \middle| \tilde{O} \right\rangle & I - \left\langle \tilde{O} \middle| A^\dagger A \middle| \tilde{O} \right\rangle \end{pmatrix} \end{aligned}$$

where $A$ and $A^\dagger$ are column or row vectors of operators $a_n$ and $a_n^\dagger$, and $I$ is the unity matrix. Then, using Eq. (1.1), it is easy to see that $B^\dagger RB$ can be expressed as

$$B^\dagger RB = \begin{pmatrix} I - \left\langle \tilde{O} \middle| \eta\eta^\dagger \middle| \tilde{O} \right\rangle & -\left\langle \tilde{O} \middle| \eta\eta \middle| \tilde{O} \right\rangle \\ -\left\langle \tilde{O} \middle| \eta^\dagger\eta^\dagger \middle| \tilde{O} \right\rangle & I - \left\langle \tilde{O} \middle| \eta^\dagger\eta \middle| \tilde{O} \right\rangle \end{pmatrix}$$

Now if we define the Bogoliubov state as the vacuum of the quasi-particles, then we find the diagonal form

$$B^\dagger RB = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}$$

which shows that $B$ diagonalizes $R$. The quasi-particle vacuum $\left|\tilde{O}\right\rangle$ can be written formally as

$$\left|\tilde{O}\right\rangle = \prod_{\mu} \eta_\mu \left|0\right\rangle$$

and can be identified with the ground the state since by destroying all quasi-particles with positive energy we have built the state of lowest energy. Thus by imposing that $R$ is diagonal in the representation diagonalizing the Bogoliubov Hamiltonian, we are led to the correct and consistent interpretation of the vacuum.

## 1.2 Perturbation of the generalized density matrix around the HFB solution

In this section we study the stability of the Hartree-Fock-Bogoliubov (HFB) solutions and also introduce the so-called theory of elementary excitations of the HFB fields (i.e., the QRPA). It generalizes the random phase theory (RPA) used to describe excitation modes associated with small amplitude oscillations of the Hartree-Fock mean field. As we will also see it will be useful to study the response of the HFB fields to some prescribed external fields and related quantities; mass parameters, zero point energy corrections, adjustment of Lagrange parameters, etc.

Let us define a generalized density matrix corresponding to some Bogoliubov vacuum denoted as $\left|\tilde{O}'\right\rangle$ corresponding to a small deviation from $\left|\tilde{O}\right\rangle$, i.e. $\left|\tilde{O}'\right\rangle = \left|\tilde{O} + \delta\tilde{O}\right\rangle$. In the representation given by the solutions of the HFB equations for some Bogoliubov vacuum $\left|\tilde{O}\right\rangle$, we denote the generalized density matrix as ${}^{(0)}R$. By definition this matrix is diagonal and, as shown above, it takes the form

$${}^{(0)}R = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix} \tag{1.16}$$

The density matrix associated with the vacuum $\left|\tilde{O}'\right\rangle$ is then defined as

$$R = \begin{pmatrix} I - \left\langle \tilde{O}' \left| \eta\eta^\dagger \right| \tilde{O}' \right\rangle & -\left\langle \tilde{O}' \left| \eta\eta \right| \tilde{O}' \right\rangle \\ -\left\langle \tilde{O}' \left| \eta^\dagger\eta^\dagger \right| \tilde{O}' \right\rangle & I - \left\langle \tilde{O}' \left| \eta^\dagger\eta \right| \tilde{O}' \right\rangle \end{pmatrix}$$

This matrix can be represented by block matrices in the form

$$R = \begin{pmatrix} R^{1,1} & R^{1,2} \\ R^{2,1} & R^{2,2} \end{pmatrix} \tag{1.17}$$

The matrix elements of the block matrices in the representation in question are

$$
\begin{aligned}
R^{1,1}_{\mu,\nu} &= \left\langle \tilde{O}' \left| \eta^\dagger_\nu \eta_\mu \right| \tilde{O}' \right\rangle \\
R^{1,2}_{\mu,\nu} &= \left\langle \tilde{O}' \left| \eta_\nu \eta_\mu \right| \tilde{O}' \right\rangle \\
R^{2,1}_{\mu,\nu} &= \left\langle \tilde{O}' \left| \eta^\dagger_\nu \eta^\dagger_\mu \right| \tilde{O}' \right\rangle \\
R^{2,2}_{\mu,\nu} &= \left\langle \tilde{O}' \left| \eta_\nu \eta^\dagger_\mu \right| \tilde{O}' \right\rangle
\end{aligned}
$$

Since $\left| \tilde{O}' \right\rangle$ is a Bogoliubov vacuum, the density matrix is idempotent and therefore satisfies the identity

$$R^2 = R \tag{1.18}$$

We further assume that $\left| \tilde{O}' \right\rangle$ does not depart too much from $\left| \tilde{O} \right\rangle$, which means that $R$ can be expanded around ${}^{(0)}R$ up to second order in the form

$$R = {}^{(0)}R + {}^{(1)}R + {}^{(2)}R$$

with

$${}^{(i)}R \ll {}^{(0)}R$$

for $i = 1, 2$. By using this expansion in equation (1.18) we are going to find constraints on the matrix elements of ${}^{(i)}R$. In effect (1.16) gives

$$
\begin{aligned}
R^2 = {}^{(0)}R^2 + {}^{(0)}R^{(1)}R + {}^{(1)}R^{(0)}R + {}^{(1)}R^{(1)}R \\
+{}^{(2)}R^{(0)}R + {}^{(0)}R^{(2)}R + \mathcal{O}\left({}^{(3)}R\right)
\end{aligned}
$$

In this expression the notation $\mathcal{O}\left({}^{(3)}R\right)$ means that the first term neglected is a third order contribution. By identifying this result with $R$ and taking into account ${}^{(0)}R^2 = {}^{(0)}R$, we obtain a set of relations

$$
\begin{aligned}
{}^{(0)}R^{(1)}R + {}^{(1)}R^{(0)}R &= {}^{(1)}R \\
{}^{(2)}R^{(0)}R + {}^{(0)}R^{(2)}R + {}^{(1)}R^2 &= {}^{(2)}R
\end{aligned}
\tag{1.19}
$$

Using the matrix representation (1.16) and (1.17) it is easy to show that the first relation reduces to

$$
\begin{pmatrix} 0 & {}^{(1)}R^{1,2} \\ {}^{(1)}R^{2,1} & 2\,{}^{(1)}R^{2,2} \end{pmatrix} = \begin{pmatrix} {}^{(1)}R^{1,1} & {}^{(1)}R^{1,2} \\ {}^{(1)}R^{2,1} & {}^{(1)}R^{2,2} \end{pmatrix}
$$

which implies

$$^{(1)}R^{1,1} = {}^{(1)}R^{2,2} = 0, \quad {}^{(1)}R^{1,2} \neq 0, {}^{(1)}R^{2,1} \neq 0$$

One concludes that the first order contribution to $R$ contains only off-diagonal blocks,

$$^{(1)}R = \begin{pmatrix} 0 & {}^{(1)}R^{1,2} \\ {}^{(1)}R^{2,1} & 0 \end{pmatrix} \tag{1.20}$$

Since the generalized density is a hermitian operator, the block matrices must satisfy

$$^{(1)}R^{1,2\dagger} ={}^{(1)} R^{2,1} \tag{1.21}$$

and it must me antisymmetric

$$^{(1)}R^{2,1T} = -{}^{(1)}R^{2,1} \tag{1.22}$$

The second relation in Eq. (1.19) determines the matrix elements of the second-order contribution to R. Again by using the matrix definition of (Eqs. (1.16),(1.20)) we find

$$\begin{pmatrix} {}^{(1)}R^{1,2(1)}R^{2,1} & {}^{(2)}R^{1,2} \\ {}^{(2)}R^{2,1} & 2^{(2)}R^{2,2} + {}^{(1)}R^{2,1(1)}R^{1,2} \end{pmatrix} = \begin{pmatrix} {}^{(2)}R^{1,1} & {}^{(2)}R^{1,2} \\ {}^{(2)}R^{2,1} & {}^{(2)}R^{2,2} \end{pmatrix}$$

This equation tells us that the matrix elements of $^{(2)}R$ are

$$\begin{aligned} {}^{(2)}R^{1,1} &= {}^{(1)}R^{1,2(1)}R^{2,1} \\ {}^{(2)}R^{2,2} &= -{}^{(1)}R^{2,1(1)}R^{1,2} \\ {}^{(2)}R^{1,2} \text{ and } {}^{(2)}R^{2,1} &\text{ are arbitrary, but second order} \end{aligned} \tag{1.23}$$

It is with this decomposition of the generalized density matrix that we study in the next section the stability of the HFB ground state.

## 1.3 Stability of the HFB vacuum and definition of the QRPA matrix

By means of the results obtained in the previous section we expand up to second order the total energy of the system calculated with the Bogoliubov vacuum $\left|\tilde{O}'\right\rangle$. This variation can be written as

$$\begin{aligned} E(R) = E\left({}^{(0)}R\right) &+ \sum_{\mu,\nu,i,j} \left[\frac{\delta E(R)}{\delta R^{i,j}_{\mu\nu}}\right]_{R={}^{(0)}R} {}^{(1)}R^{i,j}_{\mu,\nu} \\ &+ \sum_{\mu,\nu,i} \left[\frac{\delta E(R)}{\delta R^{i,i}_{\mu,\nu}}\right]_{R={}^{(0)}R} {}^{(2)}R^{i,i}_{\mu,\nu} \\ &+ \frac{1}{2} \sum_{i,j,k,l,\mu,\nu,\lambda,\sigma} \left[\frac{\delta^2 E(R)}{\delta R^{i,j}_{\mu,\nu} \delta R^{k,l}_{\lambda,\sigma}}\right]_{R={}^{(0)}R} {}^{(1)}R^{i,j}_{\mu,\nu}\, {}^{(1)}R^{k,l}_{\lambda,\sigma} \end{aligned} \tag{1.24}$$

where $i \neq j = 1,2$ and $k \neq l = 1,2$. According to Eqs. (1.20) and (1.10) we express the first order term as

$$\left[\frac{\delta E(R)}{\delta R^{i,j}_{\mu\nu}}\right]_{R={}^{(0)}R} = H^{i,j}_{\mu,\nu}$$

with $i \neq j = 1,2$. Since we work in the representation which diagonalizes $H$ this term vanishes and we are left with second order terms. The first of them, on account of Eqs. (1.21), (1.23), (1.10) and (1.15) ($H^{i,i}_{\mu,\nu} = (-1)^{i+1}\, \varepsilon_\mu \delta_{\mu,\nu}$), can be expressed as

$$\begin{aligned} \sum_{i,\mu,\nu} \left[\frac{\delta E(R)}{\delta R^{i,i}_{\mu\nu}}\right]_{R={}^{(0)}R} {}^{(2)}R^{i,i}_{\mu\nu} &= \sum_{\mu,\lambda} \epsilon_\mu ({}^{(1)}R^{1,2}_{\mu,\lambda}\, {}^{(1)}R^{2,1}_{\lambda,\mu} + {}^{(1)}R^{2,1}_{\mu,\lambda}\, {}^{(1)}R^{1,2}_{\lambda,\mu}) \\ &= \sum_{\mu,\lambda} (\epsilon_\mu + \epsilon_\lambda) {}^{(1)}R^{1,2}_{\mu,\lambda}\, {}^{(1)}R^{2,1}_{\lambda,\mu} \end{aligned}$$

As we will see later it is convenient to rewrite this contribution in a symmetric form

$$\begin{aligned} \sum_{\mu,\lambda} (\epsilon_\mu + \epsilon_\lambda) {}^{(1)}R^{1,2}_{\mu,\lambda}\, {}^{(1)}R^{2,1}_{\lambda,\mu} = \frac{1}{2} \Bigg[ &\sum_{\nu\mu\lambda\sigma} {}^{(1)}R^{2,1*}_{\mu,\lambda} (\epsilon_\mu + \epsilon_\nu) \delta_{\nu,\lambda} \delta_{\mu,\sigma}\, {}^{(1)}R^{2,1}_{\mu,\lambda} \\ &+ {}^{(1)}R^{2,1}_{\mu,\lambda} (\epsilon_\mu + \epsilon_\nu) \delta_{\nu,\lambda} \delta_{\mu,\sigma}\, {}^{(1)}R^{2,1*}_{\mu,\lambda} \Bigg] \end{aligned} \tag{1.25}$$

which can also be written in the compact form

$$\sum_{\mu,\lambda} (\epsilon_\mu + \epsilon_\lambda) {}^{(1)}R^{1,2}_{\mu,\lambda}\, {}^{(1)}R^{2,1}_{\lambda,\mu} = \frac{1}{2} \left( {}^{(1)}R^{2,1*} \quad {}^{(1)}R^{2,1} \right) \begin{pmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{pmatrix} \begin{pmatrix} {}^{(1)}R^{2,1} \\ {}^{(1)}R^{2,1*} \end{pmatrix}$$

where we have defined

$$\varepsilon_{(\nu\mu),(\sigma\lambda)} = \quad (\epsilon_\mu + \epsilon_\nu) \delta_{\nu,\lambda} \delta_{\mu,\sigma}$$

It remains to expand the last term in equation (1.24). There are many ways to proceed. We choose to start with the expression of the second variation of the energy written in the single-particle basis on which the qp are expanded:[2]

$$\delta^2 E \equiv \underbrace{\frac{1}{2}\sum_{m,n,p,q} \langle m,n|\, V\, |\widetilde{p,q}\rangle\, \delta\rho_{q,n}\delta\rho_{p,m}}_{\equiv\delta^2 E_{pot}} + \underbrace{\frac{1}{4}\sum_{m,n,p,q} \langle m,n|\, V\, |\widetilde{p,q}\rangle\, \delta\kappa_{q,p}\delta\kappa^*_{n,m}}_{\equiv\delta^2 E_{pair}} \tag{1.26}$$

and use the relation

$$\begin{pmatrix} \delta\rho & -\delta\kappa \\ \delta\kappa^* & -\delta\rho^* \end{pmatrix} = B \begin{pmatrix} 0 & {}^{(1)}R^{1,2} \\ {}^{(1)}R^{2,1} & 0 \end{pmatrix} B^\dagger \tag{1.27}$$

to rewrite this second-order variation of the energy in the form given in Eq. (1.24). From Eq. (1.27) we obtain

$$\begin{aligned} \delta\rho &= U^{(1)}R^{1,2}V^T + V^{*(1)}R^{2,1}U^\dagger \\ \delta\kappa &= -\left[U^{(1)}R^{1,2}U^T + V^{*(1)}R^{2,1}V^\dagger\right] \end{aligned} \tag{1.28}$$

We show the meaning of this matrix notation in the case of a matrix element $\delta\rho_{q,n}$.We write

$$\begin{aligned} \delta\rho_{q,n} &= \left[U^{(1)}R^{1,2}V^T + V^{*(1)}R^{2,1}U^\dagger\right]_{q,n} \\ &= \sum_{\mu,\nu}\left[U_{q,\mu}{}^{(1)}R^{1,2}_{\mu,\nu}V_{n,\nu} + V^*_{q,\mu}{}^{(1)}R^{2,1}_{\mu,\nu}U^*_{n,\nu}\right] \end{aligned}$$

After substitution in the first term of (1.26) we obtain the expression

$$\begin{aligned} \delta^2 E_{pot} = \frac{1}{2}\sum_{m,n,p,q}\sum_{\mu,\nu,\lambda,\sigma} &\langle m,n|\, V\, |\widetilde{p,q}\rangle \left(U_{q,\mu}{}^{(1)}R^{1,2}_{\mu,\nu}V_{n,\nu} + V^*_{q,\mu}{}^{(1)}R^{2,1}_{\mu,\nu}U^*_{n,\nu}\right) \\ &\times \left(U_{p,\lambda}{}^{(1)}R^{1,2}_{\lambda,\sigma}V_{m,\sigma} + V^*_{p,\lambda}{}^{(1)}R^{2,1}_{\lambda,\sigma}U^*_{m,\sigma}\right) \end{aligned}$$

It is very convenient to define the following kets

$$\begin{aligned} |U_\mu\rangle &= \sum_q U_{q,\mu}\, |q\rangle \\ |V_\mu\rangle &= \sum_q V^*_{q,\mu}\, |q\rangle \end{aligned} \tag{1.29}$$

[2] Note that the expression for $\delta^2 E$ does not explicitly account for any dependence of the potential on the density for the sake of simplicity, but the extension is relatively straightforward (see, e.g., [6]).

and we then have

$$\begin{aligned}
\delta^2 E_{pot} = \frac{1}{2} \sum_{\mu,\nu,\lambda,\sigma} \Big\{ & \langle V_\sigma, V_\nu | \, V \left| \widetilde{U_\lambda, U_\mu} \right\rangle {}^{(1)}R^{1,2}_{\mu,\nu} {}^{(1)}R^{1,2}_{\lambda,\sigma} \\
& + \langle U_\sigma, V_\nu | \, V \left| \widetilde{V_\lambda, U_\mu} \right\rangle {}^{(1)}R^{1,2}_{\mu,\nu} {}^{(1)}R^{2,1}_{\lambda,\sigma} \\
& + \langle V_\sigma, U_\nu | \, V \left| \widetilde{U_\lambda, V_\mu} \right\rangle {}^{(1)}R^{2,1}_{\mu,\nu} {}^{(1)}R^{1,2}_{\lambda,\sigma} \\
& + \langle U_\sigma, U_\nu | \, V \left| \widetilde{V_\lambda, V_\mu} \right\rangle {}^{(1)}R^{2,1}_{\mu,\nu} {}^{(1)}R^{2,1}_{\lambda,\sigma} \Big\}
\end{aligned}$$

Using Eqs. (1.21) and (1.22) and the hermiticity of the potential, we can re-write this in a form which will be more convenient later

$$\begin{aligned}
\delta^2 E_{pot} = \frac{1}{2} \sum_{\mu,\nu,\lambda,\sigma} \Big\{ & \langle V_\nu, V_\sigma | \, V \left| \widetilde{U_\mu, U_\lambda} \right\rangle {}^{(1)}R^{2,1*}_{\sigma,\lambda} {}^{(1)}R^{2,1*}_{\nu,\mu} \\
& + \langle V_\nu, U_\sigma | \, V \left| \widetilde{U_\mu, V_\lambda} \right\rangle {}^{(1)}R^{2,1*}_{\nu,\mu} {}^{(1)}R^{2,1}_{\lambda,\sigma} \\
& + \Big[ \langle V_\nu, U_\sigma | \, V \left| \widetilde{U_\mu, V_\lambda} \right\rangle {}^{(1)}R^{2,1*}_{\nu,\mu} {}^{(1)}R^{2,1}_{\lambda,\sigma} \Big]^* \\
& + \Big[ \langle V_\nu, V_\sigma | \, V \left| \widetilde{U_\mu, U_\lambda} \right\rangle {}^{(1)}R^{2,1*}_{\sigma,\lambda} {}^{(1)}R^{2,1*}_{\nu,\mu} \Big]^* \Big\}
\end{aligned}$$

Next, we define the matrix

$$B_{(\nu\mu),(\sigma\lambda)} = \langle V_\nu, V_\sigma | \, V \left| \widetilde{U_\mu, U_\lambda} \right\rangle \tag{1.30}$$

Notice that the matrix $B$ is symmetric ($B = B^T$) as can be readily verified

$$\begin{aligned}
B_{(\nu\mu),(\sigma\lambda)} &= \langle V_\nu, V_\sigma | \, V \left| \widetilde{U_\mu, U_\lambda} \right\rangle \\
&= \langle V_\sigma, V_\nu | \, V \left| \widetilde{U_\lambda, U_\mu} \right\rangle \\
&= B_{(\sigma\lambda),(\nu\mu)}
\end{aligned} \tag{1.31}$$

We also define a matrix $A$

$$A_{(\nu\mu),(\sigma\lambda)} = \langle V_\nu, U_\lambda | \, V \left| \widetilde{U_\mu, V_\sigma} \right\rangle$$

Notice that the matrix A is hermitian ($A^\dagger = A$):

$$\begin{aligned}
A_{(\nu\mu),(\sigma\lambda)} &= \langle V_\nu, U_\lambda | \, V \left| \widetilde{U_\mu, V_\sigma} \right\rangle \\
&= \langle U_\mu, V_\sigma | \, V \left| \widetilde{V_\nu, U_\lambda} \right\rangle^* \\
&= \langle V_\sigma, U_\mu | \, V \left| \widetilde{U_\lambda, V_\nu} \right\rangle^* = A^*_{(\sigma\lambda),(\nu\mu)}
\end{aligned} \tag{1.32}$$

With these definitions, we can write

$$\delta^2 E_{pot} = \frac{1}{2} \sum_{\mu\nu\lambda\sigma} \Big\{ {}^{(1)}R^{2,1*}_{\nu\mu} B_{(\nu\mu),(\sigma\lambda)} \, {}^{(1)}R^{2,1*}_{\sigma\lambda} + {}^{(1)}R^{2,1}_{\nu\mu} B^*_{(\nu\mu),(\sigma\lambda)} \, {}^{(1)}R^{2,1}_{\sigma\lambda}$$
$$+ {}^{(1)}R^{2,1*}_{\nu,\mu} A_{(\nu\mu),(\lambda\sigma)} \, {}^{(1)}R^{2,1}_{\lambda,\sigma} + {}^{(1)}R^{2,1}_{\nu,\mu} A^*_{(\nu\mu),(\lambda\sigma)} \, {}^{(1)}R^{2,1*}_{\lambda,\sigma} \Big\} \tag{1.33}$$

or in more compact notation

$$\delta^2 E_{pot} = \frac{1}{2} \begin{pmatrix} R^{2,1*} & R^{2,1} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} R^{2,1} \\ R^{2,1*} \end{pmatrix}$$

We still have the variation of the energy coming from the second term in (1.26) representing the pairing contribution. Using the definition of variation of the pairing tensor in equation (1.28) we write the second order variation in the form

$$\delta^2 E_{pair} = \frac{1}{4} \sum_{\mu,\nu,\lambda,\sigma} \sum_{m,n,p,q} \langle m,n| V |\widetilde{p,q}\rangle \left( U_{q,\mu} U_{p,\nu} \, {}^{(1)}R^{1,2}_{\mu,\nu} + V^*_{q,\mu} V^*_{p,\nu} \, {}^{(1)}R^{2,1}_{\mu,\nu} \right)$$
$$\times \left( U^*_{n,\lambda} U^*_{m,\sigma} \, {}^{(1)}R^{2,1}_{\sigma,\lambda} + V_{n,\lambda} V_{m,\sigma} \, {}^{(1)}R^{1,2}_{\sigma,\lambda} \right) \tag{1.34}$$

We re-write these terms in a more convenient form, as we did in the case of $\delta^2 E_{pot}$ above to find

$$\begin{aligned} \delta^2 E_{pair} = \frac{1}{4} \sum_{\mu,\nu,\lambda,\sigma} \Big\{ & \langle U_\nu, U_\mu | V \Big| \widetilde{U_\sigma, U_\lambda} \Big\rangle^* \, {}^{(1)}R^{2,1*}_{\nu,\mu} \, {}^{(1)}R^{2,1}_{\sigma,\lambda} \\ & - \langle V_\sigma, V_\lambda | V \Big| \widetilde{U_\nu, U_\mu} \Big\rangle \, {}^{(1)}R^{2,1*}_{\nu,\mu} \, {}^{(1)}R^{2,1*}_{\sigma,\lambda} \\ & - \langle U_\sigma, U_\lambda | V \Big| \widetilde{V_\nu, V_\mu} \Big\rangle \, {}^{(1)}R^{2,1}_{\nu,\mu} \, {}^{(1)}R^{2,1}_{\sigma,\lambda} \\ & + \langle V_\sigma, V_\lambda | V \Big| \widetilde{V_\nu, V_\mu} \Big\rangle \, {}^{(1)}R^{2,1}_{\nu,\mu} \, {}^{(1)}R^{2,1*}_{\sigma,\lambda} \Big\} \end{aligned} \tag{1.35}$$

It will be useful to symmetrize the matrix elements under the summation and write this expression as

$$\delta^2 E_{pair} = \frac{1}{4} \sum_{\mu,\nu,\lambda,\sigma}$$
$$\Big\{ \frac{1}{2} \left( \langle U_\nu, U_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle^* + \langle V_\nu, V_\mu | V \left| \widetilde{V_\sigma, V_\lambda} \right\rangle \right) {}^{(1)}R^{2,1*}_{\nu,\mu} {}^{(1)}R^{2,1}_{\sigma,\lambda}$$
$$- \frac{1}{2} \left( \langle V_\sigma, V_\lambda | V \left| \widetilde{U_\nu, U_\mu} \right\rangle + \langle V_\nu, V_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle \right) {}^{(1)}R^{2,1*}_{\nu,\mu} {}^{(1)}R^{2,1*}_{\sigma,\lambda}$$
$$- \frac{1}{2} \left( \langle U_\sigma, U_\lambda | V \left| \widetilde{V_\nu, V_\mu} \right\rangle + \langle U_\nu, U_\mu | V \left| \widetilde{V_\sigma, V_\lambda} \right\rangle \right) {}^{(1)}R^{2,1}_{\nu,\mu} {}^{(1)}R^{2,1}_{\sigma,\lambda}$$
$$+ \frac{1}{2} \left( \langle U_\nu, U_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle + \langle V_\nu, V_\mu | V \left| \widetilde{V_\sigma, V_\lambda} \right\rangle^* \right) {}^{(1)}R^{2,1}_{\nu,\mu} {}^{(1)}R^{2,1*}_{\sigma,\lambda} \Big\} \tag{1.36}$$

We now define a matrix $C$

$$C_{(\nu\mu),(\sigma\lambda)} \equiv \frac{1}{4} \left[ \langle U_\nu, U_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle^* + \langle V_\nu, V_\mu | V \left| \widetilde{V_\sigma, V_\lambda} \right\rangle \right]$$

It is easy to show that C is hermitian

$$C_{(\nu\mu),(\sigma\lambda)} = C^*_{(\sigma\lambda),(\nu\mu)}$$

We also set

$$D_{(\sigma\lambda),(\nu\mu)} = -\frac{1}{4} \left[ \langle V_\sigma, V_\lambda | V \left| \widetilde{U_\nu, U_\mu} \right\rangle + \langle V_\nu, V_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle \right]$$

Note that the matrix $D$ is symmetric by construction,

$$D_{(\sigma\lambda),(\nu\mu)} = D_{(\nu\mu),(\sigma\lambda)}$$

With these notations the contribution of the pairing term to equation (1.34) takes the form

$$\delta^2 E_{pair} = \frac{1}{2} \sum_{\mu,\nu,\lambda,\sigma} \Big\{ {}^{(1)}R^{2,1*}_{\nu,\mu} C_{(\nu\mu),(\sigma\lambda)} {}^{(1)}R^{2,1}_{\sigma,\lambda} + {}^{(1)}R^{2,1}_{\nu,\mu} C^*_{(\nu\mu),(\sigma\lambda)} {}^{(1)}R^{2,1*}_{\sigma,\lambda}$$
$$+ {}^{(1)}R^{2,1*}_{\nu,\mu} D_{(\nu\mu),(\sigma\lambda)} {}^{(1)}R^{2,1*}_{\sigma,\lambda} + {}^{(1)}R^{2,1}_{\nu,\mu} D^\dagger_{(\nu\mu),(\sigma\lambda)} {}^{(1)}R^{2,1}_{\sigma,\lambda} \Big\} \tag{1.37}$$

Collecting the different terms given by Eqs. (1.25), (1.33), and (1.37) and using the following definitions

$$W_{(\nu\mu),(\sigma\lambda)} = (\epsilon_\nu + \epsilon_\mu)\delta_{\nu,\sigma}\delta_{\mu,\lambda} + A_{(\nu\mu),(\sigma\lambda)} + C_{(\nu\mu),(\sigma\lambda)}$$
$$Z_{(\nu\mu),(\sigma\lambda)} = B_{(\nu\mu),(\sigma\lambda)} + D_{(\nu\mu),(\sigma\lambda)}$$

Let us note that, according to the properties of the matrices $A$, $C$, $B$ and $D$ mentioned above, the matrix $W$ is hermitian and the matrix $Z$ is symmetric. We can write the second-order variation of the energy in Eq. (1.26) using these matrix definitions as

$$\delta^2 E = \frac{1}{2} \sum_{\mu\nu\lambda\sigma} \Big\{ {}^{(1)}R^{2,1*}_{\nu\mu}\, W_{(\nu\mu),(\sigma\lambda)}\, {}^{(1)}R^{2,1}_{\sigma\lambda} + {}^{(1)}R^{2,1*}_{\nu\mu} Z_{(\nu\mu),(\sigma\lambda)}\, {}^{(1)}R^{2,1*}_{\sigma,\lambda}$$
$$+ {}^{(1)}R^{2,1}_{\nu,\mu} \left(Z^\dagger\right)_{(\nu\mu),(\sigma\lambda)}\, {}^{(1)}R^{2,1}_{\sigma\lambda} + {}^{(1)}R^{2,1}_{\nu,\mu} W^*_{(\nu\mu),(\sigma\lambda)}\, {}^{(1)}R^{2,1*}_{\sigma,\lambda} \Big\} \tag{1.38}$$

which we can write in the quadratic form

$$\delta^2 E = \frac{1}{2} \left( {}^{(1)}R^{2,1*} \;\; {}^{(1)}R^{2,1} \right) \begin{pmatrix} W & Z \\ Z^\dagger & W^* \end{pmatrix} \begin{pmatrix} {}^{(1)}R^{2,1} \\ {}^{(1)}R^{2,1*} \end{pmatrix} \tag{1.39}$$

In fact, according to equation (1.22) the variations of the generalized density matrix are anti-symmetric and consequently it is advantageous to take into account this property in the expression above by writing

$$\delta E = \frac{1}{2} \left( {}^{(1)}R^{2,1*}_{>} \;\; {}^{(1)}R^{2,1}_{>} \right) \begin{pmatrix} \overline{W} & \overline{Z} \\ \overline{Z}^\dagger & \overline{W}^* \end{pmatrix} \begin{pmatrix} {}^{(1)}R^{2,1}_{>} \\ {}^{(1)}R^{2,1*}_{>} \end{pmatrix} \tag{1.40}$$

where we assume $\nu < \mu$ and $\sigma < \lambda$ for a given matrix $X$

$$\overline{X}_{(\nu\mu),(\sigma\lambda)} \equiv X_{(\nu\mu),(\sigma\lambda)} + X_{(\mu\nu),(\lambda\sigma)} - X_{(\mu\nu),(\sigma\lambda)} - X_{(\nu\mu),(\lambda\sigma)}$$
$$\left[ {}^{(1)}R^{2,1}_{>} \right]_{\mu\nu} = {}^{(1)}R^{2,1}_{\mu\nu}, \text{ with ordered indices}$$

We can write the matrix elements explicitly,

$$\begin{aligned} \overline{W}_{(\nu\mu),(\sigma\lambda)} = {} & (\epsilon_\nu + \epsilon_\mu)\delta_{\nu,\sigma}\delta_{\mu,\lambda} \\ & + \langle V_\nu, U_\lambda | V \left| \widetilde{U_\mu, V_\sigma} \right\rangle + \langle V_\mu, U_\sigma | V \left| \widetilde{U_\nu, V_\lambda} \right\rangle \\ & - \langle V_\mu, U_\lambda | V \left| \widetilde{U_\nu, V_\sigma} \right\rangle - \langle V_\nu, U_\sigma | V \left| \widetilde{U_\mu, V_\lambda} \right\rangle \\ & + \langle U_\nu, U_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle^* + \langle V_\nu, V_\mu | V \left| \widetilde{V_\sigma, V_\lambda} \right\rangle \end{aligned}$$

and similarly,

$$\begin{aligned} \overline{Z}_{(\nu\mu),(\sigma\lambda)} = {} & \langle V_\nu, V_\sigma | V \left| \widetilde{U_\mu, U_\lambda} \right\rangle + \langle V_\mu, V_\lambda | V \left| \widetilde{U_\nu, U_\sigma} \right\rangle \\ & - \langle V_\mu, V_\sigma | V \left| \widetilde{U_\nu, U_\lambda} \right\rangle - \langle V_\nu, V_\lambda | V \left| \widetilde{U_\mu, U_\sigma} \right\rangle \\ & - \langle V_\nu, V_\mu | V \left| \widetilde{U_\sigma, U_\lambda} \right\rangle - \langle V_\sigma, V_\lambda | V \left| \widetilde{U_\nu, U_\mu} \right\rangle \end{aligned}$$

The matrix occurring in the quadratic form, Eq. (1.40), is the so-called QRPA matrix which plays a key role in the theory based on the Bogoliubov transformation. We are content at this stage to show how this matrix occurs in the calculation of the response of the Bogoliubov fields to a one-body external field.

To end this Section, we derive expressions of the $W$ and $Z$ matrices in terms of expectations values of double commutators with the Hamiltonian $H$ which will be useful for the developments made in Chapter 4. These expressions follow from a general theorem (see e.g. the Appendix E in the book by Ring and Schuck [1]) which asserts that the perturbed HFB vacuum $|\tilde{O}'\rangle = |\tilde{O}+\delta\tilde{O}\rangle$ can be related to the HFB vacuum $|\tilde{O}\rangle$ by means of a unitary transformation according to the formula

$$|\tilde{O}'\rangle = e^{-S}|\tilde{O}\rangle \tag{1.41}$$

with

$$S = \frac{1}{2}\sum_{\mu\nu}\left(K_{\mu\nu}\eta_\mu\eta_\nu + K^*_{\mu\nu}\eta^\dagger_\mu\eta^\dagger_\nu\right) = -S^\dagger \tag{1.42}$$

where the matrix $K$ is antisymmetric, $K^T = -K$, and the $\eta_\mu$ annihilate the vacuum $|\tilde{O}\rangle$ i.e., $\eta_\mu|\tilde{O}\rangle = 0$. Since $S$ is an antihermitian operator, $e^{-S}$ is a unitary operator. Eq. (1.42) can also be written in the matrix form

$$S = \frac{1}{2}\left(\eta^\dagger\ \eta\right)\mathcal{S}\begin{pmatrix}\eta\\ \eta^\dagger\end{pmatrix} \tag{1.43}$$

with

$$\mathcal{S} = \begin{pmatrix}0 & K^*\\ K & 0\end{pmatrix} = -\mathcal{S}^\dagger \tag{1.44}$$

Since $|\tilde{O}'\rangle$ has been assumed to be close to $|\tilde{O}\rangle$, the matrice $K$ and $\mathcal{S}$ may be assumed to be small quantities.
The generalized density matrix associated with the vacuum $|\tilde{O}'\rangle$ is

$$R = \langle\tilde{O}'|\widehat{R}|\tilde{O}'\rangle$$

where $\widehat{R}$ is the operator

$$\widehat{R} = \begin{pmatrix}I & 0\\ 0 & I\end{pmatrix} - \begin{pmatrix}\eta\\ \eta^\dagger\end{pmatrix}\left(\eta^\dagger\ \eta\right) \tag{1.45}$$

Using the relation (1.41) we get, up to first order in $S$,

$$R = \langle\tilde{O}|e^S\widehat{R}e^{-S}|\tilde{O}\rangle = \langle\tilde{O}|\widehat{R}|\tilde{O}\rangle + \langle\tilde{O}|\left[S,\widehat{R}\right]|\tilde{O}\rangle \equiv^{(0)} R +^{(1)} R$$

where the same notation as in Section 2.2 is employed in the last equality for the perturbative expansion of $R$. The zeroth order of course gives back the result (1.16), ${}^{(0)}R = \begin{pmatrix}0 & 0\\ 0 & I\end{pmatrix}$. In order to express the matrix ${}^{(1)}R$, we need to calculate the commutator of $S$ with $\widehat{R}$. Using (1.42) and the antisymmetry of the matrix $K$, we first have

$$
\begin{aligned}
[S, \eta_\lambda] &= \sum_\mu \eta_\mu^\dagger K_{\mu\lambda}^* = -\sum_\nu K_{\lambda\nu}^* \eta_\nu^\dagger \\
\left[S, \eta_\lambda^\dagger\right] &= \sum_\mu \eta_\mu K_{\mu\lambda} = -\sum_\nu K_{\lambda\nu} \eta_\nu
\end{aligned}
$$

These relations may be put under the matrix forms

$$
\begin{aligned}
\left[S, \begin{pmatrix} \eta_\lambda \\ \eta_\lambda^\dagger \end{pmatrix}\right] &= -\sum_\nu \mathcal{S}_{\lambda\nu} \begin{pmatrix} \eta_\nu \\ \eta_\nu^\dagger \end{pmatrix} \\
\left[S, \left( \eta_\lambda^\dagger \; \eta_\lambda \right)\right] &= \sum_\mu \left( \eta_\mu^\dagger \; \eta_\mu \right) \mathcal{S}_{\mu\lambda}
\end{aligned}
$$

so that, with $\widehat{R}$ given by (1.45), we get

$$
\begin{aligned}
\left[S, \widehat{R}_{\lambda\sigma}\right] &= -\left[S, \begin{pmatrix} \eta_\lambda \\ \eta_\lambda^\dagger \end{pmatrix}\right] \left( \eta_\sigma^\dagger \; \eta_\sigma \right) - \begin{pmatrix} \eta_\lambda \\ \eta_\lambda^\dagger \end{pmatrix} \left[S, \left( \eta_\sigma^\dagger \; \eta_\sigma \right)\right] \\
&= \sum_\nu \mathcal{S}_{\lambda\nu} \begin{pmatrix} \eta_\nu \\ \eta_\nu^\dagger \end{pmatrix} \left( \eta_\sigma^\dagger \; \eta_\sigma \right) - \sum_\mu \begin{pmatrix} \eta_\lambda \\ \eta_\lambda^\dagger \end{pmatrix} \left( \eta_\mu^\dagger \; \eta_\mu \right) \mathcal{S}_{\mu\sigma} \\
&= \sum_\nu \mathcal{S}_{\lambda\nu} \left( \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - \widehat{R} \right)_{\nu\sigma} - \sum_\mu \left( \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - \widehat{R} \right)_{\lambda\mu} \mathcal{S}_{\mu\sigma} \\
&= \left( \widehat{R}\mathcal{S} - \mathcal{S}\widehat{R} \right)_{\lambda\sigma}
\end{aligned}
$$

The first order density matrix therefore is

$$
{}^{(1)}R_{\lambda\sigma} = \langle \tilde{O} | \left( \widehat{R}\mathcal{S} - \mathcal{S}\widehat{R} \right)_{\lambda\sigma} | \tilde{O} \rangle = \left( {}^{(0)}R\mathcal{S} - \mathcal{S}\, {}^{(0)}R \right)_{\lambda\sigma}
$$

Using the expressions (1.16) and (1.44) of ${}^{(0)}R$ and $\mathcal{S}$, we thus obtain

$$
{}^{(1)}R = \left[ \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \begin{pmatrix} 0 & K^* \\ K & 0 \end{pmatrix} \right] = \begin{pmatrix} 0 & -K^* \\ K & 0 \end{pmatrix} \tag{1.46}
$$

We see that this expression agrees with the one found in Section 2.2, Eq. (1.20), provided we have

$$
{}^{(1)}R^{2,1} = -{}^{(1)}R^{1,2^*} = K \tag{1.47}
$$

Now, the total energy of the system calculated with the perturbed vacuum $|\tilde{O}'\rangle$ is, up to second order in $S$ and using the same notations as in Eq. (1.24),

$$
\begin{aligned}
E(R) &= \langle \tilde{O}' | H | \tilde{O}' \rangle = \langle \tilde{O} | e^S H e^{-S} | \tilde{O} \rangle \\
&= \langle \tilde{O} | H | \tilde{O} \rangle + \langle \tilde{O} | \left[ S, H \right] | \tilde{O} \rangle + \frac{1}{2} \langle \tilde{O} | \left[ S, \left[ S, H \right] \right] | \tilde{O} \rangle \\
&\equiv E({}^{(0)}R) + \delta^1 E + \delta^2 E
\end{aligned} \tag{1.48}
$$

The first order term $\delta^1 E$ vanishes because of the stationarity of the HFB energy for the vacuum $|\tilde{O}\rangle$, which requires that the mean value of the commutator of the Hamiltonian $H$ with any one-body operator is zero. As to the second order contribution

$$\delta^2 E = \frac{1}{2}\langle\tilde{O}|\,[S,[S,H]]\,|\tilde{O}\rangle = \frac{1}{2}\langle\tilde{O}|\,[[H,S]\,,S]\,|\tilde{O}\rangle$$

we may calculate it using the expression (1.42) of $S$. We get

$$\begin{aligned}\delta^2 E = \frac{1}{8}\sum_{\mu\nu\lambda\sigma}\Big\{\; & K_{\mu\nu}K_{\lambda\sigma}\langle\tilde{O}|\,[[H,\eta_\mu\eta_\nu]\,,\eta_\lambda\eta_\sigma]\,|\tilde{O}\rangle \\ & + K_{\mu\nu}K^*_{\lambda\sigma}\langle\tilde{O}|\left[[H,\eta_\mu\eta_\nu]\,,\eta^\dagger_\lambda\eta^\dagger_\sigma\right]|\tilde{O}\rangle \\ & + K^*_{\mu\nu}K_{\lambda\sigma}\langle\tilde{O}|\left[\left[H,\eta^\dagger_\mu\eta^\dagger_\nu\right],\eta_\lambda\eta_\sigma\right]|\tilde{O}\rangle \\ & + K^*_{\mu\nu}K^*_{\lambda\sigma}\langle\tilde{O}|\left[\left[H,\eta^\dagger_\mu\eta^\dagger_\nu\right],\eta^\dagger_\lambda\eta^\dagger_\sigma\right]|\tilde{O}\rangle\Big\}\end{aligned} \tag{1.49}$$

Replacing all the $K$ by ${}^{(1)}R^{2,1}$ according to Eq. (1.47) and identifying the resulting expression of $\delta^2 E$ with the previous one given in Eq. (1.38) yields

$$\begin{aligned}W_{(\mu\nu),(\lambda\sigma)} &= \frac{1}{4}\langle\tilde{O}|\left[\left[H,\eta^\dagger_\mu\eta^\dagger_\nu\right],\eta_\lambda\eta_\sigma\right]|\tilde{O}\rangle \\ Z_{(\mu\nu),(\lambda\sigma)} &= \frac{1}{4}\langle\tilde{O}|\left[\left[H,\eta^\dagger_\mu\eta^\dagger_\nu\right],\eta^\dagger_\lambda\eta^\dagger_\sigma\right]|\tilde{O}\rangle \\ W^*_{(\mu\nu),(\lambda\sigma)} &= \frac{1}{4}\langle\tilde{O}|\left[[H,\eta_\mu\eta_\nu]\,,\eta^\dagger_\lambda\eta^\dagger_\sigma\right]|\tilde{O}\rangle \\ Z^*_{(\mu\nu),(\lambda\sigma)} &= \frac{1}{4}\langle\tilde{O}|\,[[H,\eta_\mu\eta_\nu]\,,\eta_\lambda\eta_\sigma]\,|\tilde{O}\rangle\end{aligned} \tag{1.50}$$

It is easy to check that the third and the fourth equations are consistent with the first and the second ones, respectively, and also that the matrix $W$ is hermitian and the matrix $Z$ symmetric (so that $Z^* = Z^\dagger$). These latter properties of $W$ and $Z$ appear in a more transparent way if we expand the double commutators, which gives the alternative expressions

$$\begin{aligned}W_{(\mu\nu),(\lambda\sigma)} &= -\frac{1}{4}\langle\tilde{O}|\eta_\lambda\eta_\sigma H\eta^\dagger_\mu\eta^\dagger_\nu|\tilde{O}\rangle + \frac{1}{4}\langle\tilde{O}|\eta_\lambda\eta_\sigma\eta^\dagger_\mu\eta^\dagger_\nu H|\tilde{O}\rangle \\ &= -\frac{1}{4}\langle\tilde{O}|\eta_\lambda\eta_\sigma H\eta^\dagger_\mu\eta^\dagger_\nu|\tilde{O}\rangle + \frac{1}{4}\left(\delta_{\lambda\nu}\delta_{\sigma\mu} - \delta_{\lambda\mu}\delta_{\sigma\nu}\right)\langle\tilde{O}|H|\tilde{O}\rangle \\ &= W^*_{(\lambda\sigma),(\mu\nu)} \\ Z_{(\mu\nu),(\lambda\sigma)} &= \frac{1}{4}\langle\tilde{O}|H\eta^\dagger_\mu\eta^\dagger_\nu\eta^\dagger_\lambda\eta^\dagger_\sigma|\tilde{O}\rangle \\ &= Z_{(\lambda\sigma),(\mu\nu)}\end{aligned} \tag{1.51}$$

These properties ensure that the QRPA matrix

$$M = \begin{pmatrix} W & Z \\ Z^* & W^* \end{pmatrix} = \begin{pmatrix} W & Z \\ Z^\dagger & W^* \end{pmatrix} \tag{1.52}$$

defined previously is hermitian.

## 1.4 Response of HFB to a one-body external field

We choose a one body operator that we denote as $\lambda\hat{F}$:

$$\hat{F} = \sum_{\alpha\beta} F_{\alpha\beta} a_\alpha^\dagger a_\beta$$

The parameter $\lambda$ is used to vary the intensity of the external field. Let us assume that we have solved the Bogoliubov equations of the system under the influence of $\lambda\hat{F}$. In other words, that we have determined a generalized density matrix satisfying the equation

$$\left[H\left(R(\lambda), \lambda\hat{F}\right), R(\lambda)\right] = 0 \tag{1.53}$$

Our goal is to relate two generalized density matrices $R(\lambda)$ and $R(\lambda + \delta\lambda)$ for an infinitesimal change of the intensity of the field in question. The latter satisfies the equation

$$\left[H\left(R(\lambda + \delta\lambda), (\lambda + \delta\lambda)\hat{F}\right), R(\lambda + \delta\lambda)\right] = 0 \tag{1.54}$$

Since the change is infinitesimal, one can solve this equation by linearizing around the solution of (1.53). In order to use the formalism developed in the previous section we define

$$\begin{aligned} R(\lambda) &= {}^{(0)}R \\ R(\lambda + \delta\lambda) &= {}^{(0)}R + {}^{(1)}R \end{aligned}$$

We expand to first order the Bogoliubov Hamiltonian

$$\begin{aligned} H\left(R(\lambda + \delta\lambda), (\lambda + \delta\lambda)\hat{F}\right) = H\left({}^{(0)}R, \lambda\hat{F}\right) + \frac{\delta H\left(R, \lambda\hat{F}\right)}{\delta R}{}^{(1)}R \\ + \delta\lambda\mathbb{F} + \text{second order} \end{aligned} \tag{1.55}$$

The second term in the right hand side is the variation associated with the implicit dependence of the HFB solutions on the parameter $\lambda$. The third one comes from the explicit dependence of the external field. It is important to notice that the new matrix $\mathbb{F}$ which occurs in the Bogoliubov equations is expressed in the $\begin{pmatrix} a_\alpha \\ a_\alpha^\dagger \end{pmatrix}$ representation with double dimension and is related to the matrix $F$ by

$$\mathbb{F} = \begin{pmatrix} F & 0 \\ 0 & -F^* \end{pmatrix} \tag{1.56}$$

After substituting Eq. (1.55) in (1.54) we find

$$\left[ H\left( {}^{(0)}R, \lambda \hat{F} \right) + \frac{\delta H}{\delta R} {}^{(1)}R + \delta\lambda \mathbb{F}, {}^{(0)}R + {}^{(1)}R \right] = 0$$

If we take into account that ${}^{(0)}R$ is solution of (1.53) we are left with

$$\left[ H\left( {}^{(0)}R, \lambda \hat{F} \right), {}^{(1)}R \right] + \left[ \frac{\delta H}{\delta R} {}^{(1)}R, {}^{(0)}R \right] = \quad -\delta\lambda \left[ \mathbb{F}, {}^{(0)}R \right] \tag{1.57}$$

We solve this equation in the representation diagonalizing $H\left( {}^{(0)}R, \lambda \hat{F} \right)$. Consequently, all the operators must be expressed in this representation

$${}^{(0)}R = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \quad {}^{(1)}R = \begin{pmatrix} 0 & {}^{(1)}R^{1,2} \\ {}^{(1)}R^{2,1} & 0 \end{pmatrix},$$

and

$$\breve{F} = B^\dagger \begin{pmatrix} F & 0 \\ 0 & -F^* \end{pmatrix} B, \quad H\left( {}^{(0)}R, \lambda \hat{F} \right) = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}$$

For what follows we need the expression of $\breve{F}$ which is easily derived by means of definition (1.14) of the matrix $B$. We are content to give here the result

$$\breve{F} = \begin{pmatrix} F^{1,1} & F^{1,2} \\ F^{2,1} & F^{2,2} \end{pmatrix} = \begin{pmatrix} U^\dagger F U - V^\dagger F^* V & U^\dagger F V^* - V^\dagger F^* U^* \\ V^T F U - U^T F^* V & V^T F V^* - U^T F^* U^* \end{pmatrix} \tag{1.58}$$

Since $\breve{F}$ is hermitian we obtain the following relation

$$F^{2,1}_{\mu\nu} = F^{1,2*}_{\nu\mu} \tag{1.59}$$

Furthermore it is clear from Eq. (1.58) that

$$F^{1,2} = -F^{2,1*} \tag{1.60}$$

and consequently we obtain the set of relations

$$F^{2,1}_{\mu\nu} = F^{1,2*}_{\nu\mu} = -F^{2,1}_{\nu\mu}$$

In order to express the commutators in equation (1.57) we give for an arbitrary operator $\hat{A}$ with matrix representation

$$A = \begin{pmatrix} A^{1,1} & A^{1,2} \\ A^{2,1} & A^{2,2} \end{pmatrix}$$

the identity

$$\left[\hat{A}, {}^{(0)}R\right] = \begin{pmatrix} 0 & A^{1,2} \\ -A^{2,1} & 0 \end{pmatrix}$$

We also have

$$\left[H\left({}^{(0)}R, \lambda\hat{F}\right), {}^{(1)}R\right] = \begin{pmatrix} 0 & \left\{\varepsilon, {}^{(1)}R^{1,2}\right\} \\ -\left\{\varepsilon, {}^{(1)}R^{1,2}\right\} & 0 \end{pmatrix}$$

with

$$\left\{\varepsilon, {}^{(1)}R^{1,2}\right\} = \varepsilon^{(1)}R^{1,2} + {}^{(1)}R^{1,2}\varepsilon$$

Finally, we have

$$\frac{\delta H}{\delta R}{}^{(1)}R = \begin{pmatrix} \partial H^{1,1} & \partial H^{1,2} \\ \partial H^{2,1} & \partial H^{2,2} \end{pmatrix} \tag{1.61}$$

with the definition

$$\partial H^{i,j} = \sum_{k,l} \frac{\delta H^{i,j}}{\delta R^{k,l}}{}^{(1)}R^{k,l} \tag{1.62}$$

We have now all what we need to express equation (1.57) in a simple way. We are content to give the result

$$\begin{pmatrix} 0 & \left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{1,2} \\ -\left[\left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{2,1}\right] & 0 \end{pmatrix} = -\delta\lambda \begin{pmatrix} 0 & F^{1,2} \\ F^{2,1} & 0 \end{pmatrix}$$

We thus have two equations

$$\begin{aligned} \left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{1,2} &= -\delta\lambda F^{1,2} \\ \left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{2,1} &= \delta\lambda F^{2,1} \end{aligned} \tag{1.63}$$

It remains to detail a little more the form of the quantity $\partial H^{i,j}$. According to Eq. (1.62), and on account of the definition given by Eq. (1.10), we can write

$$\partial H^{i,j} = \sum_{k,l} \frac{\delta^2 E}{\delta R^{j,i}\delta R^{k,l}}\,{}^{(1)}R^{k,l}$$

or, more explicitly,

$$\left[\left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{1,2}\right]_{\mu\nu} = -\left(\varepsilon_\mu + \varepsilon_\nu\right) {}^{(1)}R^{2,1*} - \sum_{\alpha\beta}\left[\frac{\delta^2 E}{\delta R^{2,1*}_{\alpha\beta}\delta R^{2,1}_{\mu\nu}} {}^{(1)}R^{2,1*}_{\mu\nu} + \frac{\delta^2 E}{\delta R^{2,1}_{\alpha\beta}\delta R^{2,1}_{\mu\nu}} {}^{(1)}R^{2,1}_{\alpha\beta}\right]$$

$$\left[\left\{\varepsilon, {}^{(1)}R^{2,1}\right\} + \partial H^{2,1}\right]_{\mu\nu} = \left(\varepsilon_\mu + \varepsilon_\nu\right) {}^{(1)}R^{2,1} + \sum_{\alpha\beta}\left[\frac{\delta^2 E}{\delta R^{2,1*}_{\alpha\beta}\delta R^{2,1*}_{\mu\nu}} {}^{(1)}R^{2,1*}_{\mu\nu} + \frac{\delta^2 E}{\delta R^{2,1}_{\alpha\beta}\delta R^{2,1*}_{\mu\nu}} {}^{(1)}R^{2,1}_{\alpha\beta}\right] \tag{1.64}$$

These second derivatives are identified to the block matrices $W$, $Z$, etc.

$$\left\{\varepsilon, {}^{(1)}R^{2,1}\right\} + \partial H^{2,1} = W\,{}^{(1)}R^{2,1} + Z\,{}^{(1)}R^{2,1*}$$
$$\left\{\varepsilon, {}^{(1)}R^{1,2}\right\} + \partial H^{1,2} = Z^\dagger\,{}^{(1)}R^{2,1} + W^*\,{}^{(1)}R^{2,1*}$$

Consequently Eq. (1.63) can be expressed with the QRPA matrix defined by Eq. (1.39) in the matrix form

$$\begin{pmatrix} W & Z \\ Z^\dagger & W^* \end{pmatrix}\begin{pmatrix} {}^{(1)}R^{2,1} \\ {}^{(1)}R^{2,1*} \end{pmatrix} = -\delta\lambda\begin{pmatrix} F^{2,1} \\ F^{2,1*} \end{pmatrix}$$

If we denote the QRPA matrix by $M$, and if we assume that this matrix is invertible, we find the formal solution

$$\begin{pmatrix} {}^{(1)}R^{2,1} \\ {}^{(1)}R^{2,1*} \end{pmatrix} = -\delta\lambda M^{-1}\begin{pmatrix} F^{2,1} \\ F^{2,1*} \end{pmatrix} \tag{1.65}$$

We cannot give a simple form for the inverse matrix in general at this stage. We consider instead the simple case where we neglect the interaction between quasi-particles. The matrix $M$ then becomes diagonal since, in effect $Z = 0$ and $W$ is diagonal,

$$W_{(\mu\nu),(\lambda\sigma)} = (\varepsilon_\mu + \varepsilon_\nu)\delta_{\mu\lambda}\delta_{\nu\sigma}$$

Equation (1.65) combined with equation (1.58) permits one to derive the matrix elements of the perturbed generalized density matrix. We find

$${}^{(1)}R^{2,1}_{\mu,\nu} = \frac{-\delta\lambda}{\varepsilon_\mu + \varepsilon_\nu}\left[V^T F U - U^T F^* V\right]_{\mu,\nu}$$
$$\left[V^T F U - U^T F^* V\right]_{\mu,\nu} = \sum_{\beta\alpha}\left(F_{\beta\alpha}U_{\alpha\nu}V_{\beta\mu} - F^*_{\beta\alpha}V_{\alpha\nu}U_{\beta\mu}\right)$$

We have now the essential results to attack the problem of solving the Bogoliubov equations with additional constraints (Constrained HFB).

## 1.5 HFB with additional constraints

The problem to solve is defined as follows. We want to find the solution of the HFB equations with the constraints that the mean values of a chosen set of $N$ operators $\left\{\hat{F}_i\right\}, i = 1, \ldots, N$ have some desired values $\left\{\left\langle\hat{F}_i\right\rangle = f_i\right\}, i = 1, \ldots, N$. It is understood that the mean value is calculated with the HFB solution in question. This problem is solved by using the Lagrange-multiplier method, which in this case consist in minimizing the quantity

$$\left\langle \tilde{O}, \{f_i\} \left| H + \sum_{i=1}^{N} \lambda_i \hat{F}_i \right| \tilde{O}, \{f_i\} \right\rangle$$

where the parameters $\lambda_i$ have to be determined by the conditions

$$\left\langle \tilde{O}, \{f_i\} \left| \hat{F}_j \right| \tilde{O}, \{f_i\} \right\rangle = f_j, \quad j = 1, \ldots, N \tag{1.66}$$

The expectation value in Eq. (1.66) can be written in terms of traces of the matrix $\mathbb{F}_j$ defined in Eq. (1.56) and its components $F_j$, taking into account the hermiticity of $\hat{F}_j$

$$\begin{aligned} \left\langle \hat{F}_j \right\rangle &= \frac{1}{2} \sum_n (F_j)_{nn} + \frac{1}{2} \sum_{n,n'} \left[ (F_j)_{nn'} \rho_{n'n} - (F_j)^*_{nn'} \left( \delta_{nn'} - \rho^*_{n'n} \right) \right] \\ &= \frac{1}{2} \mathrm{Tr} F_j + \frac{1}{2} \mathrm{Tr} \mathbb{F}_j R \end{aligned} \tag{1.67}$$

According to our discussion in the previous paragraph this problem can be interpreted as the resolution of the HFB with $N$ external fields whose respective intensity must be determined in such a way that Eq. (1.66) is satisfied.

### *1.5.1 The case of one constraint*

We are content for the moment to consider the case of one constraint $\hat{F}$ and give an iterative procedure to solve this problem. Let us denote by $R^{(n-1)}, \lambda^{(n-1)}$ a generalized density matrix (GDM) and a Lagrange parameter such the constraint is satisfied $\left\langle \hat{F} \right\rangle_{n-1} = f$ at iteration number $n - 1$.

The diagonalization of the Bogoliubov Hamiltonian $H\left(R^{(n-1)},\lambda^{(n-1)}\right)$ provides generally a GDM denoted as $\overline{R}^{(n)}$, which is such that the constraint is no longer satisfied. Our goal is to provide a method to readjust the Lagrange parameter and derive a GDM $R^{(n)}$ to start the iteration "$n$" with $R^{(n)},\lambda^{(n)}$. In other words at each iteration we calculate with a GDM satisfying the constraints.

Let us denote the mean value of the constraint calculated with $\overline{R}^{(n)}$ by

$$\left\langle \hat{F}\left(\overline{R}^{(n)}\right)\right\rangle = f^{(n)}$$

and the mismatch of the constraint by

$$\delta f^{(n)} = f - f^{(n)}$$

Also, we introduce the definitions

$$\begin{aligned} R^{(n)} &= \overline{R}^{(n)} + {}^{(1)}R \\ \lambda^{(n)} &= \lambda^{(n-1)} + \delta\lambda \end{aligned} \tag{1.68}$$

to calculate the readjustment. It is clear that in order to satisfy the constraint $\left\langle \hat{F}\left(R^{(n)}\right)\right\rangle = f$ when $\left\langle \hat{F}\left(\overline{R}^{(n)}\right)\right\rangle = f^{(n)}$, one must determine a ${}^{(1)}R$ such that

$$\delta\left\langle \hat{F}\right\rangle \equiv \left\langle \hat{F}\left(\overline{R}^{(n)} + {}^{(1)}R\right)\right\rangle - \left\langle \hat{F}\left(\overline{R}^{(n)}\right)\right\rangle = \delta f^{(n)} \tag{1.69}$$

This can be achieved in perturbation by varying the intensity of the external field. In effect we have seen (Eq. (1.65)) that to a variation $\delta\lambda$ corresponds

$${}^{(1)}\mathbf{R} = -\delta\lambda M^{-1}\mathbf{F} \tag{1.70}$$

where the column vectors ${}^{(1)}\mathbf{R}$ and $\mathbf{F}$ are defined by Eq. (1.65). The condition in Eq. (1.69) can be calculated with a trace (see Eq. (1.67)),

$$\delta\left\langle \hat{F}\right\rangle = \frac{1}{2}\mathrm{Tr}\left[\mathbb{F}\,{}^{(1)}R\right]$$

Writing the trace in the quasi-particle representation, and using the properties of $F$ and ${}^{(1)}R$, we have

$$\begin{aligned} \delta\left\langle \hat{F}\right\rangle &= -\frac{1}{2}\mathrm{Tr}\left[F^{2,1*}\,{}^{(1)}R^{2,1} + F^{2,1}\,{}^{(1)}R^{2,1*}\right] \\ &= +\frac{1}{2}\mathrm{Tr}\left[\mathbf{F}^{\dagger}\cdot{}^{(1)}\mathbf{R}\right] \end{aligned}$$

where the change in sign in the second line is due to used Eqs. (1.59) and (1.60). Using Eq. (1.70), this becomes

$$\delta\left\langle \hat{F}\right\rangle = -\frac{1}{2}\delta\lambda \mathrm{Tr}\left[\mathbf{F}^{\dagger}\cdot M^{-1}\mathbf{F}\right] = \delta f^{(n)} \tag{1.71}$$

From Eq. (1.71) we thus obtain a $\delta\lambda$ given by

$$\delta\lambda = -\frac{2\delta f^{(n)}}{\mathrm{Tr}\left[\mathbf{F}^{\dagger}\cdot M^{-1}\mathbf{F}\right]} \tag{1.72}$$

Equation (1.68) calculated with the quantities given by Eqs. (1.72) and (1.70) solves our problem.

### *1.5.2 The case of N constraints*

The generalized density matrix is now a function of $N$ Lagrange parameters $\{\lambda_i\}$. Equation (1.70) becomes

$$^{(1)}\mathbf{R} = -\sum_{i=1}^{N}\delta\lambda_i M^{-1}\mathbf{F}_{(i)} \tag{1.73}$$

In order to obtain this expression we have written the variation as

$$^{(1)}\mathbf{R} = \delta\mathbf{R}(\{\lambda_i\}) = \sum_{i=1}^{N}\frac{\partial\mathbf{R}(\{\lambda_i\})}{\partial\lambda_i}\delta\lambda_i$$

with

$$\frac{\partial\mathbf{R}(\{\lambda_i\})}{\partial\lambda_i} = -M^{-1}\mathbf{F}_{(i)} \tag{1.74}$$

We have taken into account that a partial derivative with respect to $\lambda_i$ is associated to the variation of the density matrix when varying the intensity of the external field $F_{(i)}$, all other fields being kept fixed. Equation (1.71) is then replaced by a set of $N$ equations

$$\begin{aligned}\delta\left\langle \hat{F}_{(i)}\right\rangle &= +\frac{1}{2}\mathrm{Tr}\left[\mathbf{F}^{\dagger}_{(i)}\cdot {}^{(1)}\mathbf{R}\right] \\ &= -\frac{1}{2}\sum_j\delta\lambda_j \mathrm{Tr}\left[\mathbf{F}^{\dagger}_{(i)}\cdot M^{-1}\mathbf{F}_{(j)}\right] = \delta f^{(n)}_{(i)}\end{aligned} \tag{1.75}$$

It is convenient to define a matrix T

$$T_{l,m} = \frac{1}{2}\mathrm{Tr}\left[\mathbf{F}^{\dagger}_{(l)}\cdot M^{-1}\mathbf{F}_{(m)}\right] \tag{1.76}$$

which permits one to recast this set of equations in the form,

$$T\overrightarrow{\delta\lambda} = -\overrightarrow{\delta f}^{(n)}$$

where $\overrightarrow{\delta\lambda}$ and $\overrightarrow{\delta f}^{(n)}$ are column vectors of dimension $N$. Equation (1.72) becomes

$$\overrightarrow{\delta\lambda} = -T^{-1}\overrightarrow{\delta f}^{(n)} \tag{1.77}$$

In other words the variations of the $N$ Lagrange parameters given by (1.77) can be written as

$$\delta\lambda_i = -\sum_j \left[T^{-1}\right]_{i,j} \delta f_{(j)}^{(n)} \tag{1.78}$$

The corresponding variation of the generalized density matrix is then obtained by substituting the variations (1.78) into equation (1.74).

The general algorithm implementing the constrained HFB method presented in this section can be found in appendix A.

## 1.6 Illustration of the constrained HFB method with the multi-$O\,(4)$ model

The HFB method will be extensively used in the second part of this book with the finite interaction described in chapter 2. As a more pedagogical review of the formalism developed in this chapter, we apply it to a toy model of the nucleus, the multi-$O\,(4)$ model.

### *1.6.1 Description of the model*

The multi-$O\,(4)$ model [7, 8, 9, 10, 11, 12, 13, 14] is a simplified version of the standard pairing-plus-quadrupole nuclear model [15]. In the model, $N$ particles occupy states characterized by a half-integer angular momentum $j$ and its projection quantum number $m = -j, -j+1, \ldots, j-1, j$. The pair multiplicity of each $j$ shell is thus $\Omega_j = j + 1/2$. Here we will assume only one type of particle (e.g., neutrons). The Hamiltonian for this model is

$$\hat{H} = \hat{H}_0 + \hat{H}_Q + \hat{H}_P \tag{1.79}$$

which contains a spherical part,

$$\hat{H}_0 = \sum_j e_j^0 \hat{N}_j \tag{1.80}$$

where the $e_j^0$ are single-particle energies for the $j$ shells which we will take as given quantities, and $\hat{N}_j$ is the number operator which we can write in terms of particle creation and destruction operators,

$$\hat{N}_j = \sum_m a^\dagger_{jm} a_{jm} \tag{1.81}$$

The next term in Eq. (1.79) is the quadrupole interaction,

$$\hat{H}_Q = -\frac{1}{2}\chi \hat{D}^2 \tag{1.82}$$

where $\chi$ is the interaction strength, and

$$\begin{aligned} \hat{D} &= \sum_j d_j \hat{D}_j \\ \hat{D}_j &= \sum_m \sigma_{jm} a^\dagger_{jm} a_{jm} \end{aligned} \tag{1.83}$$

where the $d_j$ coefficients represent the magnitude of reduced quadrupole matrix elements, and the $\sigma_{jm}$ values are chosen to be

$$\sigma_{jm} = \begin{cases} +1 & |m| < \Omega_j/2 \\ -1 & |m| > \Omega_j/2 \end{cases}$$

in order to mimic the behavior of matrix elements $\langle jm \left| r^2 Y_{20} \right| jm \rangle$. The last term in Eq. (1.79) represents a pairing interaction of the form

$$\hat{H}_P = -\frac{1}{2} G \left( \hat{A}^\dagger \hat{A} + \hat{A}\hat{A}^\dagger \right) \tag{1.84}$$

where $G$ is the interaction strength and

$$\begin{aligned} \hat{A}^\dagger &= \sum_j \hat{A}^\dagger_j \\ \hat{A}^\dagger_j &= \sum_{m>0} a^\dagger_{jm} a^\dagger_{j\bar{m}} \end{aligned}$$

and where $\bar{m}$ indicates the time-reversed state of the state $m$ in the $j$ shell. The main advantage of the model defined in section 1.6.1 is that the many-body problem can be solved exactly in this case, and thereby provides a benchmark reference. The exact solution is presented in appendix B.

### *1.6.2 Constrained Hartree-Fock-Bogoliubov calculations*

Starting from the Hamiltonian defined in Eqs. (1.79), (1.80), (1.82), and (1.84) and using the fermion commutation rules for the particle operators, we write out the components explicitly and in time-ordered form,

$$\hat{H}_0 = \sum_{j,m>0} e_j^0 \left( a_{j,m}^\dagger a_{j,m} + a_{j,\bar{m}}^\dagger a_{j,\bar{m}} \right) \tag{1.85}$$

$$\begin{aligned}
\hat{H}_Q = &-\frac{1}{2}\chi \sum_{j_1,m_1>0} d_{j_1}^2 \sigma_{j_1,m_1}^2 \left( a_{j_1,m_1}^\dagger a_{j_1,m_1} + a_{j_1,\bar{m}_1}^\dagger a_{j_1,\bar{m}_1} \right) \\
&- \frac{1}{2}\chi \sum_{j_1,m_1>0} \sum_{j_2,m_2>0} d_{j_1}\sigma_{j_1,m_1} d_{j_2}\sigma_{j_2,m_2} \Big( a_{j_1,m_1}^\dagger a_{j_2,m_2}^\dagger a_{j_2,m_2} a_{j_1,m_1} \\
&+ a_{j_1,\bar{m}_1}^\dagger a_{j_2,\bar{m}_2}^\dagger a_{j_2,\bar{m}_2} a_{j_1,\bar{m}_1} + a_{j_1,m_1}^\dagger a_{j_2,\bar{m}_2}^\dagger a_{j_2,\bar{m}_2} a_{j_1,m_1} \\
&+ a_{j_1,\bar{m}_1}^\dagger a_{j_2,m_2}^\dagger a_{j_2,m_2} a_{j_1,\bar{m}_1} \Big)
\end{aligned} \tag{1.86}$$

$$\begin{aligned}
\hat{H}_P = &\frac{1}{2}G \sum_{j_1,m_1>0} \left( a_{j_1,m_1}^\dagger a_{j_1,m_1} + a_{j_1,\bar{m}_1}^\dagger a_{j_1,\bar{m}_1} \right) \\
&- G \sum_{j_1,m_1>0} \sum_{j_2,m_2>0} a_{j_1,m_1}^\dagger a_{j_1,\bar{m}_1}^\dagger a_{j_2,\bar{m}_2} a_{j_2,m_2}
\end{aligned} \tag{1.87}$$

where we have explicitly written the contribution from time-reversed terms, $(j, \bar{m})$. Adopting the shorthand notation $a = (j_a, m_a)$ and $\bar{a} = (j_a, \bar{m}_a)$, and introducing the standard density matrix $\rho_{ab} \equiv \left\langle \tilde{0} \left| a_b^\dagger a_a \right| \tilde{0} \right\rangle$ and pairing tensor $\kappa_{ab} \equiv \langle \tilde{0} | a_a a_b | \tilde{0} \rangle$ with respect to the quasiparticle ground state $|\tilde{0}\rangle$, we can use Wick's theorem to calculate expectation values of the operator products in the Hamiltonian,

$$\begin{aligned}
\left\langle \tilde{0} \left| a_a^\dagger a_b^\dagger a_b a_a \right| \tilde{0} \right\rangle &= \rho_{aa}\rho_{bb} - \rho_{ba}\rho_{ab} \\
\left\langle \tilde{0} \left| a_{\bar{a}}^\dagger a_{\bar{b}}^\dagger a_{\bar{b}} a_{\bar{a}} \right| \tilde{0} \right\rangle &= \rho_{aa}^*\rho_{bb}^* - \rho_{ba}^*\rho_{ab}^* \\
\left\langle \tilde{0} \left| a_a^\dagger a_{\bar{b}}^\dagger a_{\bar{b}} a_a \right| \tilde{0} \right\rangle &= \rho_{aa}\rho_{bb}^* + \kappa_{\bar{b}a}^*\kappa_{\bar{b}a} \\
\left\langle \tilde{0} \left| a_{\bar{a}}^\dagger a_b^\dagger a_b a_{\bar{a}} \right| \tilde{0} \right\rangle &= \rho_{aa}^*\rho_{bb} + \kappa_{b\bar{a}}^*\kappa_{b\bar{a}} \\
\left\langle \tilde{0} \left| a_a^\dagger a_{\bar{a}}^\dagger a_{\bar{b}} a_b \right| \tilde{0} \right\rangle &= \rho_{ba}\rho_{ba}^* + \kappa_{\bar{a}a}^*\kappa_{\bar{b}b}
\end{aligned}$$

where we have made use of the identities $\kappa_{ab} = 0$ and $\rho_{b\bar{a}} = 0$ for $a, b > 0$.With these results, we can now calculate the total HFB energy including constraints on the particle number and quadrupole moment,

$$
\begin{aligned}
E_{HFB} &= \left\langle \tilde{0} \left| \hat{H} + \lambda_N \hat{N} + \lambda_D \hat{D} \right| \tilde{0} \right\rangle \\
&= \sum_{a>0} \left( e_a^0 - \frac{1}{2}\chi d_a^2 \sigma_a^2 + \frac{1}{2}G + \lambda_N + \lambda_D d_a \sigma_a \right) \left(\rho_{aa} + \rho_{aa}^*\right) \\
&\quad - \frac{1}{2}\chi \sum_{a,b>0} d_a \sigma_a d_b \sigma_b \left(\rho_{aa}\rho_{bb} - \rho_{ba}\rho_{ab} + \rho_{aa}^*\rho_{bb}^* - \rho_{ba}^*\rho_{ab}^* \right. \\
&\quad \left. + \rho_{aa}\rho_{bb}^* + \rho_{aa}^*\rho_{bb} + \kappa_{\bar{b}a}^*\kappa_{\bar{b}a} + \kappa_{\bar{b}a}\kappa_{\bar{b}a}^*\right) \\
&\quad - G \sum_{a,b>0} \left(\rho_{ba}\rho_{ba}^* + \kappa_{\bar{a}a}^*\kappa_{\bar{b}b}\right)
\end{aligned}
\tag{1.88}
$$

From this point, we can proceed as described in the earlier sections of this chapter to derive the full HFB Hamiltonian and solve it. Although we will present calculations from a full HFB treatment, we also wish to present for pedagogical reasons a simpler derivation in the Hartree-Bogoliubov approximation, which can directly compared with results in [12]. To this end, we drop the term

$$
\sum_{a>0} \left( -\frac{1}{2}\chi d_a^2 \sigma_a^2 + \frac{1}{2}G \right) \left(\rho_{aa} + \rho_{aa}^*\right)
$$

and the non-diagonal terms $\rho_{ba}\rho_{ab}$, $\rho_{ba}^*\rho_{ab}^*$, $\rho_{ba}\rho_{ba}^*$, $\kappa_{\bar{b}a}^*\kappa_{\bar{b}a}$, and $\kappa_{\bar{b}a}\kappa_{\bar{b}a}^*$in Eq. (1.88). We are then left with

$$
\begin{aligned}
E_{HB} &= \sum_{a>0} \left(e_a^0 + \lambda_N + \lambda_D d_a \sigma_a\right) \left(\rho_{aa} + \rho_{aa}^*\right) \\
&\quad - \frac{1}{2}\chi \left[ \sum_{a>0} d_a \sigma_a \left(\rho_{aa} + \rho_{aa}^*\right) \right]^2 - G \left( \sum_{a>0} \kappa_{\bar{a}a}^* \right) \left( \sum_{a>0} \kappa_{\bar{a}a} \right)
\end{aligned}
\tag{1.89}
$$

Next, we calculate the HFB Hamiltonian from Eq. (1.12). For $k > 0$, we find the matrix elements

$$
\begin{aligned}
H_{k,k}^{1,1} &= e_k^0 + \lambda_N + \lambda_D d_k \sigma_k - \chi d_k \sigma_k \sum_{a>0} d_a \sigma_a \left(\rho_{aa} + \rho_{aa}^*\right) \equiv e_k \\
H_{k,\bar{k}}^{1,2} &= -G \sum_{a>0} \kappa_{\bar{a}a} \equiv \Delta \\
H_{k,\bar{k}}^{2,1} &= -\Delta^* \\
H_{k,k}^{2,2} &= -e_k
\end{aligned}
\tag{1.90}
$$

The time-reversed matrix elements are readily found by using the symmetry properties of the generalized density matrix which imply $\rho_{\bar{k}\bar{k}} = \rho_{kk}^*$ and $\kappa_{k\bar{k}} = -\kappa_{\bar{k}k}^*$ in Eq. (1.12). We find

$$
\begin{aligned}
H^{1,1}_{\bar{k},\bar{k}} &= -H^{2,2}_{k,k} = e_k \\
H^{1,2}_{\bar{k},k} &= H^{2,1}_{k,\bar{k}} = -\Delta^* \\
H^{2,1}_{\bar{k},k} &= H^{1,2}_{k,\bar{k}} = \Delta \\
H^{2,2}_{\bar{k},\bar{k}} &= -H^{1,1}_{k,k} = -e_k
\end{aligned}
\tag{1.91}
$$

We can conveniently write the components of the Hamiltonian as $2\times 2$ matrices that take into account the time-reversed state explicitly,

$$
H^{1,1} = H^{2,2} = \begin{pmatrix} e_k & 0 \\ 0 & e_k \end{pmatrix}, \quad H^{1,2} = \left(H^{2,1}\right)^T = \begin{pmatrix} 0 & \Delta \\ -\Delta^* & 0 \end{pmatrix}
\tag{1.92}
$$

In this representation, the $U$ and $V$ matrices take the form (see, e.g., chapter 7 in [1] or appendix D in [16]),

$$
U = \begin{pmatrix} u_k & 0 \\ 0 & u_k^* \end{pmatrix}, \quad V = \begin{pmatrix} 0 & -v_k^* \\ v_k & 0 \end{pmatrix}
\tag{1.93}
$$

The Hamiltonian is diagonalized by the Bogoliubov transformation in Eq. (1.14),

$$
\tilde{H} = B^\dagger H B
\tag{1.94}
$$

We could of course carry out this diagonalization numerically, but since our goal is to illustrate the formalism in this chapter as much as possible, we will solve this standard BCS problem explicitly. We can carry out the diagonalization in Eq. (1.94) for each state $k$ by performing the matrix operations using the $2\times 2$ matrices in Eqs. (1.92) and (1.93). From this point on we will assume all quantities are real and drop the complex conjugation. We find in particular the off-diagonal component

$$
\tilde{H}^{2,1} = \begin{pmatrix} 0 & 2e_k u_k v_k + \Delta\left(v_k^2 - u_k^2\right) \\ -e_k u_k v_k - \Delta\left(v_k^2 - u_k^2\right) & 0 \end{pmatrix}
$$

Then the requirement that $\tilde{H}$ be diagonal in the qp representation imposes $\tilde{H}^{2,1} = 0$, which leads to the well-known BCS equation (see, e.g., Eq. (6.48) in [1]),

$$
2\left(e_k^0 + \lambda_N + \lambda_D d_k \sigma_k - \chi d_k \sigma_k \bar{D}\right) u_k v_k + \Delta\left(v_k^2 - u_k^2\right) = 0
\tag{1.95}
$$

where have written

$$
\bar{D} \equiv \sum_{a>0} d_a \sigma_a \left(\rho_{aa} + \rho_{aa}^*\right)
\tag{1.96}
$$

We also have from Eq. (1.7),

$$
\begin{aligned}
\rho_{kk} &= v_k^2 \\
\kappa_{k\bar{k}} &= -\kappa_{\bar{k}k} = u_k v_k
\end{aligned}
\tag{1.97}
$$

from which

$$\Delta = -G \sum_{a>0} \kappa_{\bar{a}a} = G \sum_{a>0} u_a v_a \tag{1.98}$$

The standard solutions of Eq. (1.95) are

$$\begin{aligned} u_k^2 &= \frac{1}{2}\left(1 + \frac{e_k^0 - \chi d_k \sigma_k \bar{D} + \lambda_N + \lambda_D d_k \sigma_k}{\sqrt{\left(\varepsilon_k + \lambda_N + \lambda_D d_k \sigma_k\right)^2 + \Delta^2}}\right) \\ v_k^2 &= \frac{1}{2}\left(1 - \frac{e_k^0 - \chi d_k \sigma_k \bar{D} + \lambda_N + \lambda_D d_k \sigma_k}{\sqrt{\left(\varepsilon_k + \lambda_N + \lambda_D d_k \sigma_k\right)^2 + \Delta^2}}\right) \end{aligned} \tag{1.99}$$

where we take $u_k$ and $v_k$ to be the positive roots. All that remains is to determine the values of the Lagrange multipliers $\lambda_N$ and $\lambda_D$ to recover the desired average particle number $2\sum_{k>0} v_k^2 = N$ and average deformation $2\sum_{k>0} d_k \sigma_k v_k^2 = D_0$. In order to illustrate the formalism developed in section 1.5 for the adjustment of multiple constraints, we apply it to the problem at hand. The constraint matrices $F$ that appear in Eq. (1.56) can be written explicitly as $2\times 2$ matrices for each state $k>0$ and its time-reversed partner. Thus, for the number operator

$$F_N\left(k\right) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.100}$$

and for the deformation operator

$$F_D\left(k\right) = d_k \sigma_k \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.101}$$

Transforming $\mathbb{F}$ to the qp representation, Eq. (1.58) gives

$$\begin{aligned} F_N^{2,1}\left(k\right) &= V^T F_N U - U^T F_N^* V \\ &= 2u_k v_k \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{aligned} \tag{1.102}$$

and similarly

$$F_D^{2,1}\left(k\right) = 2u_k v_k d_k \sigma_k \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{1.103}$$

We also need the inverted diagonal matrix $M^{-1}$ which appears in Eq. (1.65),

$$M^{-1}\left(k\right) = \begin{pmatrix} \frac{1}{2E_k} & 0 \\ 0 & \frac{1}{2E_k} \end{pmatrix} \tag{1.104}$$

with $E_k$ the quasiparticle energy. We now have the necessary ingredients to calculate the matrix $T$ whose elements are defined in Eq. (1.76). Taking the traces over all states $k$, we obtain

$$T_{N,N} = -4 \sum_{k>0} \frac{(u_k v_k)^2}{E_k} \tag{1.105}$$

$$T_{N,D} = T_{D,N} = -4 \sum_{k>0} \frac{(u_k v_k)^2 d_k \sigma_k}{E_k} \tag{1.106}$$

$$T_{D,D} = -4 \sum_{k>0} \frac{(u_k v_k d_k \sigma_k)^2}{E_k} \tag{1.107}$$

The resulting $2 \times 2$ matrix is easy to invert, and Eq. (1.77) gives the adjustment to the Lagrange multipliers,

$$\begin{pmatrix} \delta\lambda_N \\ \delta\lambda_D \end{pmatrix} = \begin{pmatrix} T_{N,N} & T_{N,D} \\ T_{D,N} & T_{D,D} \end{pmatrix}^{-1} \begin{pmatrix} N - N^{(n)} \\ D - D^{(n)} \end{pmatrix} \tag{1.108}$$

which can be evaluated numerically at each iteration $n$. The corresponding variation in the generalized density is given by Eq. (1.73),

$$\begin{pmatrix} {}^{(1)}R^{2,1} \\ {}^{(1)}R^{2,1*} \end{pmatrix} = -\delta\lambda_N M^{-1} \begin{pmatrix} F_N^{2,1} \\ F_N^{2,1*} \end{pmatrix} - \delta\lambda_D M^{-1} \begin{pmatrix} F_D^{2,1} \\ F_D^{2,1*} \end{pmatrix} \tag{1.109}$$

We can again focus on the individual states $k$ and $\bar{k}$ and calculate

$${}^{(1)}R^{2,1}(k) = -\frac{u_k v_k}{2E_k} (\delta\lambda_N + \delta\lambda_D d_k \sigma_k) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{1.110}$$

We can relate this back to variations in $\rho$ and $\kappa$ through Eqs. (1.28) and (1.21),

$$\begin{aligned} \delta\rho(k) &= U^{(1)}R^{1,2}V^T + V^{*(1)}R^{2,1}U^\dagger \\ &= -\frac{(u_k v_k)^2}{2E_k} (\delta\lambda_N + \delta\lambda_D d_k \sigma_k) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{1.111}$$

Similarly, we calculate

$$\begin{aligned} \delta\kappa(k) &= -\left[U^{(1)}R^{1,2}U^T + V^{*(1)}R^{2,1}V^\dagger\right] \\ &= -\frac{u_k v_k}{2E_k} (\delta\lambda_N + \delta\lambda_D d_k \sigma_k) \left(u_k^2 - v_k^2\right) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{aligned} \tag{1.112}$$

Since we are working directly with the $u_k$ and $v_k$ coefficients, it will be convenient to relate the variations of $\delta\rho(k)$ and $\delta\kappa(k)$ to those coefficients. With the help of Eq. (1.97), we write

$$\begin{aligned} \delta\rho_{kk} &= 2v_k\delta v_k \\ &= -\frac{(u_k v_k)^2}{2E_k}\left(\delta\lambda_N + \delta\lambda_D d_k\sigma_k\right) \end{aligned} \tag{1.113}$$

and

$$\begin{aligned} -\delta\kappa_{\bar{k}k} &= v_k\delta u_k + u_k\delta v_k \\ &= \frac{u_k v_k}{2E_k}\left(\delta\lambda_N + \delta\lambda_D d_k\sigma_k\right)\left(u_k^2 - v_k^2\right) \end{aligned} \tag{1.114}$$

Combining these two equations, we find

$$\begin{aligned} \delta v_k &= -\frac{u_k^2 v_k}{4E_k}\left(\delta\lambda_N + \delta\lambda_D d_k\sigma_k\right) \\ \delta u_k &= \frac{u_k}{2E_k}\left(\delta\lambda_N + \delta\lambda_D d_k\sigma_k\right)\left(\frac{3}{2}u_k^2 - v_k^2\right) \end{aligned} \tag{1.115}$$

After the $u_k$ and $v_k$ coefficients are adjusted in a given iteration via

$$\begin{aligned} u_k &\to u_k + \delta u_k \\ v_k &\to v_k + \delta v_k \end{aligned} \tag{1.116}$$

the new values can be mixed with the old to slow down variations from one iteration to the next and improve convergence (see, e.g., [1, 17]). Then new values of $\bar{D}$ and $\Delta$ can be calculated using Eqs. (1.96) and (1.98), and new values of the coefficients $u_k$ and $v_k$ follow from Eq. (1.99). This iterative process is repeated until the change in the $u_k$ and $v_k$ coefficients is smaller than some predetermined value $\varepsilon$ (in the present calculations, we used $\varepsilon = 10^{-8}$).

Then the total HB energy is given by

$$E_{HB} = 2\sum_{a>0} e_a^0 v_a^2 - 2\chi\left(\sum_{a>0} d_a\sigma_a v_a^2\right)^2 - \frac{\Delta^2}{G} \tag{1.117}$$

and the single quasiparticle energies are given by

$$E_k \equiv \sqrt{\left(e_k^0 - \chi d_k\sigma_k\bar{D} + \lambda_N + \lambda_D d_k\sigma_k\right)^2 + \Delta^2} \tag{1.118}$$

For the numerical example described in section B.5, we perform constrained Hartree-Bogoliubov calculations with the solution given by Eq. (1.99), as well as a full constrained HFB calculation with the method described in the earlier sections of this chapter starting from the complete expression for the energy in Eq. (1.88). The resulting total HB and HFB energies are plotted as a function of deformation $D_0$ in Fig. 1.1. Both HB and HFB curves display minima at approximately the same deformations ($\approx \pm 31$ for HB, $\approx \pm 29$ for HFB), and a local maximum at zero deformation. The HFB energies are systematically lower than the HB ones. Note that the ground-state energy we calculated in the exact solution in section B.5 was $-16.944$, somewhat lower than the HB minima (with deformation $D_0 = \pm 30.627$ and energy -13.780). Thus the HB an HFB calculations reveal the dual minima in the energy surface that give rise to the shape mixing, but they only give a very approximate value for the ground-state energy. A more accurate estimate of the ground-state energy should include correlations beyond the HFB approximation.

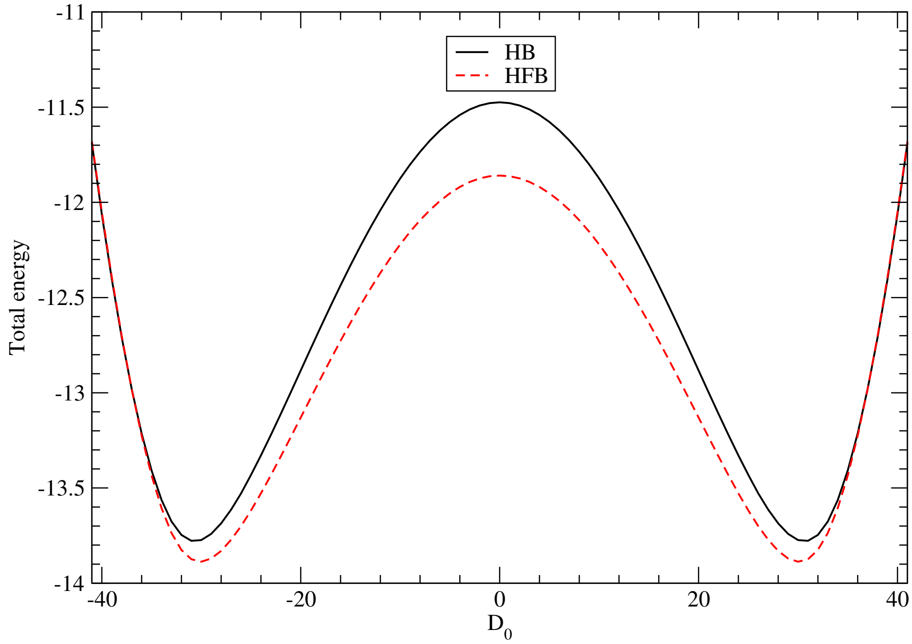


**Fig. 1.1** Energy surfaces obtained from HB and HFB calculations with the multi-$O\,(4)$ model presented in section 1.6.1, as a function of the constrained deformation $D_0$.

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Chapter 2

# Matrix elements of the finite-range interaction

In this chapter we give explicit expression for the matrix elements of the finite-range interaction used in the second part of the book in the deformed harmonic-oscillator basis. The components of the interaction explicitly given are: the central (Gaussian) part, the spin-orbit part, a density-dependent contribution, and both the exact and Slater approximation to the Coulomb interaction.

Microscopic approaches using phenomenological effective interactions of the Skyrme [1, 2] and finite-range [3, 4] type have a long history of successful applications to a variety of nuclear-physics phenomena [6, 7, 5, 8]. These interactions are parameterizations which usually include a density-dependent part, as suggested by Brueckner's G-matrix theory [9, 10], and are based on the hypothesis that nuclear properties can be well reproduced at the mean-field approximation with these forces. This is essentially the philosophy of the Brueckner-Hartree-Fock approach [11], The parameters of the interaction can then be adjusted within this framework using a judicious choice of nuclear data, such as the properties of nuclear matter and of select finite nuclei [12, 4, 13]. The calculations in the second part of this book will rely on a finite-range effective interaction [3, 4], which we describe in this chapter.

## 2.1 General form of the interaction

The finite-range effective interaction potential used in this work takes the form [3, 4]

$$\begin{aligned} V(\mathbf{r}_1,\mathbf{r}_2) = &\sum_{i=1}^{2}\left(W_i + B_i\hat{P}_\sigma - H_i\hat{P}_\tau - M_i\hat{P}_\sigma\hat{P}_\tau\right)e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu_i^2} \\ &+ iW_{LS}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right)\times\delta(\mathbf{r}_1-\mathbf{r}_2)\left(\overrightarrow{\nabla}_1-\overrightarrow{\nabla}_2\right)\cdot(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2) \\ &+ t_0\left(1+x_0\hat{P}_\sigma\right)\delta^3(\mathbf{r}_1-\mathbf{r}_2)\,\rho^\alpha\left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right) \\ &+ \frac{e^2\delta_{q_1,\mathrm{proton}}\delta_{q_2,\mathrm{proton}}}{|\mathbf{r}_1-\mathbf{r}_2|} \end{aligned} \tag{2.1}$$

where $\hat{P}_\sigma$ and $\hat{P}_\tau$ are spin- and isospin-exchange operators, $\rho$ is the total nuclear density, $\boldsymbol{\sigma}_1$ and $\boldsymbol{\sigma}_2$ are vectors whose components are the Pauli spin matrices, and the remaining parameters are listed in Table 2.1. Throughout this book, we have used the D1S parameterization given in table 2.1.

| | $i$ | $\mu_i$ (fm) | $W_i$ (MeV) | $B_i$ (MeV) | $H_i$ (MeV) | $M_i$ $(MeV)$ | $t_0$ (MeV $\cdot\mathrm{fm}^{3(\alpha+1)}$) | $x_0$ | $\alpha$ | $W_{LS}$ $(\mathrm{MeV}\cdot\mathrm{fm}^5)$ |
|---|---|---|---|---|---|---|---|---|---|---|
| D1 | 1 | 0.7 | -402.40 | -100.00 | -496.17 | -23.561 | 1350.0 | 1 | 1/3 | 115 |
| | 2 | 1.2 | -21.297 | -11.772 | 37.270 | -68.810 | | | | |
| D1S | 1 | 0.7 | 1720.30 | 1300.0 | -1813.53 | 1397.6 | 1390.6 | 1 | 1/3 | 130 |
| | 2 | 1.2 | 103.639 | -163.483 | 162.812 | -223.933 | | | | |
| D1N | 1 | 0.8 | -2047.6 | 1700.0 | -2414.9 | 1519.4 | 1609.5 | 1 | 1/3 | 115 |
| | 2 | 1.2 | 293.02 | -300.78 | 414.59 | -316.84 | | | | |
| D1M | 1 | 0.50 | -12797.57 | 14048.85 | -15144.43 | 11963.89 | 1562.22 | 1 | 1/3 | 115.36 |
| | 2 | 1.00 | 490.95 | -752.27 | 675.12 | -693.57 | | | | |

**Table 2.1** Different Parameterization for the finite-range effective interaction in Eq. (2.1). The values are adapted from [14, 15, 16].

## 2.2 The deformed harmonic-oscillator basis

In applications to fission presented subsequently, the HFB equations have been solved by expanding the qp states onto finite bases constituted of truncated sets of axially deformed harmonic oscillator (HO) states. This choice is very convenient since the matrix elements of the different terms of the finite-range interaction 2.1 then assumes a closed analytical form (see, e.g., Refs [17, 18] for a review of the numerical methods that are used in this context)[1]. Such a deformed HO basis can be written in cylindrical coordinates $(\rho, \varphi, z)$ as

$$\begin{aligned}\Phi_{n_r,\Lambda,n_z}(\mathbf{r}; b_\perp, b_z) &= \Phi_{n_r,\Lambda}(\rho, \varphi; b_\perp)\,\Phi_{n_z}(z; b_z) \\ &= \Phi_{n_r,|\Lambda|}(\rho; b_\perp)\,\frac{e^{\mathrm{i}\Lambda\varphi}}{\sqrt{2\pi}}\Phi_{n_z}(z; b_z)\end{aligned} \tag{2.2}$$

with the radial-component function

$$\Phi_{n_r,|\Lambda|}(\rho; b_\perp) = \mathcal{N}_{n_r}^{|\Lambda|}\eta^{|\Lambda|/2}e^{-\eta/2}L_{n_r}^{|\Lambda|}(\eta) \tag{2.3}$$

defined in terms of associated Laguerre polynomials $L_{n_r}^{|\Lambda|}(\eta)$ as a function of

$$\eta \equiv \rho^2/b_\perp^2$$

The quantity $\Lambda$ corresponds to the projection of the orbital angular momentum onto the symmetry axis $Oz$, whereas $n_r$ and $n_z$ count the number of nodes of the wave function along the radial and $z$ directions, respectively. In Eq. (2.3) the normalization constant given by

[1] Let us mention that using an axially deformed HO basis does not necessarily imply that nuclear shapes have to be restricted to axially symmetric ones. In fact, triaxial shapes can be described using such a basis by allowing a mixing of the orbital momentum projection quantum number $\Lambda$ in the expansion of the HFB qp states, although such a mixing is convenient in practice only for relatively small triaxiality - which is generally the case along fission paths.

$$\mathcal{N}_{n_r,|\Lambda|} \equiv \frac{1}{b_\perp}\left[\frac{2n_r!}{(n_r+|\Lambda|)!}\right]^{1/2} \tag{2.4}$$

The Cartesian, z-axis-component function in Eq. (2.2),

$$\Phi_{n_z}(z;b_z) = \mathcal{N}_{n_z} e^{-\xi^2/2} H_{n_z}(\xi) \tag{2.5}$$

is expressed in terms of Hermite polynomials $H_{n_z}(\xi)$ with

$$\xi \equiv z/b_z$$

and normalization constant

$$\mathcal{N}_{n_z} \equiv \frac{1}{\left(b_z\sqrt{\pi}2^{n_z}n_z!\right)^{1/2}}$$

The harmonic-oscillator functions defined in Eqs. (2.2) and (2.5) satisfy the orthonormalization conditions

$$\int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi\, \Phi^*_{n_r,\Lambda}(\rho,\varphi;b_\perp)\, \Phi_{n'_r,\Lambda'}(\rho,\varphi;b_\perp) = \delta_{n_r,n'_r}\delta_{\Lambda,\Lambda'}$$

$$\int_{-\infty}^{\infty} dz\, \Phi_{n_z}(z;b_z)\, \Phi_{n'_z}(z;b_z) = \delta_{n_z,n'_z}$$

The parameters $b_\perp$ and $b_z$ appearing in the harmonic-oscillator function definitions are usually treated as variational parameters in HFB calculations, and chosen to minimize the energy. These parameters can also be written in terms of harmonic-oscillator energies

$$\hbar\omega_\perp = \frac{\hbar^2}{mb_\perp^2}, \quad \hbar\omega_z = \frac{\hbar^2}{mb_z^2}, \quad \omega_0 \equiv \omega_\perp^2\omega_z$$

where $m$ is the nucleon mass. The quantum numbers of the basis, $n_r = 0,1,2,\ldots$, $\Lambda = 0,\pm1,\pm2,\ldots$, $n_z = 0,1,2,\ldots$, are truncated for a given maximum shell number $N$ according to the relation [19]

$$\hbar\omega_\perp(2n_r+|\Lambda|+1) + \hbar\omega_z\left(n_z+\frac{1}{2}\right) \le \hbar\omega_0(N+2)$$

In addition, a maximum value $n_z^{(\max)}$ can be imposed on the $n_z$ quantum number. Through a systematic study of the optimal values of $\hbar\omega_\perp$ and $\hbar\omega_z$ for $^{240}$Pu as a function of quadrupole ($Q_{20}$) and octupole ($Q_{30}$) constraints, we have obtained the following relations for $N = 13$ and $n_z^{(\max)} = 25$, by fitting the individual $\hbar\omega_0$ and $q \equiv \omega_\perp/\omega_z$ with the functional form

$$f(Q_{30}, Q_{20}) = \sum_{i,j} c_{ij} Q_{30}^i Q_{20}^j \tag{2.6}$$

The numerical values of the $c_{ij}$ coefficients for $\hbar\omega_0$ and the ratio $q$ are given in tables 2.2 and 2.3, respectively. From this, we can then calculate

$$\hbar\omega_\perp = q^{1/3}\hbar\omega_0$$
$$\hbar\omega_z = q^{-2/3}\hbar\omega_0$$

| $i$ | $j$ | $c_{ij}$ |
|---|---|---|
| 0 | 0 | 7.916212603959e+00 |
| 0 | 1 | 4.416886583910e-03 |
| 0 | 2 | -8.119414361741e-06 |
| 1 | 0 | 1.401836208522e-01 |
| 1 | 1 | -1.046648642584e-03 |
| 1 | 2 | 1.618642016886e-06 |
| 2 | 0 | -5.828609820447e-03 |
| 2 | 1 | 4.468841617704e-05 |
| 2 | 2 | -7.011156064446e-08 |
| 3 | 0 | 6.498801501801e-05 |
| 3 | 1 | -4.805951376011e-07 |
| 3 | 2 | 6.592668106802e-10 |
| 4 | 0 | -2.438595317082e-07 |
| 4 | 1 | 1.551342759362e-09 |
| 4 | 2 | -1.401951420300e-12 |

**Table 2.2** Coefficients for $\hbar\omega_0$ using the functional form of Eq. (2.6).

| $i$ | $j$ | $c_{ij}$ |
|---|---|---|
| 0 | 0 | 9.574894959751e-01 |
| 0 | 1 | 8.261269094176e-03 |
| 0 | 2 | -6.909503821655e-06 |
| 1 | 0 | 2.005584042966e-02 |
| 1 | 1 | -1.854775781290e-04 |
| 1 | 2 | 3.043733634606e-07 |
| 2 | 0 | -5.096586816081e-05 |
| 2 | 1 | 1.227377881974e-06 |
| 2 | 2 | -2.708065016489e-09 |

**Table 2.3** Coefficients for $q \equiv \omega_\perp/\omega_z$ using the functional form of Eq. (2.6).

Including the spin quantum number $\sigma = \pm 1/2$, the basis kets can be written as

$$|\alpha\rangle = |n_r^\alpha, \Lambda_\alpha, n_z^\alpha, \sigma_\alpha\rangle$$

and the total angular-momentum projection on the symmetry axis of the nucleus is $\Omega_\alpha = \Lambda_\alpha + \sigma_\alpha$. If axial symmetry is preserved, then the projection $\Omega$ is a good quantum number for the system, and the mean and pairing field matrices discussed in sections 2.3.2 and 2.3.3, respectively, will adopt a block-diagonal structure, with the blocks labeled by $\Omega$. Following the notation in [20], we write the time-reversed basis states as

$$|\bar{\alpha}\rangle = 2\sigma_\alpha \, |\underline{\alpha}\rangle$$

where

$$|\underline{\alpha}\rangle = |n_r^\alpha, -\Lambda_\alpha, n_z^\alpha, -\sigma_\alpha\rangle$$

## 2.3 Form of the HFB equations

### 2.3.1 Total energy of the system

Compact forms of the HFB equations have previously been given for various symmetries [4, 20]. For convenience, we present here forms of those equations appropriate for axially symmetric solutions.

The total energy of the system, including constraints on the nucleon numbers, can be written as [4]

$$E \equiv \left\langle \tilde{0} \left| \hat{H} - \lambda_n \hat{N}_n - \lambda_p \hat{N}_p \right| \tilde{0} \right\rangle$$

or, more explicitly,

$$\begin{aligned} E = & \sum_{q,\alpha\beta} \left(T_{\alpha\beta} - \lambda_q \delta_{\alpha\beta}\right) \rho^q_{\beta\alpha} + \frac{1}{2} \sum_{qq',\alpha\beta\gamma\delta} \bar{V}^{qq'}_{\alpha\beta\gamma\delta} \rho^{q'}_{\delta\beta} \rho^q_{\gamma\alpha} \\ & + \frac{1}{4} \sum_{qq',\alpha\beta\gamma\delta} \bar{V}^{qq'}_{\alpha\beta\gamma\delta} \kappa^{q'}_{\delta\gamma} \left(\kappa^q_{\beta\alpha}\right)^* \end{aligned}$$

where the indices $\alpha, \beta, \gamma, \delta$ span the basis states, $q, q' = 0, 1$ designate neutron and proton states, respectively, the $\rho^q_{\beta\alpha} \equiv \left\langle \tilde{0} \left| a^{q\dagger}_\alpha a^q_\beta \right| \tilde{0} \right\rangle$ are the matrix elements of the one-body density, and the $\kappa^q_{\beta\alpha} \equiv \left\langle \tilde{0} \left| a^q_\beta a^q_\alpha \right| \tilde{0} \right\rangle$ are the matrix elements of the pairing tensor. Let us note that, implicit in the above expression of the energy, is the assumption that the HFB vacuum is the direct product of a proton and neutron vacuum; otherwise $\rho$ and $\kappa$ would not necessarily be diagonal in $q$. The coefficients $T_{\alpha\beta}$ are matrix elements of the kinetic-energy operator, and the anti-symmetrized matrix elements of the density-dependent effective interaction are given by

$$\begin{aligned}\bar{V}^{qq'}_{\alpha\beta\gamma\delta} &\equiv \left\langle \alpha\beta \left| V \right| \widetilde{\gamma\delta} \right\rangle \\ &= \langle \alpha\beta \left| V \right| \gamma\delta \rangle - \langle \alpha\beta \left| V \right| \delta\gamma \rangle\end{aligned}$$

with the properties

$$\begin{aligned}\bar{V}_{\beta\alpha\gamma\delta} &= -\bar{V}_{\alpha\beta\gamma\delta} \\ \bar{V}_{\alpha\beta\delta\gamma} &= -\bar{V}_{\alpha\beta\gamma\delta}\end{aligned}$$

For convenience, we define

$$\begin{aligned}E_{kin} &\equiv \sum_{q,\alpha\beta} \left(T_{\alpha\beta} - \lambda_q \delta_{\alpha\beta}\right) \rho^q_{\beta\alpha} \\ E_{pot} &\equiv \frac{1}{2} \sum_{qq',\alpha\beta\gamma\delta} \bar{V}^{qq'}_{\alpha\beta\gamma\delta} \rho^{q'}_{\delta\beta} \rho^q_{\gamma\alpha} \\ E_{pair} &\equiv \frac{1}{4} \sum_{qq',\alpha\beta\gamma\delta} \bar{V}^{qq'}_{\alpha\beta\gamma\delta} \kappa^{q'}_{\delta\gamma} \left(\kappa^q_{\beta\alpha}\right)^*\end{aligned} \tag{2.7}$$

so that

$$E = E_{kin} + E_{pot} + E_{pair}$$

The matrix elements of the density and pairing tensor operators satisfy the properties

$$\begin{aligned}\rho^{q*}_{\alpha\beta} &= \rho^q_{\beta\alpha} \\ \rho^q_{\bar{\alpha}\bar{\beta}} &= \rho^{q*}_{\alpha\beta} \\ \rho^q_{\bar{\alpha}\beta} &= \rho^q_{\alpha\bar{\beta}} = 0 \quad \text{for } \alpha, \beta > 0\end{aligned}$$

and

$$\begin{aligned}\kappa_{\beta\alpha} &= -\kappa_{\alpha\beta} \\ \kappa_{\bar{\alpha}\beta} &= -\kappa^*_{\alpha\bar{\beta}} \\ \kappa_{\alpha\beta} &= \kappa_{\bar{\alpha}\bar{\beta}} = 0 \quad \text{for } \alpha, \beta > 0\end{aligned}$$

Then, using the hermiticity of the matrix elements, we can simplify the expression above to get

$$\begin{aligned}E_{kin} &= 2 \sum_{q;\alpha,\beta>0} \left(T_{\alpha\beta} - \lambda_q \delta_{\alpha\beta}\right) \rho^q_{\beta\alpha} \\ &= 4 \sum_{q;\alpha>\beta>0} \left(T_{\alpha\beta} - \lambda_q \delta_{\alpha\beta}\right) \rho^q_{\beta\alpha} + 2 \sum_{q;\alpha} \left(T_{\alpha\alpha} - \lambda_q \delta_{\alpha\alpha}\right) \rho^q_{\alpha\alpha}\end{aligned}$$

Or, in a more compact form,

$$\boxed{E_{kin} = 4 \sum_{q;\alpha \geq \beta > 0} \frac{1}{1+\delta_{\alpha\beta}} \left(T_{\alpha\beta} - \lambda_q \delta_{\alpha\beta}\right) \rho^q_{\beta\alpha}}$$

and similarly,

$$\boxed{E_{pot} = 2 \sum_{q;\alpha \geq \gamma > 0} \frac{1}{1+\delta_{\alpha\gamma}} \Gamma^{q,nr}_{\alpha\gamma}\left(pot\right) \rho^q_{\gamma\alpha}}$$

where we have defined the Hartree-Fock field (with no re-arrangement terms) as

$$\Gamma^{q,nr}_{\alpha\gamma}\left(pot\right) \equiv \sum_{q',\beta\delta} \bar{V}^{qq'}_{\alpha\beta\gamma\delta} \rho^{q'}_{\delta\beta} \tag{2.8}$$

and which satisfies the properties

$$\begin{aligned}
\Gamma^{q,nr}_{\bar{\alpha}\bar{\gamma}}\left(pot\right) &= \left[\Gamma^{q,nr}_{\alpha\gamma}\left(pot\right)\right]^* \\
\Gamma^{q,nr}_{\gamma\alpha}\left(pot\right) &= \left[\Gamma^{q,nr}_{\alpha\gamma}\left(pot\right)\right]^*
\end{aligned}$$

Next, we simplify the pairing contribution to the total energy,

$$\boxed{E_{pair} = -2 \sum_{q;\alpha \geq \beta > 0} \frac{1}{1+\delta_{\alpha\beta}} \mathrm{Re}\left\{\Delta^q_{\alpha\bar{\beta}} \kappa_{\beta\bar{\alpha}}\right\}}$$

where we have defined the pairing field for $\alpha, \beta > 0$

$$\begin{aligned}
\Delta^q_{\alpha\bar{\beta}} &\equiv \frac{1}{2} \sum_{q';\gamma,\delta>0} \left[\bar{V}^{qq'}_{\alpha\bar{\beta}\gamma\bar{\delta}} \kappa^{q'}_{\bar{\delta}\gamma} + \bar{V}^{qq'}_{\alpha\bar{\beta}\bar{\gamma}\delta} \kappa^{q'}_{\delta\bar{\gamma}}\right] \\
&= \frac{1}{2} \sum_{q';\gamma,\delta>0} \left[-\bar{V}^{qq'}_{\alpha\bar{\beta}\gamma\bar{\delta}} \kappa^{q'*}_{\delta\bar{\gamma}} + \bar{V}^{qq'}_{\alpha\bar{\beta}\bar{\gamma}\delta} \kappa^{q'}_{\delta\bar{\gamma}}\right]
\end{aligned}$$

and which satisfies the properties

$$\begin{aligned}
\Delta^q_{\bar{\alpha}\beta} &= -\left(\Delta^q_{\alpha\bar{\beta}}\right)^* \\
\Delta^q_{\bar{\beta}\alpha} &= -\Delta^q_{\alpha\bar{\beta}}
\end{aligned}$$

### 2.3.2 The Hartree-Fock field

The Hartree-Fock field defined in Eq. (2.8) did not include the so-called "re-arrangement" terms. The more general definition of the field, which includes re-arrangement terms, is

$$\begin{aligned}\Gamma^q_{\alpha\gamma} &= \frac{\partial}{\partial\rho^q_{\gamma\alpha}}E_{pot} + \frac{\partial}{\partial\rho^q_{\gamma\alpha}}E_{pair} \\ &\equiv \Gamma^q_{\alpha\gamma}\left(pot\right) + \Gamma^q_{\alpha\gamma}\left(pair\right)\end{aligned}$$

The second term, $\Gamma^q_{\alpha\gamma}\left(pair\right)$, arises if the effective interaction contains an explicit density dependence (which is the case of the interaction (2.1)). It is expressed as

$$\begin{aligned}\Gamma^q_{\alpha\gamma}\left(pair\right) &\equiv \frac{\partial}{\partial\rho^q_{\gamma\alpha}}\frac{1}{4}\sum_{q_1q_2,\alpha'\beta'\gamma'\delta'} V^{q_1q_2}_{\alpha'\beta'\gamma'\delta'}\kappa^{q_2}_{\delta'\gamma'}\left(\kappa^{q_1}_{\beta'\alpha'}\right)^* \\ &= \frac{1}{4}\sum_{q_1q_2,\alpha'\beta'\gamma'\delta'}\left(\frac{\partial}{\partial\rho^q_{\gamma\alpha}}V^{q_1q_2}_{\alpha'\beta'\gamma'\delta'}\right)\kappa^{q_2}_{\delta'\gamma'}\left(\kappa^{q_1}_{\beta'\alpha'}\right)^*\end{aligned} \tag{2.9}$$

As we will see in section 2.4.6, the density-dependent term in the effective interaction of Eq. (2.1) will contribute matrix elements in Eq. (2.9) of the form

$$\begin{aligned}V^{qq'}_{\alpha\beta\gamma\delta} &= t_0\left(\delta_{\sigma_\alpha,\sigma_\gamma}\delta_{\sigma_\beta,\sigma_\delta} - \delta_{\sigma_\alpha,\sigma_\delta}\delta_{\sigma_\beta,\sigma_\gamma}\right)\left(1-x_0\right)\delta_{qq'} \\ &\times\int d^3r\,\Phi^*_\alpha\left(\mathbf{r}\right)\Phi^*_\beta\left(\mathbf{r}\right)\Phi_\gamma\left(\mathbf{r}\right)\Phi_\delta\left(\mathbf{r}\right)\rho^\lambda\left(\mathbf{r}\right)\end{aligned}$$

which vanish for $x_0 = 1$. Therefore, the Hartree-Fock field reduces to

$$\Gamma^q_{\alpha\gamma} = \frac{\partial}{\partial\rho^q_{\gamma\alpha}}E_{pot} \tag{2.10}$$

At this point, it is useful to separate the contributions to $\Gamma^q_{\alpha\gamma}$ into density-dependent and density-independent terms. For the density-independent part of the field, we have

$$\boxed{\Gamma^{q,di}_{\alpha\gamma} = \sum_{q';\beta\geq\delta>0}\frac{1}{1+\delta_{\beta\delta}}\left[F_{\alpha\beta\gamma\delta}\rho^{q'}_{\delta\beta} + F_{\alpha\delta\gamma\beta}\left(\rho^{q'}_{\delta\beta}\right)^*\right]}$$

where we have defined

$$\begin{aligned}F_{\alpha\beta\gamma\delta} &\equiv \left\langle\alpha\beta\left|V\right|\gamma\delta\right\rangle - \left\langle\alpha\beta\left|V\right|\delta\gamma\right\rangle + \left\langle\alpha\bar{\delta}\left|V\right|\gamma\bar{\beta}\right\rangle - \left\langle\alpha\bar{\delta}\left|V\right|\bar{\beta}\gamma\right\rangle \\ &= \left\langle\alpha\beta\left|V\right|\gamma\delta\right\rangle - \left\langle\alpha\beta\left|V\right|\delta\gamma\right\rangle + 4\sigma_\beta\sigma_\delta\left(\left\langle\alpha\underline{\delta}\left|V\right|\gamma\underline{\beta}\right\rangle - \left\langle\alpha\underline{\delta}\left|V\right|\underline{\beta}\gamma\right\rangle\right)\end{aligned} \tag{2.11}$$

For real-valued density matrix elements, the field reduces to

$$\Gamma^{q,di}_{\alpha\gamma} = \sum_{q';\beta\geq\delta>0}\frac{1}{1+\delta_{\beta\delta}}\left(F_{\alpha\beta\gamma\delta} + F_{\alpha\delta\gamma\beta}\right)\rho^{q'}_{\delta\beta}$$

The density-dependent field ($\Gamma^{q,dd}_{\alpha\gamma}$) can be obtained directly from the differentiation in Eq. (2.10). The spatial dependence of the one-body density has the form

$$\rho^q(\mathbf{r}) = \sum_{\alpha'\gamma'} \delta_{\sigma_{\alpha'},\sigma_{\gamma'}} \Phi^*_{\alpha'}(\mathbf{r}) \Phi_{\gamma'}(\mathbf{r}) \rho^q_{\gamma'\alpha'} \tag{2.12}$$

Imposing the symmetries of the density matrix elements, this expression reduces to

$$\rho^q(\mathbf{r}) = 4 \sum_{\alpha'\geq\gamma'>0} \frac{\delta_{\sigma_{\alpha'},\sigma_{\gamma'}}}{1+\delta_{\alpha'\gamma'}} \mathrm{Re}\left[\Phi^*_{\alpha'}(\mathbf{r}) \Phi_{\gamma'}(\mathbf{r}) \rho^q_{\gamma'\alpha'}\right] \tag{2.13}$$

Thus, for a generic function of the density, we write the derivative with respect $\rho^q_{\gamma\alpha}$ using Eq. (2.12),

$$\frac{\partial}{\partial \rho^q_{\gamma\alpha}} f(\rho^q(\mathbf{r})) = \delta_{\sigma_\alpha,\sigma_\gamma} \Phi^*_\alpha(\mathbf{r}) \Phi_\gamma(\mathbf{r}) f'(\rho^q(\mathbf{r}))$$

where $f'$ is the derivative of the function $f$.

### 2.3.3 The pairing field

The pairing field is given in general by

$$\begin{aligned} \Delta^q_{\alpha\beta} &\equiv \frac{\partial}{\partial\left(\kappa^q_{\beta\alpha}\right)^*} E_{pair} \\ &= \frac{1}{2} \sum_{q',\gamma\delta} V^{qq'}_{\alpha\beta\gamma\delta} \kappa^{q'}_{\delta\gamma} \end{aligned}$$

Taking into account the symmetry properties of the matrix elements,

$$\boxed{\Delta^q_{\alpha\bar{\beta}} = \sum_{q',\gamma\geq\delta>0} \frac{1}{1+\delta_{\gamma\delta}} G_{\alpha\beta\gamma\delta} \kappa^{q'}_{\delta\bar{\gamma}}}$$

where we have defined

$$G_{\alpha\beta\gamma\delta} \equiv V_{\alpha\bar{\beta}\bar{\gamma}\delta} - V_{\alpha\bar{\beta}\delta\bar{\gamma}} - V_{\alpha\bar{\beta}\gamma\bar{\delta}} + V_{\alpha\bar{\beta}\bar{\delta}\gamma}$$

## 2.4 Matrix elements in an axially deformed harmonic-oscillator basis

### 2.4.1 Matrix element of the kinetic-energy operator

The contribution from the kinetic-energy operator follows from Eq. (2.7)

$$\frac{\partial}{\partial \rho_{ki}^{q}} E_{kin} = T_{ik} - \lambda_q \delta_{ik}$$

where

$$T_{ik} = \left\langle i \left| -\frac{\hbar^2}{2m} \nabla^2 \right| k \right\rangle$$

We can use the fact that the harmonic-oscillator basis functions satisfy the harmonic-oscillator Schrödinger equation, which in cylindrical coordinates takes the form

$$\begin{aligned}&\left( -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m\omega_\perp^2 r^2 + \frac{1}{2} m\omega_z^2 z^2 \right) \Phi_{n_r,\Lambda} \left(\rho, \Lambda; b_\perp\right) \Phi_{n_z} \left(z; b_z\right) \\ &= E \Phi_{n_r,\Lambda} \left(\rho, \Lambda; b_\perp\right) \Phi_{n_z} \left(z; b_z\right)\end{aligned}$$

with

$$E = \hbar\omega_\perp \left(2n_r + |\Lambda| + 1\right) + \hbar\omega_z \left(n_z + \frac{1}{2}\right)$$

along with recurrence relations for the Laguerre and Hermite polynomials to calculate

$$\begin{aligned}\left\langle n_r', \Lambda', n_z', \sigma' \left| -\frac{\hbar^2}{2m} \nabla^2 \right| n_r, \Lambda, n_z, \sigma \right\rangle = \delta_{\Lambda'\Lambda} \delta_{\sigma'\sigma} \\ \times \left\{ \delta_{n_z' n_z} \left\langle n_r', \Lambda' \left| -\frac{\hbar^2}{2m} \nabla_r^2 \right| n_r, \Lambda \right\rangle \right. \\ \left. + \delta_{n_r' n_r} \left\langle n_z' \left| -\frac{\hbar^2}{2m} \nabla_z^2 \right| n_z \right\rangle \right\}\end{aligned}$$

with

$$\begin{aligned}\left\langle n_r', \Lambda' \left| -\frac{\hbar^2}{2m} \nabla_r^2 \right| n_r, \Lambda \right\rangle = \frac{\hbar\omega_\perp}{2} \left\{ \delta_{n_r' n_r} \left(2n_r + |\Lambda| + 1\right) \right. \\ + \delta_{n_r', n_r - 1} \sqrt{n_r \left(n_r + |\Lambda|\right)} \\ \left. + \delta_{n_r', n_r + 1} \sqrt{\left(n_r + 1\right)\left(n_r + |\Lambda| + 1\right)} \right\}\end{aligned}$$

and

$$\left\langle n_z' \left| -\frac{\hbar^2}{2m}\nabla_z^2 \right| n_z \right\rangle = \frac{\hbar\omega_z}{2}\left\{\delta_{n_z' n_z}\left(n_z + \frac{1}{2}\right) \right.$$
$$-\frac{1}{2}\delta_{n_z', n_z-2}\sqrt{n_z\left(n_z-1\right)}$$
$$\left. -\frac{1}{2}\delta_{n_z', n_z+2}\sqrt{\left(n_z+1\right)\left(n_z+2\right)}\right\}$$

See also the discussion in section 2.4.5.

### *2.4.2 Matrix elements of the central contribution*

For the central terms in Eq. (2.1),

$$V_{cent}\left(\mathbf{r}_1, \mathbf{r}_2\right) = \left(W + B\hat{P}_\sigma - H\hat{P}_\tau - M\hat{P}_\sigma\hat{P}_\tau\right) e^{-(\mathbf{r}_1-\mathbf{r}_2)^2/\mu^2}$$

To calculate the matrix elements needed in Eq. (2.11) it is convenient to separate the spin, isospin, and spatial parts,

$$\langle ij \left| V \right| kl\rangle = \langle ij \left| V_\sigma \right| kl\rangle \langle ij \left| V_\tau \right| kl\rangle \langle ij \left| V_r \right| kl\rangle$$

After some simplifications, we can write for $\sigma_i = \sigma_k$ and $\sigma_j = \sigma_l$:

$$\begin{aligned}
&F_{ijkl} + F_{ilkj} \\
&= \left[2\left(W - H\delta_{qq'}\right) + \left(B - M\delta_{qq'}\right)\right]\left(\langle ij \left| V_r \right| kl\rangle + \langle il \left| V_r \right| kj\rangle\right) \\
&\quad - \left[\left(B\delta_{qq'} - M\right) + \left(W\delta_{qq'} - H\right)\delta_{\sigma_i\sigma_j}\right]\left(\langle ij \left| V_r \right| lk\rangle + \langle il \left| V_r \right| jk\rangle\right) \\
&\quad - \left[\left(B\delta_{qq'} - M\right) + \left(W\delta_{qq'} - H\right)\delta_{\sigma_i,-\sigma_j}\right]\left(\left\langle i\underline{l} \left| V_r \right| \underline{j}k\right\rangle + \left\langle i\underline{j} \left| V_r \right| \underline{l}k\right\rangle\right)
\end{aligned}$$

and for $\sigma_i = -\sigma_k$ and $\sigma_j = -\sigma_k$:

$$\begin{aligned}
F_{ijkl} + F_{ilkj} = \left(W\delta_{qq'} - H\right)&\left[\delta_{\sigma_i,-\sigma_j}\left(\left\langle i\underline{l} \left| V_r \right| \underline{j}k\right\rangle - \langle ij \left| V_r \right| lk\rangle\right)\right. \\
&\left. -\delta_{\sigma_i,\sigma_j}\left(\langle il \left| V_r \right| jk\rangle + \left\langle i\underline{j} \left| V_r \right| \underline{l}k\right\rangle\right)\right]
\end{aligned}$$

while the remaining cases give

$$F_{ijkl} + F_{ilkj} = 0$$

For the spatial part of the matrix elements, we recall the results in [17]. A matrix element of the gaussian function in a cylindrical harmonic-oscillator basis can be separated into radial and Cartesian components,

$$\langle ij \left| V_r \right| kl\rangle = V_{ijkl}^{(r)} V_{ijkl}^{(z)} \tag{2.14}$$

where, in cylindrical coordinates $(r, \varphi, z)$,

$$
\begin{aligned}
V_{ijkl}^{(r)} \equiv & \int_0^\infty r_1 dr_1 \int_0^{2\pi} d\varphi_1 \int_0^\infty r_2 dr_2 \int_0^{2\pi} d\varphi_2 \\
& \Phi^*_{n_r^{(i)},\Lambda_i}(r_1,\varphi_1;b_\perp)\, \Phi^*_{n_r^{(j)},\Lambda_j}(r_2,\varphi_2;b_\perp) \\
& V(r_1,\varphi_1;r_2,\varphi_2)\, \Phi_{n_r^{(k)},\Lambda_k}(r_1,\varphi_1;b_\perp)\, \Phi_{n_r^{(l)},\Lambda_l}(r_2,\varphi_2;b_\perp)
\end{aligned}
$$

and

$$
\begin{aligned}
V_{ijkl}^{(z)} \equiv & \int_{-\infty}^\infty dz_1 \int_{-\infty}^\infty dz_2\, \Phi_{n_z^{(i)}}(z_1;b_z)\, \Phi_{n_z^{(j)}}(z_2;b_z) \\
& V(z_1;z_2)\, \Phi_{n_z^{(k)}}(z_1;b_z)\, \Phi_{n_z^{(l)}}(z_2;b_z)
\end{aligned}
$$

In [17], explicit forms were derived for $V_{ijkl}^{(r)}$ and $V_{ijkl}^{(z)}$ with the gaussian interaction. We have

$$
\begin{aligned}
V_{ijkl}^{(r)} = & \frac{G_\perp - 1}{G_\perp + 1} \sum_{n_r=0}^{n_{\bar{j},l}} \sum_{n=0}^{n_{\bar{i},k}} T^{n,-\Lambda_i+\Lambda_k}_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} T^{n_r,-\Lambda_j+\Lambda_l}_{n_r^{(j)},-\Lambda_j;n_r^{(l)},\Lambda_l} \\
& \times \bar{I}(n_r,-\Lambda_j+\Lambda_l;n,-\Lambda_i+\Lambda_k)
\end{aligned}
$$

with

$$
G_\perp \equiv 1 + \frac{\mu^2}{b_\perp^2} \tag{2.15}
$$

and

$$
\begin{aligned}
n_{\mu,\nu} &\equiv n_r^{(\mu)} + n_r^{(\nu)} + \frac{|\Lambda_\mu| + |\Lambda_\nu| - |\Lambda_\mu + \Lambda_\nu|}{2} \\
n_{\bar{\mu},\nu} &\equiv n_r^{(\mu)} + n_r^{(\nu)} + \frac{|\Lambda_\mu| + |\Lambda_\nu| - |-\Lambda_\mu + \Lambda_\nu|}{2}
\end{aligned} \tag{2.16}
$$

The $T$ coefficients are given by

$$
\begin{aligned}
T^{n,k_1+k_2}_{n_1,k_1;n_2,k_2} = & (-1)^{n_1+n_2-n} \sqrt{\frac{n!\,(n_1+|k_1|)!\,(n_2+|k_2|)!}{n_1!n_2!\,(n+|k_1+k_2|)!}} \\
& \times \sum_{m_1=0}^{n_1} \sum_{m_2=0}^{n_2} \delta_{n \le n_{1,2}-m_1-m_2} C^{n,k_1+k_2}_{n_1,k_1,m_1;n_2,k_2,m_2}
\end{aligned}
$$

where the Kronecker-delta function $\delta_{n \le n_{1,2}-m_1-m_2}$ ensures that we always have $n \le n_{1,2}$,

$$
\begin{aligned}
C^{n,k_1+k_2}_{n_1,k_1,m_1;n_2,k_2,m_2} \equiv & (-1)^{m_1+m_2} \binom{n_1}{m_1} \binom{n_2}{m_2} \binom{n_{1,2}-m_1-m_2}{n} \\
& \times \frac{(n_{1,2}+|k_1+k_2|-m_1-m_2)!}{(n_1+|k_1|-m_1)!\,(n_2+|k_2|-m_2)!}
\end{aligned}
$$

The coefficient $\bar{I}$ is given by

$$\bar{I}\left(n_1, k_1; n_2, k_2\right) \equiv \delta_{k_1+k_2,0} \frac{\sqrt{n_1!\left(n_1+|k|\right)! n_2!\left(n_2+|k|\right)!}}{\left(G_{\perp}+1\right)^{n_1+n_2+|k|}} \Xi\left(n_1, n_2, |k|\right)$$

and

$$\Xi\left(n_1, n_2, |k|\right)=\frac{1}{\left(n_1+n_2+|k|\right)!}\binom{n_1+n_2+|k|}{n_1}\binom{n_1+n_2+|k|}{n_2}$$

Next, for the term $V_{ijkl}^{(z)}$ in Eq. (2.14), we have

$$\begin{aligned} V_{ijkl}^{(z)}= & \sqrt{\frac{G_z-1}{G_z+1}} \sum_{m_z=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T_{n_z^{(i)}, n_z^{(k)}}^{m_z} \\ & \times \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T_{n_z^{(j)}, n_z^{(l)}}^{n_z} \bar{I}\left(m_z, n_z\right) \end{aligned} \tag{2.17}$$

where the ",2" notation indicates that the summations are incremented in steps of 2, and with

$$G_z \equiv 1+\frac{\mu^2}{b_z^2} \tag{2.18}$$

The $T$ coefficients for the Cartesian term are given by

$$T_{k_1, k_2}^k=\frac{\sqrt{k_1!k_2!k!}}{\left(\frac{k_1-k_2+k}{2}\right)!\left(\frac{k_2-k_1+k}{2}\right)!\left(\frac{k_1+k_2-k}{2}\right)!}$$

and the $\bar{I}$ coefficient by

$$\bar{I}(m, n)=\sqrt{\frac{m!n!}{2^{m+n}}} \frac{(-1)^{(m-n)/2}}{\left(\frac{m+n}{2}\right)!\left(1+G_z\right)^{(m+n)/2}}\binom{m+n}{n}$$

#### 2.4.2.1 Modification for large oscillator number in $z$ direction

In the case where the $n_z$ quantum numbers are large, Eq. (2.17) requires the evaluation of sums of products of large ($T$) and small ($\bar{I}$) coefficients, which can be numerically unstable. As shown in [21, 17], we can replace Eq. (2.17) with

$$V_{ijkl}^{(z)}=\frac{\mu}{\sqrt{2\pi^3} b_z} \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T_{n_z^{(j)}, n_z^{(l)}}^{n_z} \bar{F}_{n_z^{(i)}, n_z^{(k)}}^{n_z} \tag{2.19}$$

where

$$\bar{F}^{n_z}_{n_z^{(i)},n_z^{(k)}} \equiv \frac{\Gamma\left(\xi - n_z^{(i)}\right)\Gamma\left(\xi - n_z^{(k)}\right)\Gamma\left(\xi - n_z\right)}{z^{\xi}\sqrt{n_z! n_z^{(i)}! n_z^{(k)}!}} \times {}_2F_1\left(-n_z^{(i)}, -n_z^{(k)}; -\xi + n_z + 1; 1 - z\right) \tag{2.20}$$

where ${}_2F_1(a, b; c; z)$ is a hypergeometric function, and

$$\xi \equiv \frac{n_z^{(i)} + n_z^{(k)} + n_z + 1}{2} \tag{2.21}$$

and

$$z \equiv 1 + \frac{\mu^2}{2b^2} \tag{2.22}$$

### 2.4.3 Matrix elements of the Coulomb contribution

$$\left\langle ij \left| V_C^{(D)} \right| kl \right\rangle = e^2 \delta_{\sigma_i,\sigma_k} \delta_{\sigma_j,\sigma_l} \delta_{\sigma_j,\sigma_l} \delta_{-\Lambda_i+\Lambda_k-\Lambda_j+\Lambda_l,0} \delta_{q,p} \delta_{q',p} \times \mathcal{I}_{ijkl}$$

where we have defined the integral

$$\mathcal{I}_{ijkl} \equiv \int d^3r_1 \int d^3r_2 \Phi_i^*(\mathbf{r}_1) \Phi_j^*(\mathbf{r}_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \Phi_k(\mathbf{r}_1) \Phi_l(\mathbf{r}_2)$$

Using the integral identity

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} du \, \frac{e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2/u^2}}{u^2}$$

we can write

$$\mathcal{I}_{ijkl} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \frac{du}{u^2} C_{ijkl}^{(r)}(u) \times C_{ijkl}^{(z)}(u) \tag{2.23}$$

where

$$C_{ijkl}^{(r)}(u) \equiv \int_0^{2\pi} d\varphi_1 \int_0^{\infty} \rho_1 d\rho_1 \int_0^{2\pi} d\varphi_2 \int_0^{\infty} \rho_2 d\rho_2 \Phi^*_{n_r^{(i)},\Lambda_i}(\rho_1, \varphi_1) \Phi^*_{n_r^{(j)},\Lambda_j}(\rho_2, \varphi_2) e^{-(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2)^2/u^2} \Phi_{n_r^{(k)},\Lambda_k}(\rho_1, \varphi_1) \Phi_{n_r^{(l)},\Lambda_l}(\rho_2, \varphi_2)$$

and

$$C_{ijkl}^{(z)}(u) \equiv \int_{-\infty}^{\infty} dz_1 \int_{-\infty}^{\infty} dz_2 \Phi^*_{n_z^{(i)}}(z_1) \Phi^*_{n_z^{(j)}}(z_2) e^{-(z_1 - z_2)^2/u^2} \Phi_{n_z^{(k)}}(z_1) \Phi_{n_z^{(l)}}(z_2) \tag{2.24}$$

Using the techniques described in [17], we can write

$$C_{ijkl}^{(z)}(u) = \left[\frac{G_z(u)-1}{G_z(u)+1}\right]^{1/2} \sum_{n=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} T^{n}_{n_z^{(j)},n_z^{(l)}} \times \sum_{m=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T^{m}_{n_z^{(i)},n_z^{(k)}} \frac{1}{(G_z(u)+1)^{(m+n)/2}} \bar{J}_z(m,n) \tag{2.25}$$

where $G_z(u)$ is given by Eq. (2.18) with the integration variable $u$ replacing $\mu$, and

$$\bar{J}_z(m,n) \equiv \frac{(-1)^{(m-n)/2}\sqrt{m!n!}}{2^{(m+n)/2}\left(\frac{m+n}{2}\right)!}\binom{m+n}{m}$$

with the implicit requirement that $m+n$ is even. For the radial coefficients, we can show that

$$C_{ijkl}^{(r)}(u) = \sum_{n_r=0}^{n_{\bar{j}l}} T^{n_r}_{n_r^{(j)},-\Lambda_j;n_r^{(l)},\Lambda_l} \sum_{n=0}^{n_{\bar{i}k}} T^{n}_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} \frac{G_\perp(u)-1}{G_\perp(u)+1} \times \frac{\bar{J}_r(n,n_r,-\Lambda_i+\Lambda_k)}{(G_\perp(u)+1)^{n+n_r+|-\Lambda_i+\Lambda_k|}}$$

where $G_\perp(u)$ is given by Eq. (2.15) with the integration variable $u$ replacing $\mu$, and

$$\bar{J}_r(n_1,n_2,\Lambda) = \sqrt{n_1!\,(n_1+|\Lambda|)\,n_2!\,(n_2+|\Lambda|)}\,\Xi(n_1,n_2,|\Lambda|)$$

and

$$\Xi(n_2,n_1,|\Lambda|) = \frac{1}{(n_1+n_2+|\Lambda|)!}\binom{n_1+n_2+|\Lambda|}{n_1}\binom{n_1+n_2+|\Lambda|}{n_2}$$

We have thus re-written Eq. (2.23) in the form

$$
\begin{aligned}
\mathcal{I}_{ijkl} = & \sum_{n_r=0}^{n_{\bar{j}l}} T^{n_r}_{n_r^{(j)},-\Lambda_j;n_r^{(l)},\Lambda_l} \sum_{n=0}^{n_{\bar{i}k}} T^{n}_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} \bar{J}_r\left(n,n_r,-\Lambda_i+\Lambda_k\right) \\
& \times \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} \sum_{m=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T^{m}_{n_z^{(i)},n_z^{(k)}} T^{n_z}_{n_z^{(j)},n_z^{(l)}} \bar{J}_z\left(m,n_z\right) \\
& \times \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{du}{u^2} \frac{\frac{G_\perp(u)-1}{G_\perp(u)+1}}{\left(G_\perp\left(u\right)+1\right)^{n+n_r+\left|-\Lambda_i+\Lambda_k\right|}} \\
& \times \frac{\left[\frac{G_z(u)-1}{G_z(u)+1}\right]^{1/2}}{\left(G_z\left(u\right)+1\right)^{(m+n_z)/2}}
\end{aligned}
\tag{2.26}
$$

We define the integral

$$
\begin{aligned}
M\left(p,q\right) \equiv & \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{du}{u^2} \frac{G_\perp\left(u\right)-1}{G_\perp\left(u\right)+1} \frac{1}{\left(G_\perp\left(u\right)+1\right)^p} \\
& \times \left[\frac{G_z\left(u\right)-1}{G_z\left(u\right)+1}\right]^{1/2} \frac{1}{\left(G_z\left(u\right)+1\right)^{q/2}}
\end{aligned}
\tag{2.27}
$$

and introduce the coefficients

$$
\begin{aligned}
D^{(r)}_{ijkl}\left(p\right) \equiv & \sum_{n_r=0}^{n_{\bar{j}l}} \sum_{m_r=0}^{n_{\bar{i}k}} \delta_{m_r+n_r,p} T^{n_r}_{n_r^{(j)},-\Lambda_j;n_r^{(l)},\Lambda_l} T^{m_r}_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} \\
& \times \bar{J}_r\left(m_r,n_r,-\Lambda_i+\Lambda_k\right)
\end{aligned}
\tag{2.28}
$$

and

$$
\begin{aligned}
D^{(z)}_{ijkl}\left(q\right) \equiv & \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} \sum_{m_z=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} \delta_{m_z+n_z,q} T^{n_z}_{n_z^{(j)},n_z^{(l)}} T^{m_z}_{n_z^{(i)},n_z^{(k)}} \\
& \times \bar{J}_z\left(m_z,n_z\right)
\end{aligned}
$$

Note that Kronecker delta symbols were introduced to group the terms in the summations by the sum of the indices (i.e., $m_r+n_r$ for $D^{(r)}_{ijkl}\left(p\right)$ and $m_z+n_z$ for $D^{(z)}_{ijkl}\left(q\right)$) because the remaining integral over $u$, defined in Eq. (2.27), only depends on the sum of these indices. Then Eq. (2.26) can be cast in the form

$$
\begin{aligned}
\mathcal{I}_{ijkl} = & \sum_{p=0}^{n_{\bar{i}k}+n_{\bar{j}l}} \sum_{q=\left|n_z^{(i)}-n_z^{(k)}\right|+\left|n_z^{(j)}-n_z^{(l)}\right|}^{n_z^{(i)}+n_z^{(k)}+n_z^{(j)}+n_z^{(l)}} D^{(r)}_{ijkl}\left(p\right) \\
& \times M\left(p+\left|-\Lambda_i+\Lambda_k\right|,q\right) D^{(z)}_{ijkl}\left(q\right)
\end{aligned}
\tag{2.29}
$$

All that remains now is to further evaluate the integral in Eq. (2.27). We can re-write this integral as

$$M\left(p,2r\right)=\frac{1}{\sqrt{\pi}b_z}\int_0^{\infty}dt\frac{1}{\left(2+t\right)^{p+1}\left(2+\frac{b_\perp^2}{b_z^2}t\right)^{r+1/2}}$$

and note that

$$\int_0^{\infty}dt\frac{1}{\left(2+\alpha t\right)^k\left(2+t\right)^l}=\frac{\alpha^{l-1}}{2^{k+l-1}}\frac{\Gamma\left(k+l-1\right)\Gamma\left(k\right)}{\Gamma\left(k+l\right)}\times\ {}_2F_1\left(l,k+l-1,k+l,1-\alpha\right)\tag{2.30}$$

where ${}_2F_1\left(a,b;c;z\right)$ is a hypergeometric function. This last result can be obtained by first making the variable substitution $2+\alpha t=2/y$ in the integral, which then becomes

$$\int_0^{\infty}dt\frac{1}{\left(2+\alpha t\right)^k\left(2+t\right)^l}=\frac{\alpha^{l-1}}{2^{k+l-1}}\int_0^1 dy\ \frac{y^{k+l-2}}{\left[1-\left(1-\alpha\right)y\right]^l}\tag{2.31}$$

Equation (2.30) then follows from identifying the right-hand side of Eq. (2.31) with the integral definition of the hypergeometric function (see, e.g., (15.3.1) in [22]),

$${}_2F_1\left(a,b,c,z\right)\equiv\frac{\Gamma\left(c\right)}{\Gamma\left(b\right)\Gamma\left(c-b\right)}\int_0^1 dt\quad\frac{t^{b-1}\left(1-t\right)^{c-b-1}}{\left(1-tz\right)^a}$$

Note that for deformed systems $b_z>b_\perp$, and the hypergeometric function of $1-\alpha$ above converges.

#### 2.4.3.1 Modification for large oscillator number in $z$ direction

In the case where the $n_z$ quantum numbers are large, we use the results in [17] to replace Eq. (2.25) with

$$C_{ijkl}^{(z)}\left(u\right)=\frac{u}{\sqrt{2\pi^3}b_z}\sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}}T^{n_z}_{n_z^{(j)},n_z^{(l)}}\bar{F}^{n_z}_{n_z^{(i)},n_z^{(k)}}\left(u\right)$$

where $\bar{F}^{n_z}_{n_z^{(i)},n_z^{(k)}}$ is given by Eq. (2.20). Equation (2.29) can then be re-written as

$$\mathcal{I}_{ijkl} = \sum_{p=0}^{n_{\bar{i}k}+n_{\bar{j}l}} D_{ijkl}^{(r)}(p) \sum_{n_z=\left|n_z^{(j)}-n_z^{(l)}\right|,2}^{n_z^{(j)}+n_z^{(l)}} \bar{D}_{ijkl}^{(z)}(n_z) \times \bar{M}\left(p+\left|-\Lambda_i+\Lambda_k\right|, n_z^{(i)}, n_z^{(k)}, n_z\right) \tag{2.32}$$

where $D_{ijkl}^{(r)}(p)$ is the same coefficient defined in Eq. (2.28). Next, we have defined

$$\bar{D}_{ijkl}^{(z)}(n_z) \equiv \frac{1}{\sqrt{2\pi^3}} T_{n_z^{(j)},n_z^{(l)}}^{n_z} \frac{\Gamma\left(\xi-n_z^{(i)}\right)\Gamma\left(\xi-n_z^{(k)}\right)\Gamma\left(\xi-n_z\right)}{\sqrt{n_z!n_z^{(i)}!n_z^{(k)}!}} \tag{2.33}$$

with $\xi$ given by Eq. (2.21) and

$$\bar{M}\left(p, n_z^{(i)}, n_z^{(k)}, n_z\right) \equiv \frac{2}{\sqrt{\pi}b_z}\int_0^\infty \frac{du}{u} \frac{\frac{G_\perp(u)-1}{G_\perp(u)+1}}{\left(G_\perp(u)+1\right)^p\left(1+\frac{u^2}{2b_z^2}\right)^\xi} \times {}_2F_1\left(-n_z^{(i)}, -n_z^{(k)}; -\xi+n_z+1; -\frac{u^2}{2b_z^2}\right) \tag{2.34}$$

The coefficient in Eq. (2.33) can be re-written as

$$\bar{D}_{ijkl}^{(z)}(n_z) = \frac{T_{n_z^{(j)},n_z^{(l)}}^{n_z}}{2^\xi\sqrt{n_z^{(i)}!n_z^{(k)}!n_z!}}\left(n_z^{(i)}+n_z^{(k)}-n_z-1\right)!! \times\left(-n_z^{(i)}+n_z^{(k)}+n_z-1\right)!!\left(n_z^{(i)}-n_z^{(k)}+n_z-1\right)!! \tag{2.35}$$

and the integral in Eq. (2.34) can be re-written as

$$\bar{M}\left(p, n_z^{(i)}, n_z^{(k)}, n_z\right) = \frac{2^\xi}{\sqrt{\pi}b_z}\int_0^\infty dt\, \frac{{}_2F_1\left(-n_z^{(i)}, -n_z^{(k)}; -\xi+n_z+1; -\frac{b_\perp^2}{2b_z^2}t\right)}{(2+t)^{p+1}\left(2+\frac{b_\perp^2}{b_z^2}t\right)^\xi} \tag{2.36}$$

Next, we expand the hypergeometric function in a power series,

$${}_2F_1\left(-n_z^{(i)}, -n_z^{(k)}; -\xi+n_z+1; -\frac{\beta t}{2}\right) = \sum_{r=0}^{\min\left(n_z^{(i)},n_z^{(k)}\right)} \frac{\left(-n_z^{(i)}\right)_r\left(-n_z^{(k)}\right)_r}{\left(-\xi+n_z+1\right)_r r!} \times\left(-\frac{\beta t}{2}\right)^r \tag{2.37}$$

where the notation $(z)_r$ indicates a rising Pochhammer symbol, and where

$$\beta \equiv \frac{b_\perp^2}{b_z^2}$$

Note that since both $n_z^{(i)}$ and $n_z^{(k)}$ are integers in Eq. (2.37), the series terminates after a finite number of terms, and since $\xi$ is always a half-integer number, there are no singularities caused by the terms in the denominator. Then the integral in Eq. (2.36) becomes

$$\begin{aligned}\bar{M}\left(p, n_z^{(i)}, n_z^{(k)}, n_z\right) = \frac{2^\xi}{\sqrt{\pi} b_z} &\sum_{r=0}^{\min\left(n_z^{(i)}, n_z^{(k)}\right)} \frac{\left(-n_z^{(i)}\right)_r \left(-n_z^{(k)}\right)_r}{\left(-\xi + n_z + 1\right)_r r!} \left(-\frac{\beta}{2}\right)^r \\ &\times \int_0^\infty dt \, \frac{t^r}{(2+t)^{p+1} (2+\beta t)^\xi}\end{aligned}$$

We can evaluate the remaining integral by making the substitution

$$2 + \beta t \equiv \frac{2}{y}$$

Then, we can show that the exponents satisfy the required relations for the integral to converge and

$$\begin{aligned}\int_0^\infty dt \, \frac{t^r}{(2+t)^{p+1} (2+\beta t)^\xi} &= \frac{\beta^{p-r}}{2^{p+\xi-r}} \int_0^1 dy \, \frac{y^{p+\xi-r-1} (1-y)^r}{\left[1 - (1-\beta) y\right]^{p+1}} \\ &= \frac{\beta^{p-r}}{2^{p+\xi-r}} B\left(p+\xi-r, r+1\right) \\ &\quad \times {}_2F_1\left(p+1, p+\xi-r; p+\xi+1; 1-\beta\right) \\ &= \frac{B\left(p+\xi-r, r+1\right)}{2^{p+\xi-r}} \\ &\quad \times {}_2F_1\left(\xi, r+1; p+\xi+1; 1-\beta\right)\end{aligned}$$

where $B(x, y)$ is the Beta function. Using this result, and after some simplifications, we obtain

$$\begin{aligned}\bar{M}\left(p, n_z^{(i)}, n_z^{(k)}, n_z\right) = &\frac{1}{2^p \sqrt{\pi} \left(p+\xi\right) b_z} \sum_{r=0}^{\min\left(n_z^{(i)}, n_z^{(k)}\right)} C_r \beta^r \\ &\times {}_2F_1\left(\xi, r+1; p+\xi+1; 1-\beta\right)\end{aligned}$$

where

$$C_r \equiv \begin{cases} 1 & r = 0 \\ \prod_{q=0}^{r-1} \frac{\left(q - n_z^{(i)}\right)\left(q - n_z^{(k)}\right)}{\left(q - \xi + n_z + 1\right)\left(q - p - \xi + 1\right)} & r > 0 \end{cases}$$

With this result we have all the ingredients needed to calculate the Coulomb integral in Eq. (2.32).

### 2.4.4 Matrix elements of the spin-orbit contribution

The spin-orbit energy is given by [23]

$$E_{so} = -\frac{W_0}{2} \int d^3 r \left\{ \rho(\mathbf{r}) \boldsymbol{\nabla} \cdot \mathbf{J}(\mathbf{r}) + \sum_q \rho_q(\mathbf{r}) \boldsymbol{\nabla} \cdot \mathbf{J}_q(\mathbf{r}) \right\}$$

where the density for charge $q$ is

$$\begin{aligned} \rho_q(\mathbf{r}) &\equiv \sum_{\alpha,\beta,\sigma} \rho^{(q)}_{\beta\alpha} \Phi^*_\alpha(\mathbf{r},\sigma) \Phi_\beta(\mathbf{r},\sigma) \\ &\equiv \sum_{\alpha,\beta,\sigma} \rho^{(q)}_{\beta\alpha} R_{\alpha\beta}(\mathbf{r},\sigma) \end{aligned} \tag{2.38}$$

and the current is

$$\mathbf{J}_q(\mathbf{r}) \equiv -\mathrm{i} \sum_{\alpha,\beta,\sigma,\sigma'} \rho^{(q)}_{\beta\alpha} \Phi^*_\alpha(\mathbf{r},\sigma) \boldsymbol{\nabla}\Phi_\beta(\mathbf{r},\sigma') \times \langle \sigma | \boldsymbol{\sigma} | \sigma' \rangle$$

where the components of $\boldsymbol{\sigma}$ are the Pauli spin matrices. We calculate the divergence

$$\begin{aligned} \boldsymbol{\nabla} \cdot \mathbf{J}_q(\mathbf{r}) &= -\mathrm{i} \sum_{\alpha,\beta,\sigma,\sigma'} \rho^{(q)}_{\beta\alpha} \boldsymbol{\nabla} \cdot \left[ \Phi^*_\alpha(\mathbf{r},\sigma) \boldsymbol{\nabla}\Phi_\beta(\mathbf{r},\sigma') \times \langle \sigma | \boldsymbol{\sigma} | \sigma' \rangle \right] \\ &= -\mathrm{i} \sum_{\alpha,\beta,\sigma,\sigma'} \rho^{(q)}_{\beta\alpha} \langle \sigma | \boldsymbol{\sigma} | \sigma' \rangle \cdot \boldsymbol{\nabla}\Phi^*_\alpha(\mathbf{r},\sigma) \times \boldsymbol{\nabla}\Phi_\beta(\mathbf{r},\sigma') \\ &\equiv \sum_{\alpha,\beta,\sigma,\sigma'} \rho^{(q)}_{\beta\alpha} \Delta_{\alpha\beta}(\mathbf{r},\sigma,\sigma') \end{aligned}$$

and define

$$R_{ik}(\mathbf{r}) \equiv \sum_\sigma R_{ik}(\mathbf{r},\sigma)$$

and

$$\Delta_{ik}(\mathbf{r}) \equiv \sum_{\sigma,\sigma'} \Delta_{ik}(\mathbf{r},\sigma,\sigma')$$

From this, it follows that

$$\frac{\partial}{\partial \rho_{ki}^{(q')}} \rho_q(\mathbf{r}) = \delta_{q,q'} R_{ik}(\mathbf{r})$$

and

$$\frac{\partial}{\partial \rho_{ki}^{(q')}} \boldsymbol{\nabla} \cdot \mathbf{J}_q(\mathbf{r}) = \delta_{q,q'} \Delta_{ik}(\mathbf{r})$$

and therefore,

$$\begin{aligned}\langle ij\,|V_{so}|\,kl\rangle &= \frac{\partial^2}{\partial \rho_{lj}^{(q_{jl})} \partial \rho_{ki}^{(q_{ik})}} E_{so} \\ &= -\frac{W_0}{2}\left(1+\delta_{q_{ik},q_{jl}}\right) \int d^3r \left[R_{ik}(\mathbf{r})\,\Delta_{jl}(\mathbf{r}) + R_{jl}(\mathbf{r})\,\Delta_{ik}(\mathbf{r})\right]\end{aligned} \tag{2.39}$$

Note that this result contains the exchange part of the matrix element, which appears as the $\delta_{q_{ik},q_{jl}}$ term.

#### 2.4.4.1 Explicit form of $R_{ik}(\mathrm{r})$ and $\Delta_{jl}(\mathrm{r})$

We write

$$\begin{aligned}R_{ik}(\mathbf{r}) &= \sum_{\sigma} \Phi_i^*(\mathbf{r},\sigma)\,\Phi_k(\mathbf{r},\sigma) \\ &= \frac{e^{i(\Lambda_k-\Lambda_i)\varphi}}{2\pi} \delta_{\sigma_i,\sigma_k} \tilde{\Phi}_i(\rho,z)\,\tilde{\Phi}_k(\rho,z)\end{aligned}$$

where we have written

$$\Phi_n(\mathbf{r},\sigma) \equiv \frac{e^{i\Lambda_n\varphi}}{\sqrt{2\pi}} \tilde{\Phi}_n(\rho,z)\,\chi_\sigma$$

to separate the dependence of the basis states on $(\rho, z)$ alone. Next we have

$$\begin{aligned}\Delta_{ik}(\mathbf{r}) &= \sum_{\sigma,\sigma'} -\mathrm{i}\,\langle\sigma\,|\boldsymbol{\sigma}|\,\sigma'\rangle \cdot \boldsymbol{\nabla}\Phi_i^*(\mathbf{r},\sigma) \times \boldsymbol{\nabla}\Phi_k(\mathbf{r},\sigma') \\ &= -\mathrm{i}\,\langle\sigma_i\,|\boldsymbol{\sigma}|\,\sigma_k\rangle \cdot \boldsymbol{\nabla}\Phi_i^*(\mathbf{r}) \times \boldsymbol{\nabla}\Phi_k(\mathbf{r})\end{aligned}$$

We further write

$$\begin{aligned}\langle\sigma_i\,|\boldsymbol{\sigma}|\,\sigma_k\rangle &= \delta_{\sigma_i,-\sigma_k}\hat{x} + 2\mathrm{i}\sigma_k\delta_{\sigma_i,-\sigma_k}\hat{y} + 2\sigma_k\delta_{\sigma_i,\sigma_k}\hat{z} \\ &= \delta_{\sigma_i,-\sigma_k}\left(\cos\varphi\hat{\rho} - \sin\varphi\hat{\varphi}\right) + 2\mathrm{i}\sigma_k\delta_{\sigma_i,-\sigma_k}\left(\sin\varphi\hat{\rho} + \cos\varphi\hat{\varphi}\right) \\ &\quad +2\sigma_k\delta_{\sigma_i,\sigma_k}\hat{z} \\ &= \delta_{\sigma_i,-\sigma_k}e^{2\mathrm{i}\sigma_k\varphi}\hat{\rho} + 2\mathrm{i}\sigma_k\delta_{\sigma_i,-\sigma_k}e^{2\mathrm{i}\sigma_k\varphi}\hat{\varphi} + 2\sigma_k\delta_{\sigma_i,\sigma_k}\hat{z}\end{aligned}$$

Now, since $i$ and $k$ are from the same symmetry block then $\Omega_i = \Omega_k$, and

$$\Lambda_k - \Lambda_i + 2\sigma_k - 2\sigma_i = 0$$

Therefore,

$$\langle \sigma_i |\boldsymbol{\sigma}| \sigma_k \rangle e^{\mathrm{i}(\Lambda_k - \Lambda_i)\varphi} = \delta_{\sigma_i,-\sigma_k}\hat{\rho} + 2\mathrm{i}\sigma_k\delta_{\sigma_i,-\sigma_k}\hat{\varphi} + 2\sigma_k\delta_{\sigma_i,\sigma_k}\hat{z}$$

Then, carrying out the vector operations,

$$\begin{aligned}\Delta_{ik}(\mathbf{r}) = \frac{1}{2\pi}\Bigg\{ & -\delta_{\sigma_i,-\sigma_k}\left[\frac{\Lambda_i}{\rho}\tilde{\Phi}_i\partial_z\tilde{\Phi}_k + \partial_z\tilde{\Phi}_i\frac{\Lambda_k}{\rho}\tilde{\Phi}_k\right] \\ & -2\sigma_k\delta_{\sigma_i,-\sigma_k}\left[\partial_\rho\tilde{\Phi}_i\partial_z\tilde{\Phi}_k - \partial_z\tilde{\Phi}_i\partial_\rho\tilde{\Phi}_k\right] \\ & +2\sigma_k\delta_{\sigma_i,\sigma_k}\left[\partial_\rho\tilde{\Phi}_i\frac{\Lambda_k}{\rho}\tilde{\Phi}_k + \frac{\Lambda_i}{\rho}\tilde{\Phi}_i\partial_\rho\tilde{\Phi}_k\right]\Bigg\}\end{aligned}$$

#### 2.4.4.2 Separation of coordinates

Returning to Eq. (2.39), we can write

$$\langle ij |V_{so}| kl\rangle = -\frac{W_0}{2}\left(1 + \delta_{q_{ik},q_{jl}}\right)\left(I_{ik;jl} + I_{jl;ik}\right)$$

where we have defined the integral

$$\begin{aligned}I_{ik;jl} &\equiv \int d^3r\, R_{ik}(\mathbf{r})\,\Delta_{jl}(\mathbf{r}) \\ &= \int d^3r_1 \int d^3r_2\, \delta^3(\mathbf{r}_1 - \mathbf{r}_2)\, R_{ik}(\mathbf{r}_1)\,\Delta_{jl}(\mathbf{r}_2)\end{aligned}$$

Using the techniques outlined in [17], we can show that

$$\delta^3(\mathbf{r}_1 - \mathbf{r}_2) = \sum_{n_r,\Lambda,n_z} f_{n_r,\Lambda,n_z}(\mathbf{r}_1)\,\hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r}_2)$$

where

$$f_{n_r,\Lambda,n_z}(\mathbf{r}_1) \equiv e^{-\eta_1/2}e^{-\xi_1^2/2}\Phi^*_{n_r,\Lambda,n_z}(\mathbf{r}_1)$$

and

$$\hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r}_2) \equiv e^{\eta_2/2}e^{\xi_2^2/2}\Phi_{n_r,\Lambda,n_z}(\mathbf{r}_2)$$

with the variables $\eta$ and $\xi$ defined as in section 2.2. Thus, we need to calculate the integrals

$$R_{ik}^{(n_r,\Lambda,n_z)} \equiv \int d^3r_1 R_{ik}(\mathbf{r}_1) f_{n_r,\Lambda,n_z}(\mathbf{r}_1) \tag{2.40}$$

and

$$\Delta_{jl}^{(n_r,\Lambda,n_z)} \equiv \int d^3r_2 \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r}_2) \Delta_{jl}(\mathbf{r}_2) \tag{2.41}$$

from which we will obtain

$$I_{ik;jl} = \sum_{n_r,\Lambda,n_z} R_{ik}^{(n_r,\Lambda,n_z)} \Delta_{jl}^{(n_r,\Lambda,n_z)}$$

#### 2.4.4.3 Calculation of the integral $R_{ik}^{(n_r,\Lambda,n_z)}$ in Eq. (2.40)

Expanding the products of harmonic-oscillator functions as in [17], we get

$$\begin{aligned} R_{ik}^{(n_r,\Lambda,n_z)} = & \frac{1}{\sqrt{\pi}b_\perp} \frac{1}{(\pi b_z^2)^{1/4}} \delta_{\sigma_i,\sigma_k} \delta_{\Lambda-\Lambda_i+\Lambda_k,0} \\ & \times \left[ \sum_{m=0}^{n_{i,k}} T^m_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} I(n_{i,k}-m,-\Lambda_i+\Lambda_k,n_r,\Lambda;b) \right] \\ & \times \left[ \sum_{n=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T^n_{n_z^{(i)},n_z^{(k)}} I(n,n_z;b) \right] \end{aligned}$$

where

$$I(n_1,\Lambda_1,n_2,\Lambda_2;b) \equiv \int_0^\infty \rho d\rho \int_0^{2\pi} d\varphi \, e^{-\rho^2/b^2} \Phi_{n_1,\Lambda_1}(\rho,\varphi;b) \Phi_{n_2,\Lambda_2}(\rho,\varphi;b)$$

and

$$I(n_1,n_2;b) \equiv \int_{-\infty}^{+\infty} dz \, e^{-z^2/b^2} \Phi_{n_1}(z;b) \Phi_{n_2}(z;b)$$

Note that this implies we always have $\Lambda = 0$ (since $i$ and $k$ are from the same block, $\Omega_i = \Omega_k$, and since $\sigma_i = \sigma_k$ we must therefore have $\Lambda_i = \Lambda_k$). We can separate this further as

$$R_{ik}^{(n_r,\Lambda,n_z)} = R_{ik}^{(n_r,\Lambda)} R_{ik}^{(n_z)} \tag{2.42}$$

with

$$R_{ik}^{(n_r,\Lambda)} \equiv \frac{1}{\sqrt{\pi}b_\perp}\delta_{\sigma_i,\sigma_k}\delta_{\Lambda-\Lambda_i+\Lambda_k,0} \times \left[\sum_{m=0}^{n_{i,k}} T^m_{n_r^{(i)},-\Lambda_i;n_r^{(k)},\Lambda_k} I\left(n_{i,k}-m,-\Lambda_i+\Lambda_k,n_r,\Lambda;b\right)\right]$$

$$R_{ik}^{(n_z)} \equiv \frac{1}{\left(\pi b_z^2\right)^{1/4}}\left[\sum_{n=\left|n_z^{(i)}-n_z^{(k)}\right|,2}^{n_z^{(i)}+n_z^{(k)}} T^n_{n_z^{(i)},n_z^{(k)}} I\left(n,n_z;b\right)\right]$$

Using the generating-function methods in [17] we calculate the remaining integrals explicitly,

$$\begin{aligned}
I\left(n_1,\Lambda_1,n_2,\Lambda_2;b\right) = {} & \frac{(-1)^{n_1+n_2}}{2^{n_{1,2}+1}n_{1,2}!}\sqrt{n_1!\left(n_1+|\Lambda_1|\right)!}\sqrt{n_2!\left(n_2+|\Lambda_2|\right)!}\delta_{\Lambda_1+\Lambda_2,0} \\
& \times\sum_{p=0}^{n_{1,2}}(-1)^p\binom{n_{1,2}}{p}\sum_{q=0}^{p}\binom{p}{q}\binom{n_{1,2}-p}{\frac{n_{1,2}-p-\Lambda_1}{2}} \\
& \times\delta_{2q-p,2n_1+|\Lambda_1|-n_{1,2}}\delta_{n_{1,2}-p-\Lambda_1,\text{even}}\delta_{p-n_{1,2}\le\Lambda_1\le n_{1,2}-p}
\end{aligned}$$

and

$$I\left(n_1,n_2;b\right) = \frac{\left(n_1+n_2-1\right)!!}{2^{(n_1+n_2+1)/2}\sqrt{n_1!n_2!}}\left(-1\right)^{(n_1+n_2)/2}\frac{(-1)^{n_1}+(-1)^{n_2}}{2}$$

#### 2.4.4.4 Calculation of the integral $\boldsymbol{\Delta_{jl}^{(n_r,\Lambda,n_z)}}$ in Eq. (2.41)

For the integral $\Delta_{ik}^{(n_r,\Lambda,n_z)}$, it will be convenient to re-introduce the $\varphi$ dependence explicitly. We then write

$$\begin{aligned}
\Delta_{ik}^{(n_r,\Lambda,n_z)} &= -\delta_{\sigma_i,-\sigma_k}\left(I_{\varphi z}-I_{z\varphi}\right)-2\sigma_k\delta_{\sigma_i,-\sigma_k}\left(I_{\rho z}-I_{z\rho}\right) \\
&\quad +2\sigma_k\delta_{\sigma_i,\sigma_k}\left(I_{\rho\varphi}-I_{\varphi\rho}\right) \\
&= -\delta_{\sigma_i,-\sigma_k}\left(I_{\varphi z}+2\sigma_k I_{\rho z}\right)+\delta_{\sigma_i,-\sigma_k}\left(I_{z\varphi}+2\sigma_k I_{z\rho}\right) \\
&\quad +2\sigma_k\delta_{\sigma_i,\sigma_k}\left(I_{\rho\varphi}-I_{\varphi\rho}\right) \\
&\equiv A_{ik}^{(n_r,\Lambda)}A_{ik}^{(n_z)}+B_{ik}^{(n_r,\Lambda)}B_{ik}^{(n_z)}+Z_{ik}^{(n_r,\Lambda)}Z_{ik}^{(n_z)}
\end{aligned}$$

with

$$
\begin{aligned}
I_{\varphi z} &\equiv \int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\, e^{2\mathrm{i}\sigma_k\varphi}\mathrm{i}\partial_\varphi \Phi_i^*(\mathbf{r})\,\partial_z\Phi_k(\mathbf{r})\\
I_{z\varphi} &\equiv \int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\, e^{2\mathrm{i}\sigma_k\varphi}\mathrm{i}\partial_z \Phi_i^*(\mathbf{r})\,\partial_\varphi\Phi_k(\mathbf{r})\\
I_{\rho z} &\equiv \int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\, e^{2\mathrm{i}\sigma_k\varphi}\partial_\rho \Phi_i^*(\mathbf{r})\,\partial_z\Phi_k(\mathbf{r})\\
I_{z\rho} &\equiv \int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\, e^{2\mathrm{i}\sigma_k\varphi}\partial_z \Phi_i^*(\mathbf{r})\,\partial_\rho\Phi_k(\mathbf{r})\\
I_{\rho\varphi} &\equiv -\mathrm{i}\int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\,\partial_\rho \Phi_i^*(\mathbf{r})\,\partial_\varphi\Phi_k(\mathbf{r})\\
I_{\varphi\rho} &\equiv \mathrm{i}\int d^3r\, \hat{\Phi}_{n_r,\Lambda,n_z}(\mathbf{r})\,\partial_\varphi \Phi_i^*(\mathbf{r})\,\partial_\rho\Phi_k(\mathbf{r})
\end{aligned}
$$

To proceed further, we separate the radial $(\rho,\varphi)$ and $z$ dependence of each term in $\Delta_{ik}^{(n_r,\Lambda,n_z)}$,

$$
\begin{aligned}
-\delta_{\sigma_i,-\sigma_k}\left(I_{\varphi z}+2\sigma_k I_{\rho z}\right) &\equiv A_{ik}^{(n_r,\Lambda)}A_{ik}^{(n_z)}\\
\delta_{\sigma_i,-\sigma_k}\left(I_{z\varphi}+2\sigma_k I_{z\rho}\right) &\equiv B_{ik}^{(n_r,\Lambda)}B_{ik}^{(n_z)}\\
2\sigma_k\delta_{\sigma_i,\sigma_k}\left(I_{\rho\varphi}-I_{\varphi\rho}\right) &\equiv Z_{ik}^{(n_r,\Lambda)}Z_{ik}^{(n_z)}
\end{aligned}
$$

Next, we introduce the general integrals of the form

$$
\begin{aligned}
I_{\alpha,\mu}^{(n_r,\Lambda)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) \equiv \int_0^\infty \rho d\rho \int_0^{2\pi} & d\varphi\, \rho^\alpha e^{\mathrm{i}\mu\varphi}\hat{\Phi}_{n_r,\Lambda}(\rho,\varphi)\\
&\times \Phi_{n_1,\Lambda_1}^*(\rho,\varphi)\,\Phi_{n_2,\Lambda_2}(\rho,\varphi)
\end{aligned}
\tag{2.43}
$$

and

$$
I^{(n_z)}\left(n_1;n_2\right) \equiv \int_{-\infty}^{\infty} dz\, \hat{\Phi}_{n_z}(z)\,\Phi_{n_1}(z)\,\Phi_{n_2}(z) \tag{2.44}
$$

Using recurrence relations for the derivatives of harmonic-oscillator functions, we can then write

$$
\begin{aligned}
A_{ik}^{(n_r,\Lambda)} = -\frac{\delta_{\sigma_i,-\sigma_k}}{b_\perp}\Bigg\{ & \sqrt{n_r^{(i)}+|\Lambda_i|}\left(1-\delta_{\Lambda_i,0}\right)\left(-s_{-\Lambda_i}+2\sigma_k\right)\\
&\times I_{0,2\sigma_k+s_{-\Lambda_i}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i+s_{-\Lambda_i};n_r^{(k)},\Lambda_k\right)\\
&+\sqrt{n_r^{(i)}}\left[-s_{-\Lambda_i}\left(1-\delta_{\Lambda_i,0}\right)-2\sigma_k\left(1+\delta_{\Lambda_i,0}\right)\right]\\
&\times I_{0,2\sigma_k-s_{-\Lambda_i}}^{(n_r,\Lambda)}\left(n_r^{(i)}-1,\Lambda_i-s_{-\Lambda_i};n_r^{(k)},\Lambda_k\right)\\
&-\frac{2\sigma_k}{b_\perp}I_{1,2\sigma_k}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i;n_r^{(k)},\Lambda_k\right)\Bigg\}
\end{aligned}
$$

$$A_{ik}^{(n_z)} = \frac{1}{b_z}\left[\sqrt{\frac{n_z^{(k)}}{2}}I^{(n_z)}\left(n_z^{(i)}; n_z^{(k)}-1\right) - \sqrt{\frac{n_z^{(k)}+1}{2}}I^{(n_z)}\left(n_z^{(i)}; n_z^{(k)}+1\right)\right]$$

$$\begin{aligned}
B_{ik}^{(n_r,\Lambda)} = \frac{\delta_{\sigma_i,-\sigma_k}}{b_\perp}\Bigg\{ & \sqrt{n_r^{(k)}+|\Lambda_k|}\left(1-\delta_{\Lambda_k,0}\right)\left(-s_{\Lambda_k}+2\sigma_k\right) \\
& \times I_{0,2\sigma_k+s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i; n_r^{(k)},\Lambda_k-s_{\Lambda_k}\right) \\
& +\sqrt{n_r^{(k)}}\left[-s_{\Lambda_k}\left(1-\delta_{\Lambda_k,0}\right)-2\sigma_k\left(1+\delta_{\Lambda_k,0}\right)\right] \\
& \times I_{0,2\sigma_k-s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i; n_r^{(k)}-1,\Lambda_k+s_{\Lambda_k}\right) \\
& -\frac{2\sigma_k}{b_\perp}I_{1,2\sigma_k}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i; n_r^{(k)},\Lambda_k\right)\Bigg\}
\end{aligned}$$

$$B_{ik}^{(n_z)} = \frac{1}{b_z}\left[\sqrt{\frac{n_z^{(i)}}{2}}I^{(n_z)}\left(n_z^{(i)}-1; n_z^{(k)}\right) - \sqrt{\frac{n_z^{(i)}+1}{2}}I^{(n_z)}\left(n_z^{(i)}+1; n_z^{(k)}\right)\right]$$

$$\begin{aligned}
Z_{ik}^{(n_r,\Lambda)} = \frac{2\sigma_k\delta_{\sigma_i,\sigma_k}}{b_\perp^2}s_{-\Lambda_i}\left(1-\delta_{\Lambda_i,0}\right)\Bigg\{ & -2\sqrt{n_r^{(i)}+|\Lambda_i|}\sqrt{n_r^{(k)}} \\
& \times I_{0,s_{-\Lambda_i}-s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i+s_{-\Lambda_i}; n_r^{(k)}-1,\Lambda_k+s_{\Lambda_k}\right) \\
& +2\sqrt{n_r^{(i)}}\sqrt{n_r^{(k)}+|\Lambda_k|} \\
& \times I_{0,-s_{-\Lambda_i}+s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)}-1,\Lambda_i-s_{-\Lambda_i}; n_r^{(k)},\Lambda_k-s_{\Lambda_k}\right) \\
& +\frac{1}{b_\perp}\sqrt{n_r^{(k)}+|\Lambda_k|}I_{1,s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i; n_r^{(k)},\Lambda_k-s_{\Lambda_k}\right) \\
& +\frac{1}{b_\perp}\sqrt{n_r^{(k)}}I_{1,-s_{\Lambda_k}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i; n_r^{(k)}-1,\Lambda_k+s_{\Lambda_k}\right) \\
& -\frac{1}{b_\perp}\sqrt{n_r^{(i)}+|\Lambda_i|}I_{1,s_{-\Lambda_i}}^{(n_r,\Lambda)}\left(n_r^{(i)},\Lambda_i+s_{-\Lambda_i}; n_r^{(k)},\Lambda_k\right) \\
& -\frac{1}{b_\perp}\sqrt{n_r^{(i)}}I_{1,-s_{-\Lambda_i}}^{(n_r,\Lambda)}\left(n_r^{(i)}-1,\Lambda_i-s_{-\Lambda_i}; n_r^{(k)},\Lambda_k\right)\Bigg\}
\end{aligned}$$

$$Z_{ik}^{(n_z)} \equiv I^{(n_z)}\left(n_z^{(i)}; n_z^{(k)}\right)$$

and where

$$s_k \equiv \begin{cases} 1 & k \geq 0 \\ -1 & k < 0 \end{cases} \tag{2.45}$$

The remaining integrals can be evaluated using the formula for products of harmonic-oscillator functions in [17]. For the integral in Eq. (2.43) with $\alpha = 0$ and $\mu = 0$,

$$\boxed{I_{0,0}^{(n_r,\Lambda=0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = \frac{1}{\sqrt{\pi}b_\perp} T^{n_r}_{n_1,-\Lambda_1;n_2,\Lambda_2}\delta_{-\Lambda_1+\Lambda_2,0}\delta_{0\le n_r\le n_{\bar{1},2}}}$$

For $\alpha = 0$ and $\mu = \pm 1$,

$$\boxed{I_{0,\pm 1}^{(n_r,\Lambda=0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = \frac{1}{b_\perp}\delta_{-\Lambda_1+\Lambda_2+\mu,0}\sum_{m=0}^{n_{\bar{1},2}} T^{m}_{n_1,-\Lambda_1;n_2,\Lambda_2}\mathcal{N}_{m,1}\frac{(2m-1)!!}{2^{m+1}m!}}$$

Next, for $\alpha = 0$ and $\mu = \pm 2$ we have two cases of interest, first for $|-\Lambda_1+\Lambda_2| = 0$,

$$\boxed{I_{0,\pm 2}^{(n_r,\Lambda=0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = \frac{1}{\sqrt{\pi}b_\perp}\delta_{-\Lambda_1+\Lambda_2+\mu,0}\delta_{0\le n_r\le n_{\bar{1},2}}T^{n_r}_{n_1,-\Lambda_1;n_2,\Lambda_2}}$$

and for $|-\Lambda_1+\Lambda_2| = 2$,

$$\boxed{\begin{aligned} I_{0,\pm 2}^{(n_r,\Lambda=0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = {} & \frac{1}{\sqrt{2\pi}}\delta_{-\Lambda_1+\Lambda_2+\mu,0} \\ & \times\Bigg[\delta_{0\le n_r\le n_{1,2}}\sum_{m=n_r}^{n_{\bar{1},2}} T^{m}_{n_1,-\Lambda_1;n_2,\Lambda_2}\mathcal{N}_{m,2} \\ & -\delta_{1\le n_r\le n_{\bar{1},2}+1}n_r T^{n_r-1}_{n_1,-\Lambda_1;n_2,\Lambda_2}\mathcal{N}_{n_r-1,2}\Bigg]\end{aligned}}$$

Next, for $\alpha = 1$ and $\mu = 0$ we find

$$\boxed{I_{1,0}^{(0,0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = -\delta_{\Lambda_1,\Lambda_2}\sum_{m=0}^{n_{\bar{1},2}} T^{m}_{n_1,-\Lambda_1;n_2,\Lambda_2}\frac{(2m-3)!!}{2^{m+1}m!}}$$

and for $\alpha = 1$ and $\mu = \pm 1$

$$\boxed{\begin{aligned} I_{1,\pm 1}^{(n_r,\Lambda=0)}\left(n_1,\Lambda_1;n_2,\Lambda_2\right) = {} & \frac{b_\perp}{\sqrt{2\pi}}\delta_{-\Lambda_1+\Lambda_2+\mu,0} \\ & \times\Big[\left(n_r+1\right)T^{n_r}_{n_1,-\Lambda_1;n_2,\Lambda_2}\mathcal{N}_{n_r,1}\delta_{0\le n_r\le n_{\bar{1},2}} \\ & -n_r T^{n_r-1}_{n_1,-\Lambda_1;n_2,\Lambda_2}\mathcal{N}_{n_r-1,1}\delta_{1\le n_r\le n_{\bar{1},2}+1}\Big]\end{aligned}}$$

For the $I^{(n_z)}$ integral in Eq. (2.44), we have

$$\boxed{I^{(n_z)}(n_1;n_2) = \frac{1}{\left(\pi b_z^2\right)^{1/4}} T^{n_z}_{n_1,n_2} \delta_{|n_1-n_2|\leq n_z\leq n_1+n_2}}$$

#### 2.4.4.5 Modification for large oscillator number in $z$ direction

In the case where the $n_z$ quantum numbers are large, we need to re-write the integral $R_{ik}^{(n_z)}$ which appears in Eq. (2.42) in a form that is more stable numerically. Writing this integral explicitly, we have

$$R^n_{n_1,n_2} \equiv \int_{-\infty}^{\infty} dz\, \phi^*_{n_1}(z;b) \left[e^{-\frac{z^2}{2b^2}} \phi^*_n(z;b)\right] \phi_{n_2}(z;b)$$

In appendix D of [17] the integral

$$\langle n_1 |f_n| n_2\rangle = K_z^{1/2} \lambda_n \int_{-\infty}^{\infty} dz\, \Phi_{n_1}(z;b)\, e^{-z^2/\left(2Gb^2\right)} \Phi_n\left(z; G^{1/2} b\right) \Phi_{n_2}(z;b)$$

where

$$\begin{aligned} K_z &\equiv \frac{\pi\mu^2}{G^{1/2}} \\ \lambda_n &\equiv G^{-n/2} \\ G &\equiv 1 + \frac{\mu^2}{b^2} \end{aligned}$$

is evaluated to

$$\begin{aligned} \langle n_1 |f_n| n_2\rangle = &\frac{\mu b^{-1/2}}{\sqrt{2\pi^{5/2}}} \frac{\Gamma(\xi - n_1)\,\Gamma(\xi - n_2)\,\Gamma(\xi - n)}{z^{\xi}\sqrt{n! n_1! n_2!}} \\ &\times {}_2F_1(-n_1, -n_2; -\xi + n + 1; 1 - z) \end{aligned}$$

Taking the limit as $\mu \to 0$, we can then deduce

$$\begin{aligned} R^n_{n_1,n_2} &= \lim_{\mu\to 0} \frac{\langle n_1 |f_n| n_2\rangle}{K^{1/2}\lambda_n} \\ &= \frac{b^{-1/2}}{\sqrt{2\pi^{7/2}}} \frac{\Gamma(\xi - n_1)\,\Gamma(\xi - n_2)\,\Gamma(\xi - n)}{\sqrt{n! n_1! n_2!}} \end{aligned}$$

which can also be written as

$$\boxed{R^n_{n_1,n_2} = \frac{1}{\sqrt{2\pi^{1/2} b}} \frac{(-n_1 + n_2 + n - 1)!!\,(n_1 - n_2 + n - 1)!!\,(n_1 + n_2 - n - 1)!!}{2^{(n_1+n_2+n)/2}\sqrt{n! n_1! n_2!}}}$$

### 2.4.5 Two-body center-of-mass correction

The kinetic energy of the center of mass is written

$$K = \frac{\mathbf{P}^2}{2mA}$$

where $m$ is the nucleon mass, and $A$ is the number of nucleons. This energy must be subtracted from the Hartree-Fock Hamiltonian. The total momentum $P$ can be decomposed into the individual nucleon momenta,

$$\begin{aligned} K &= \frac{1}{2mA}\left(\sum_{i=1}^{A} \mathbf{p}_i\right)^2 \\ &= \frac{1}{2mA}\left(\sum_i \mathbf{p}_i^2 + 2\sum_{i>j} \mathbf{p}_i \cdot \mathbf{p}_j\right) \end{aligned}$$

where the individual momentum operator can be written in coordinate space

$$\mathbf{p} = \frac{\hbar}{i}\boldsymbol{\nabla}$$

The operator $\mathbf{P}^2$ can therefore be written in second-quantized form as

$$\begin{aligned} \mathbf{P}^2 &= \sum_{ij} \left\langle i \left| \mathbf{p}^2 \right| j \right\rangle a_i^\dagger a_j + \frac{1}{2}\sum_{ijkl} \left\langle ij \left| 2\mathbf{p}_1 \cdot \mathbf{p}_2 \right| kl \right\rangle a_i^\dagger a_j^\dagger a_l a_k \\ &= \sum_{ij} \left\langle i \left| \mathbf{p}^2 \right| j \right\rangle a_i^\dagger a_j + \sum_{ijkl} \left\langle ij \left| \mathbf{p}_1 \cdot \mathbf{p}_2 \right| kl \right\rangle a_i^\dagger a_j^\dagger a_l a_k \end{aligned}$$

The expectation value of this operator in the Hartree-Fock ground state is

$$\left\langle \Phi \left| \mathbf{P}^2 \right| \Phi \right\rangle = \sum_{ij} \left\langle i \left| \mathbf{p}^2 \right| j \right\rangle \rho_{ji} + \sum_{ijkl} \left\langle ij \left| \mathbf{p}_1 \cdot \mathbf{p}_2 \right| \widetilde{kl} \right\rangle \rho_{ki}\rho_{lj}$$

where $\left|\widetilde{kl}\right\rangle = |kl\rangle - |lk\rangle$ enforces antisymmetrization. Therefore, we can separate the kinetic energy into one- and two-body contributions

$$K = K_1 + K_2$$

where

$$K_1 = \frac{-\hbar^2}{2mA}\sum_{ij} \left\langle i \left| \boldsymbol{\nabla}^2 \right| j \right\rangle \rho_{ji}$$

and

$$K_2 = \frac{-\hbar^2}{2mA} \sum_{ijkl} \left\langle ij \left| \boldsymbol{\nabla}_1 \cdot \boldsymbol{\nabla}_2 \right| \widetilde{kl} \right\rangle \rho_{ki} \rho_{lj}$$

The one-body contribution, $K_1$, simply introduces a well-known $(1 - 1/A)$ multiplication factor to the matrix elements of the kinetic-energy operator derived in section 2.4.1. For the remainder of this section, we focus on the two-body contribution, $K_2$. The field that corresponds to this energy is

$$\begin{aligned}
\Gamma_{ik}^{(K)} &= \frac{\partial}{\partial \rho_{ki}} K_2 \\
&= \frac{-\hbar^2}{mA} \sum_{jl} \left( \left\langle i \left| \boldsymbol{\nabla} \right| k \right\rangle \cdot \left\langle j \left| \boldsymbol{\nabla} \right| l \right\rangle - \left\langle i \left| \boldsymbol{\nabla} \right| l \right\rangle \cdot \left\langle j \left| \boldsymbol{\nabla} \right| k \right\rangle \right) \rho_{lj}
\end{aligned}$$

It will be useful to express the derivatives in terms of ladder operators,

$$\begin{aligned}
\partial_+ &\equiv \partial_x + i\partial_y \\
\partial_- &\equiv \partial_x - i\partial_y
\end{aligned}$$

so that

$$\boldsymbol{\nabla}_1 \cdot \boldsymbol{\nabla}_2 = \frac{1}{2} \left( \partial_+^{(1)} \partial_-^{(2)} + \partial_-^{(1)} \partial_+^{(2)} \right) + \partial_{z_1} \partial_{z_2}$$

From this point, we can calculate the direct and exchange contributions explicitly.

#### 2.4.5.1 The Direct contribution

we calculate the direct contribution to the field defined by

$$\begin{aligned}
\Gamma_{ik}^{(q,K,D)} &= \frac{-\hbar^2}{mA} \sum_{jl} \sum_{q'} \left\langle ij \left| \boldsymbol{\nabla}_1 \cdot \boldsymbol{\nabla}_2 \right| kl \right\rangle \rho_{lj}^{(q')} \\
&= \frac{-\hbar^2}{mA} \sum_{q'} \left( \frac{1}{2} \left\langle i \left| \partial_+ \right| k \right\rangle \sum_{jl} \left\langle j \left| \partial_- \right| l \right\rangle \rho_{lj}^{(q')} \right. \\
&\quad + \frac{1}{2} \left\langle i \left| \partial_- \right| k \right\rangle \sum_{jl} \left\langle j \left| \partial_+ \right| l \right\rangle \rho_{lj}^{(q')} \\
&\quad \left. + \left\langle i \left| \partial_z \right| k \right\rangle \sum_{jl} \left\langle j \left| \partial_z \right| l \right\rangle \rho_{lj}^{(q')} \right)
\end{aligned}$$

Since $\Omega_i = \Omega_k$ and $\Omega_j = \Omega_l$, the conditions $\sigma_i = \sigma_k$ and $\sigma_j = \sigma_l$ imposed by the matrix elements imply that $\Lambda_i = \Lambda_k$ and $\Lambda_j = \Lambda_l$, respectively. Then by using the recurrence relations for derivatives of harmonic-oscillator functions it is easy to show that

$$\langle i \,|\partial_\pm|\, k\rangle = \langle j \,|\partial_\pm|\, l\rangle = 0$$

Thus we are left with

$$\begin{aligned}\Gamma_{ik}^{(q,K,D)} &= \frac{-\hbar^2}{mA}\langle i \,|\partial_z|\, k\rangle \sum_{q'}\sum_{jl}\langle j \,|\partial_z|\, l\rangle \rho_{lj}^{(q')} \\ &= \frac{-\hbar^2}{mA}\delta_{\sigma_i,\sigma_k} I_{ik}^{(z)} \sum_{jl}\delta_{\sigma_j,\sigma_l} I_{jl}^{(z)} \rho_{lj}\end{aligned}$$

where we have defined

$$I_{ij}^{(z)} \equiv \int d^3r\, \Phi_i^*(\mathbf{r}) \frac{\partial}{\partial z}\Phi_j(\mathbf{r}) \tag{2.46}$$

We can explicitly take into account time-reversed states and order the indices to get

$$\Gamma_{ik}^{(q,K,D)} = \frac{-\hbar^2}{mA}\delta_{\sigma_i,\sigma_k} I_{ik}^{(z)}\left[\sum_{j>l>0} 2\delta_{\sigma_j,\sigma_l}\left(I_{jl}^{(z)} + I_{lj}^{(z)}\right)\rho_{lj} + \sum_{j>0} 2I_{jj}^{(z)}\rho_{jj}\right]$$

Now, using recurrence relations, we can show that

$$I_{jj}^{(z)} = 0$$

and integrating by parts, we can show that

$$I_{lj}^{(z)} = -I_{jl}^{(z)}$$

and therefore the direct contribution vanishes,

$$\Gamma_{ik}^{(q,K,D)} = 0$$

### 2.4.5.2 The Exchange contribution

We calculate

$$\begin{aligned}\Gamma_{ik}^{(q,K,E)} &= \frac{\hbar^2}{mA}\sum_{q'}\sum_{jl}\langle i \,|\boldsymbol{\nabla}|\, l\rangle \cdot \langle j \,|\boldsymbol{\nabla}|\, k\rangle \rho_{lj}^{(q')} \\ &= \frac{\hbar^2}{mA}\sum_{jl}\delta_{\sigma_i,\sigma_l}\delta_{\sigma_j,\sigma_k}\left[\frac{1}{2}\left(I_{il}^{(+)}I_{jk}^{(-)} + I_{il}^{(-)}I_{jk}^{(+)}\right) + I_{il}^{(z)}I_{jk}^{(z)}\right]\rho_{lj}^{(q)}\end{aligned}$$

where we have defined

$$I_{ij}^{(\pm)} \equiv \int d^3r\, \Phi_i^*(\mathbf{r})\, \partial_\pm \Phi_j(\mathbf{r}) \tag{2.47}$$

For convenience, we define

$$I_{il;jk} \equiv \frac{1}{2}\left(I_{il}^{(+)} I_{jk}^{(-)} + I_{il}^{(-)} I_{jk}^{(+)}\right) + I_{il}^{(z)} I_{jk}^{(z)} \tag{2.48}$$

so that

$$\Gamma_{ik}^{(q,K,E)} = \frac{\hbar^2}{mA}\sum_{jl} \delta_{\sigma_i,\sigma_l}\delta_{\sigma_j,\sigma_k} I_{il;jk}\rho_{lj}^{(q)}$$

Taking explicitly into account time-reversed states and ordering of indices, we can write this as

$$\begin{aligned}\Gamma_{ik}^{(q,K,E)} = \frac{\hbar^2}{mA}\sum_{j\geq l>0}\frac{\rho_{lj}^{(q)}}{1+\delta_{jl}}\Big\{&\delta_{\sigma_i,\sigma_l}\delta_{\sigma_j,\sigma_k} I_{il;jk} + 4\sigma_j\sigma_l\delta_{\sigma_i,-\sigma_l}\delta_{-\sigma_j,\sigma_k} I_{i\underline{l};\underline{j}k}\\ &+\delta_{\sigma_i,\sigma_j}\delta_{\sigma_l,\sigma_k} I_{ij;lk} + 4\sigma_j\sigma_l\delta_{\sigma_i,-\sigma_j}\delta_{-\sigma_l,\sigma_k} I_{i\underline{j};\underline{l}k}\Big\}\end{aligned}$$

and with the help of the identity

$$\delta_{\sigma_i,\sigma_l}\delta_{\sigma_j,\sigma_k} = \delta_{\sigma_i,\sigma_k}\delta_{\sigma_j,\sigma_l}\delta_{\sigma_i,\sigma_j} + \delta_{\sigma_i,-\sigma_k}\delta_{\sigma_j,-\sigma_l}\delta_{\sigma_i,-\sigma_j}$$

we get

$$\begin{aligned}\Gamma_{ik}^{(q,K,E)} = \frac{\hbar^2}{mA}\sum_{j\geq l>0}\frac{\rho_{lj}^{(q)}}{1+\delta_{jl}}&\Big\{\delta_{\sigma_i,\sigma_k}\delta_{\sigma_j,\sigma_l}\Big[\delta_{\sigma_i,\sigma_j}\left(I_{il;jk} + I_{ij;lk}\right)\\ &+\delta_{\sigma_i,-\sigma_j}\left(I_{i\underline{l};\underline{j}k} + I_{i\underline{j};\underline{l}k}\right)\Big]\\ &+\delta_{\sigma_i,-\sigma_k}\delta_{\sigma_j,-\sigma_l}\Big[\delta_{\sigma_i,\sigma_j}\left(I_{ij;lk} - I_{i\underline{l};\underline{j}k}\right)\\ &+\delta_{\sigma_i,-\sigma_j}\left(I_{il;jk} - I_{i\underline{j};\underline{l}k}\right)\Big]\Big\}\end{aligned}$$

This is the field that must be subtracted from the Hartree-Fock field to correct for the two-body contributions of the center-of-mass motion. Next, we will give the explicit form of the integrals $I_{il;jk}$ defined in Eq. (2.48).

First we note that in cylindrical coordinates,

$$\partial_\pm = e^{\pm \mathrm{i}\varphi}\left(\frac{\partial}{\partial\rho} \pm \mathrm{i}\frac{1}{\rho}\frac{\partial}{\partial\varphi}\right)$$

Using recurrence relations for the derivatives of harmonic-oscillator functions, we can then show that the integral in Eq. (2.47) can be written as

$$\begin{aligned}I_{ij}^{(\pm)} = \sqrt{\pi}\delta_{n_z^{(i)},n_z^{(j)}} \Big\{ & \left(1 \mp s_{\Lambda_j}\right)\left(1-\delta_{\Lambda_j,0}\right)\sqrt{n_r^{(j)}+|\Lambda_j|} \\ & \times I_{0,s_{\Lambda_j}\pm 1}^{(0,0)}\left(n_r^{(i)},\Lambda_i;n_r^{(j)},\Lambda_j-s_{\Lambda_j}\right) \\ & -\left[\left(1\pm s_{\Lambda_j}\right)+\left(1\mp s_{\Lambda_j}\right)\delta_{\Lambda_j,0}\right]\sqrt{n_r^{(j)}} \\ & \times I_{0,-s_{\Lambda_j}\pm 1}^{(0,0)}\left(n_r^{(i)},\Lambda_i;n_r^{(j)}-1,\Lambda_j+s_{\Lambda_j}\right) \\ & -\frac{1}{b_\perp} I_{1,\pm 1}^{(0,0)}\left(n_r^{(i)},\Lambda_i;n_r^{(j)},\Lambda_j\right)\Big\}\end{aligned}$$

where $s_\Lambda$ was defined in Eq. (2.45), and the remaining integrals $I_{\alpha,\mu}^{(n_r,\Lambda)}$ were calculated in section 2.4.4. Next, for the integrals $I_{\alpha\beta}^{(z)}$ defined in Eq. (2.46), we can similarly show that

$$I_{\alpha\beta}^{(z)} = \frac{1}{b_z}\delta_{n_r^{(\alpha)},n_r^{(\beta)}}\delta_{\Lambda_\alpha,\Lambda_\beta}\left[\sqrt{\frac{n_z^{(\beta)}}{2}}\delta_{n_z^{(\alpha)},n_z^{(\beta)}-1} - \sqrt{\frac{n_z^{(\beta)}+1}{2}}\delta_{n_z^{(\alpha)},n_z^{(\beta)}+1}\right]$$

### *2.4.6 The density-dependent contribution*

We start with the potential function

$$V\left(\mathbf{r}_1,\mathbf{r}_2\right) \equiv t_0\left(1+x_0P_\sigma\right)\rho^\lambda\left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right)\delta^3\left(\mathbf{r}_1-\mathbf{r}_2\right) \tag{2.49}$$

where $\rho(\mathbf{r})$ is the spatial one-body nucleon density given by the sum of neutron and proton densities,

$$\rho(\mathbf{r}) = \rho_n(\mathbf{r}) + \rho_p(\mathbf{r})$$

with

$$\rho_q(\mathbf{r}) = \sum_{i'\gamma'}\delta_{\sigma_{i'},\sigma_{\gamma'}}\Phi_{i'}^*(\mathbf{r})\,\Phi_{\gamma'}(\mathbf{r})\,\rho_{\gamma' i'}^q$$

The total energy corresponding to the density-dependent potential is

$$E_{DD} \equiv \frac{1}{4}\sum_{qq',ijkl}\left[\left\langle ij\,|V|\,\widetilde{kl}\right\rangle\rho_{lj}^{q'}\rho_{ki}^{q} + \left\langle ij\,|V|\,\widetilde{kl}\right\rangle^*\left(\rho_{lj}^{q'}\right)^*\left(\rho_{ki}^{q}\right)^*\right] \tag{2.50}$$

After some simplifications, this can be written in the form

$$
\begin{aligned}
E_{DD} = & \frac{1}{4} t_0 \left(1 - x_0\right) \int d^3 r\, \rho^{\lambda+2}\left(\mathbf{r}\right) \\
& + t_0 \left(\frac{1}{2} + x_0\right) \int d^3 r\, \rho^{\lambda}\left(\mathbf{r}\right) \rho_n\left(\mathbf{r}\right) \rho_p\left(\mathbf{r}\right)
\end{aligned}
$$

from which we deduce the corresponding Hartree-Fock field [4], which includes the so-called "re-arrangement" terms [24]

$$
\begin{aligned}
\varGamma_{ik}^{q} &= \frac{\partial E_{DD}}{\partial \rho_{ki}^{q}} \\
&= t_0 \delta_{\sigma_i,\sigma_k} \int d^3 r\, \varPhi_i^*\left(\mathbf{r}\right) \varPhi_k\left(\mathbf{r}\right) \left\{ \left[1 + \frac{x_0}{2} + \frac{1}{4}\lambda\left(1 - x_0\right)\right] \rho^{\lambda+1}\left(\mathbf{r}\right) \right. \\
&\quad \left. - \left(\frac{1}{2} + x_0\right) \rho^{\lambda}\left(\mathbf{r}\right) \rho_q\left(\mathbf{r}\right) + \left(\frac{1}{2} + x_0\right) \lambda \rho^{\lambda-1}\left(\mathbf{r}\right) \rho_n\left(\mathbf{r}\right) \rho_p\left(\mathbf{r}\right) \right\}
\end{aligned}
$$

If we define the integral

$$
D_{\alpha\gamma}^{\left(qq'\right)} \equiv \int d^3 r\, \varPhi_\alpha^*\left(\mathbf{r}\right) \varPhi_\gamma\left(\mathbf{r}\right) \rho^{\lambda-1}\left(\mathbf{r}\right) \rho_q\left(\mathbf{r}\right) \rho_{q'}\left(\mathbf{r}\right) \tag{2.51}
$$

we can then write

$$
\begin{aligned}
\varGamma_{ik}^{q} = & t_0 \delta_{\sigma_i,\sigma_k} \left\{ \left[1 + \frac{x_0}{2} + \frac{1}{4}\lambda\left(1 - x_0\right)\right] D_{ik}^{(tt)} - \left(\frac{1}{2} + x_0\right) D_{ik}^{(tq)} \right. \\
& \left. + \left(\frac{1}{2} + x_0\right) \lambda D_{ik}^{(np)} \right\}
\end{aligned}
$$

where the superscript $t$ refers to the total density: $\rho_t\left(\mathbf{r}\right) = \rho_n\left(\mathbf{r}\right) + \rho_p\left(\mathbf{r}\right)$. For a non-integer exponent $\lambda$, the integrals in Eq. (2.51) cannot in general be performed analytically and must instead be evaluated numerically, e.g. by a quadrature method.

The contribution to the total energy of the system from the density-dependent part of the interaction is given in Eq. (2.50) and be written in terms of a Hartree-Fock field with no re-arrangement terms,

$$
E_{DD} = \frac{1}{4} \sum_{q,ik} \left[\varGamma_{ik}^{q,\mathrm{nr}} \rho_{ki}^{q} + \left(\varGamma_{ik}^{q,\mathrm{nr}}\right)^* \left(\rho_{ki}^{q}\right)^*\right]
$$

where

$$
\varGamma_{ik}^{q,\mathrm{nr}} \equiv \sum_{q',jl} \left\langle ij \left|V\right| \widetilde{kl} \right\rangle \rho_{lj}^{q'}
$$

Starting from Eq. (2.49), and using the integrals in Eq. (2.51) we can show that this is

$$\Gamma_{ik}^{q,\mathrm{nr}} = t_0 \delta_{\sigma_i,\sigma_k} \left[ \left(1 + \frac{x_0}{2}\right) D_{ik}^{(tt)} - \left(\frac{1}{2} + x_0\right) D_{ik}^{(tq)} \right]$$

Finally, we reiterate the discussion at the end of [20] concerning the contribution of the density-dependent potential in Eq. (2.49) to the pairing field. This contribution is given by

$$\Delta_{ij}^{q} = \frac{1}{2} \sum_{q',kl} \left\langle ij \left| V \right| \widetilde{kl} \right\rangle \kappa_{lk}^{q'}$$

which we can write in terms of spin-exchange ($P_\sigma$), isospin-exchange ($P_\tau$), and spatial-exchange ($P_r$) operators,

$$\Delta_{ij}^{q} = \frac{1}{2} \sum_{q',kl} \left\langle ij \left| V \left(1 - P_\sigma P_\tau P_r\right) \right| kl \right\rangle \kappa_{lk}^{q'}$$

Note however that because $V$ contains $\delta^3(\mathbf{r}_1 - \mathbf{r}_2)$, the operator $P_r$ has no effect. Furthermore, the states $k$ and $l$ are forced to correspond to the same particle type by the pairing tensor $\kappa_{lk}^{q'}$, therefore the operator $P_\tau$ also has no effect. Thus we are left with

$$\Delta_{ij}^{q} = \frac{1}{2} \sum_{q',kl} \left\langle ij \left| V \left(1 - P_\sigma\right) \right| kl \right\rangle \kappa_{lk}^{q'} \tag{2.52}$$

If we assign $x_0 = 1$ in Eq. (2.49), then the density-dependent matrix element in Eq. (2.52) is proportional to the term

$$\left(1 + P_\sigma\right)\left(1 + P_\sigma\right) = 1 - P_\sigma P_\sigma = 0$$

In other words, by choosing $x_0 = 1$, we eliminate the contribution of the density-dependent potential in Eq. (2.49) to the pairing field.

### *2.4.7 The Slater approximation to the Coulomb exchange term*

The matrix elements derived in section 2.4.3 can be used to calculate both the direct and exchange Coulomb terms, however these calculations can be computationally demanding, especially for the exchange term. As an alternate approach, an approximation due to Slater [25] can be used for the exchange energy,

$$E_{C,\mathrm{Slater}}^{(E)} = -\frac{3}{4} e^2 \left(\frac{3}{\pi}\right)^{1/3} \int d^3 r \rho_p^{4/3}(\mathbf{r})$$

and the corresponding contribution to the Hartree-Fock field is

$$\begin{aligned}
\Gamma_{ik}^{(C,E)} &= \frac{\partial}{\partial \rho_{ki}} E_{C,\text{Slater}}^{(E)} \\
&= -e^2 \left(\frac{3}{\pi}\right)^{1/3} \delta_{\sigma_i,\sigma_k} \delta_{q_i,q_k} \delta_{q_i,p} \int d^3 r \Phi_i^* \left(\mathbf{r}\right) \Phi_k \left(\mathbf{r}\right) \rho_p^{1/3} \left(\mathbf{r}\right)
\end{aligned}$$

As in the case of the integrals in Eq. (2.51), these remaining integrals must be carried out numerically. The Slater approximation can be used for all HFB iterations to accelerate the calculations. The last HFB iteration could be performed using the exact form of the Coulomb field if additional accuracy is required at a minimal additional computational cost.

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Chapter 3
# The Generator Coordinate Method

This chapter describes in detail the formalism of the Generator Coordinate Method and its use in constructing both static and dynamic collective states of the nucleus, starting from constrained Hartree-Fock-Bogoliubov solutions. The full formalism is then reduced to a Schrödinger-like equation, and the calculation of its inertial tensor and zero-point energies is presented. Next, the calculations are extended beyond the adiabatic approximation and the Schrödinger Collective Intrinsic Model is derived. The multi-$O(4)$ schematic model introduced in chapter 2 is used throughout this chapter to illustrate the formalism.

The Generator Coordinate Method (GCM) is a quantum many-body technique whose purpose is to incorporate correlations of collective character in many-body wave functions. It was first introduced by Hill and Wheeler in the context of nuclear fission in 1953 [1]. The method has subsequently been extended as a general tool by Griffin and Wheeler [2]. Its principle is to express the wave function of a many-body system as a superposition of mean-field states depending on a set of continuous parameters called "generator coordinates" and to determine the expansion coefficients by means of a variational principle. One then obtain an integral equation for the unknown coefficients called the Hill-Wheeler (HW) equation.This approach can be seen as a continuous version of the configuration interaction method commonly employed in atomic physics and quantum chemistry. It has been extensively applied in the last fifty years to a variety of problems in atomic, molecular and nuclear physics.

In the microscopic approach of fission presented in this book, two versions of the GCM method are employed: a static one which is used for constructing initial states having an average deformation localized within the ground state well – the first well – of the fission barrier (see Section 5.0.4), and a time-dependent version whose purpose is to describe the time-dependent evolution of the initial state toward scission. Fission fragment observables are then deduced from the flux of the evolving wave function through scission (see Section 4.3.3). In both cases, the wave function of the fissioning system is expressed as a superposition of HFB states obtained from the constrained HFB calculations described in Section 2.5, the constraints being chosen so as to include the different kinds of nuclear deformations encountered by the nucleus on its way to scission. Therefore the generator coordinates are taken as different sorts of nuclear deformation parameters.

For the sake of completeness we recall in the first section of this chapter the derivation of the HW equation and how the kernels of this integral equation – the GCM kernels – can be calculated. We also present a simple method of solving the HW equation, first in the standard approach and then, when particle-number projection is included in the formalism. The second and third sections describe methods of reducing the HW integral equation to a Schrödinger-like differential equation. Such a reduction considerably decreases the size of practical calculations, especially when several generator coordinates have to be used. In addition, as remarked in [3], this reduction allows one to nicely connect the GCM description to usual theories of the fission process. In section 3.2 the reduction is made under the assumption that the HFB states included in the GCM configuration mixing are invariant under time-reversal symmetry. A much more general method, the Schrödinger Collective Intrinsic Model (SCIM) which does not rely on this assumption is next developed in Section 3.3. Whereas the simple approach of section 3.2 can describe only adiabatic collective evolution in even-even fissioning nuclei, the SCIM is able to incorporate non-adiabatic effects such as the coupling of the collective motion to intrinsic quasi-particle excitations and also to describe the fission of odd and odd-odd nuclei.

## 3.1 The Hill-Wheeler equation

### *3.1.1 General formalism*

The Generator Coordinate (GC) Method consists of choosing for a many-body system a trial state of the form [2]

$$|\Psi\rangle = \int d^n q\, f(q)|\Phi_q\rangle \tag{3.1}$$

where $q = (q_1, q_2, \ldots, q_n)$ is a set of $n$ real generator coordinates extending *a priori* from $-\infty$ to $+\infty$. In the case of fission, the $q_i$ may be thought as parameters measuring different kinds of nuclear deformations e.g., multipole deformations of the whole nucleus or, close to scission, parameters describing pre-fragments configurations (see Section 4.1). The $|\Phi_q\rangle$ are obtained from constrained HFB calculations including – in addition to the usual two particle-number constraints – constraints over $n$ operators $Q_i$ chosen in order to impose the required values of the deformation parameters:

$$\langle\Phi_q|Q_i|\Phi_q\rangle = q_i, \qquad i = 1, \ldots, n \tag{3.2}$$

Let us note that two states $|\Phi_q\rangle$ and $|\Phi_{q'}\rangle$ with $q \neq q'$ are usually not orthogonal. The $f(q)$ are unknown functions – in general complex – playing the role of coefficients in the configuration mixing expansion. In the spirit of microscopic approaches they are determined from a variational principle involving the many-body Hamiltonian $H$. In the standard GCM approach the many-body state (3.1) is considered as a stationary trial state and the variational principle is applied to the energy, i.e. to the expectation value of $H$ (the case of a time-dependent state $|\Psi(t)\rangle$ is treated below)

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{3.3}$$

Since $E$ is real, it suffices to consider variations with respect to $f^*(q)$, the variations with respect to $f(q)$ yielding the complex conjugate equation. One has

$$\begin{aligned}\delta E =& \left[\frac{1}{\langle\Psi|\Psi\rangle}\frac{\delta\langle\Psi|H|\Psi\rangle}{\delta f^*(q)} - \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle^2}\frac{\delta\langle\Psi|\Psi\rangle}{\delta f^*(q)}\right]\delta f^*(q) \\ =& \frac{1}{\langle\Psi|\Psi\rangle}\int d^n q\,\delta f^*(q)\int d^n q'\,\left[\langle\Phi_q|H|\Phi_{q'}\rangle - E\langle\Phi_q|\Phi_{q'}\rangle\right] f(q')\end{aligned} \tag{3.4}$$

The condition $\delta E = 0$ for any variation $\delta f^*(q)$ then yields

$$\int d^n q'\,\left[\langle\Phi_q|H|\Phi_{q'}\rangle - E\langle\Phi_q|\Phi_{q'}\rangle\right] f(q') = 0, \qquad \forall q \tag{3.5}$$

which is the Hill-Wheeler equation. This equation represents a set of $n$ integral equations with two kinds of kernels, the norm or overlap kernel

$$N(q,q') = \langle\Phi_q|\Phi_{q'}\rangle \tag{3.6}$$

and the Hamiltonian kernel

$$H(q,q') = \langle\Phi_q|H|\Phi_{q'}\rangle \tag{3.7}$$

In subsequent developments it will be convenient to also introduce the energy kernel

$$h(q,q') = \frac{H(q,q')}{N(q,q')} \equiv \frac{\langle\Phi_q|H|\Phi_{q'}\rangle}{\langle\Phi_q|\Phi_{q'}\rangle} \tag{3.8}$$

The three kernels above may be collectively denoted as the GCM kernels. Closed formulas have been derived to express these kernels [4] and fully analytical expressions can be obtained in simple cases (see next Subsection). Once the GCM kernels are known, the HW equation (3.5) can be solved. The usual method of solving this integral equation consists of discretizing the continuous generator coordinates $q_i$ on a mesh. In this way the HW integral equation takes the form of a generalized eigenvalue equation. Such an approach is briefly presented in Section 3.1.3.

The above formalism can be readily extended to the case of a time-dependent GC state

$$|\Psi(t)\rangle = \int d^n q\, f(q,t)|\Phi_q\rangle \tag{3.9}$$

Here the mixing coefficients $f$ depend on time in addition to the generator coordinates $q = (q_1, q_2, \ldots, q_n)$. The time-dependent version of the stationary HW equation (3.5) can then be obtained by applying a variational principle to the action integral between two times $t_1$ and $t_2$ built with $|\Psi(t)\rangle$

$$\mathcal{A}(t_1,t_2) = \int_{t_1}^{t_2} \frac{\langle\Psi(t)|}{\langle\Psi(t)|\Psi(t)\rangle^{1/2}}\left(H - i\hbar\frac{\partial}{\partial t}\right)\frac{|\Psi(t)\rangle}{\langle\Psi(t)|\Psi(t)\rangle^{1/2}} \tag{3.10}$$

the values $f(q,t_1)$ and $f(q,t_2)$ being held fixed. As before the variations may be expressed with respect to only $f^*(q,t)$, and one easily gets, assuming that $|\Psi(t)\rangle$ is normalized to unity

$$\langle \Phi_q| \left( H - i\hbar \frac{\partial}{\partial t} \right) |\Psi(t)\rangle = 0, \qquad \forall q \tag{3.11}$$

that is

$$\int d^n q' \left[ \langle \Phi_q|H|\Phi_{q'}\rangle f(q',t) - \langle \Phi_q|\Phi_{q'}\rangle i\hbar \frac{\partial f(q',t)}{\partial t} \right] = 0, \qquad \forall q \tag{3.12}$$

This equation obviously possesses the same structure as the stationary Hill-Wheeler equation (3.5), the energy $E$ being simply replaced with the operator $i\hbar\partial/\partial t$. However, in order to be solved, Eq. (3.12) needs an initial condition $f(q, t = t_0)$. The latter can be obtained from the initial state $|\Psi(t = t_0)\rangle$ chosen as a starting point for the fission process by inverting the relation

$$|\Psi(t = t_0)\rangle = \int d^n q\, f(q, t = t_0)|\Phi_q\rangle \tag{3.13}$$

By making the scalar product of this equation on the left with $\langle \Phi_{q'}|$ and discretizing the $q_i$ on a mesh, the $f(q, t = t_0)$ can then be obtained by standard matrix inversion.

It is interesting to note that the stationary HW equation (3.5) can be cast into the form of an continuous eigenvalue equation. In fact, the norm kernel $N(q,q')$ is hermitian and positive. Then, according to Fredholm's theorems [5, 6], the kernel $N$ can be diagonalized by means of a continuous unitary matrix $U$ and its eigenvalues are real and positive which can be written[1]

$$\int d^n q'\, N(q,q')\, U(q',\xi) = U(q,\xi) D^2(\xi), \qquad D^2(\xi) \;\; \text{real} \tag{3.14}$$

$$\text{with} \quad \begin{cases} \displaystyle\int d^n q\, U^*(q,\xi) U(q,\xi') = \delta(\xi - \xi') \\ \displaystyle\int d\xi\, U(q,\xi) U^*(q',\xi) = \delta^n(q - q') \equiv \prod_{i=1}^{n} \delta(q_i - q_i') \end{cases} \tag{3.15}$$

From these relations, one obtains

[1] If the GC integration domain is bounded or, more generally, if the kernel $N(q,q')$ is a Hilbert-Schmidt operator (i.e. $\left|\iint d^n q d^n q' N(q,q')\right| < \infty$) the eigenvalues and eigenfunctions of $N$ constitute denumerable sets. We assume here that this is not necessarily the case. Therefore, provided the kernel $N(q,q')$ obeys appropriate convergence conditions when the $q_i$ and $q_i'$ go to infinity, its eigenvalues and eigenfunctions are to be labelled by means of a continuous parameter $\xi$.

$$N(q,q') = \int d\xi\, U(q,\xi)\, D^2(\xi)\, U^*(q',\xi) = \int d\xi\, N^{1/2}(q,\xi)\, N^{1/2^*}(q',\xi) \tag{3.16}$$

$$\text{with } \; N^{1/2}(q,\xi) = U(q,\xi)\, D(\xi), \quad D(\xi) = \sqrt{D^2(\xi)}.$$

According to Fredholm's theorem, zero is an accumulation point for the spectrum of $N$. We eliminate from the "matrix" $U$ the eigenvector "columns" corresponding to eigenvalues $D^2(\xi) < \varepsilon^2$ where $\varepsilon$ is an arbitrary small number. By doing this, one can define the inverse $N^{-1/2}$ of $N^{1/2}$,

$$N^{-1/2}(\xi,q) = D^{-1}(\xi)\, U^*(q,\xi), \qquad |D(\xi)| \geq \varepsilon \tag{3.17}$$

and a kernel $\overline{H}(\xi,\xi')$ such that

$$H(q,q') = \int' d\xi \int' d\xi'\, N^{1/2}(q,\xi)\, \overline{H}(\xi,\xi')\, N^{1/2^*}(q',\xi') \tag{3.18}$$

Here the symbol $\int'$ means integration in the range of values of $\xi$ such that $|D(\xi)| \geq \varepsilon$. Expressions (3.16) and (3.18) then show that the HW equation (3.5) can be cast into the simpler form

$$\int' \overline{H}(\xi,\xi')\, \overline{f}(\xi')\, d\xi' = E\, \overline{f}(\xi), \qquad \forall \xi \tag{3.19}$$

with

$$\overline{f}(\xi) = \int d^n q\, f(q)\, N^{1/2^*}(q,\xi) \tag{3.20}$$

The integral equation (3.19) is rigorously equivalent to the HW equation (3.5). We may call it the reduced HW equation.

Let us notice that the function $\overline{f}(\xi)$ is normalized to unity. In fact from Eqs. (3.16), (3.6) and (3.1) and assuming that the GCM state $|\Psi\rangle$ is normalized to unity, one obtains

$$\int' d\xi\, \left|\overline{f}(\xi)\right|^2 = \int d^n q \int d^n q'\, f^*(q)\, N(q,q')\, f(q') = \langle \Psi | \Psi \rangle = 1 \tag{3.21}$$

In addition it is easy to show that two solutions $|\Psi_E\rangle$ and $|\Psi_{E'}\rangle$ of the HW equations for two different energies $E$ and $E'$ are orthogonal. Consequently the corresponding GCM weight functions $f_E(q)$ and $f_{E'}(q)$ are such that

$$\int d^n q \int d^n q'\, f_E^*(q)\, N(q,q')\, f_{E'}(q') = \langle \Psi_E | \Psi_{E'} \rangle = \delta_{EE'} \tag{3.22}$$

In the same way as above, one then deduces

$$\int' d\xi\, \overline{f}_E^*(\xi)\, \overline{f}_{E'}(\xi) = \langle \Psi_E | \Psi_{E'} \rangle = \delta_{EE'} \tag{3.23}$$

The functions $\overline{f}(\xi)$ thus behave like standard orthonormal quantum-mechanical wave functions. One can call them the "collective wave functions" of the system. In the same spirit, the kernel $\overline{H}(\xi, \xi')$ of Eq. (3.19) whose eigenfunctions are the $\overline{f}(\xi)$ may be called the "collective Hamiltonian kernel".

Let us note that the above expressions allow one to express the GCM state $|\Psi\rangle$ as an expansion over orthonormal states. In fact, using (3.1) and (3.1), we find

$$|\Psi\rangle = \int d\xi \, \overline{f}(\xi) |\overline{\Phi}_\xi\rangle \tag{3.24}$$

$$\text{with} \;\; |\overline{\Phi}_\xi\rangle = \int d^n q \, N^{-1/2^*}(\xi, q) \, |\Phi_q\rangle \tag{3.25}$$

and it is easy to check that the $|\overline{\Phi}_\xi\rangle$ constitute an orthonormal set:

$$\langle \overline{\Phi}_\xi | \overline{\Phi}_{\xi'} \rangle = \delta(\xi - \xi') \tag{3.26}$$

Finally, let us mention that the above formalism can be applied in a similar fashion to the time-dependent HW equation (3.12). The result is

$$\int' \overline{H}(\xi, \xi') \, \overline{f}(\xi', t) \, d\xi' = i\hbar \frac{\partial \overline{f}(\xi, t)}{\partial t} \tag{3.27}$$

with

$$\overline{f}(\xi, t) = \int d^n q \, f(q, t) \, N^{1/2^*}(q, \xi) \tag{3.28}$$

which is an integral time-dependent Schrödinger-like equation for the time-dependent collective wave function $\overline{f}(\xi, t)$.

The integral equation (3.27) is rigorously equivalent to the time-dependent HW equation (3.12). We may call it the reduced time-dependent HW equation.

### *3.1.2 Calculation of GCM kernels*

In this section, we illustrate the formalism developed in [4] for the calculation of GCM overlaps, Eqs. (3.6) and (3.7), by applying it to the multi-$O(4)$ model described in section 1.6.1 and appendix B. First, we calculate the overlap kernel between HB states at different deformations using Eq. (3.41) in [4],

$$\langle \Phi_D | \, \Phi_{D'} \rangle = \langle 0 | \, \Phi_{D'} \rangle \, \langle \Phi_D | \, 0 \rangle \det \left[ I + M^D \right] \tag{3.29}$$

where the first two coefficients on the right-hand side are determined from the $u$ coefficients of the HB solution at the appropriate deformation,

$$\langle 0|\,\Phi_{D'}\rangle = \prod_{\mu>0} u_\mu^{D'}$$
$$\langle \Phi_D|\,0\rangle = \prod_{\mu>0} u_\mu^{D}$$

and the matrix $M^D$ is given by Eq. (3.33) in [4],

$$M^D = \tan\theta^D \tau^{DD'} \tan\theta^{D'} \left(\tau^{DD'}\right)^\dagger$$

with $\tan\theta^D$ (and $\tan\theta^{D'}$) a diagonal matrix with elements along the diagonal given by

$$\left(\tan\theta^D\right)_{\mu\mu} = \frac{v_\mu^D}{u_\mu^D} \tag{3.30}$$

The matrix $\tau^{DD'}$ represents the overlap of the single-particle basis states between the two deformations. In our case, these states remain the same for all deformations $D$, and therefore $\tau^{DD'}$ is simply the identity matrix. Thus, in our simple example,

$$M_{\mu\mu}^D = \frac{v_\mu^D v_\mu^{D'}}{u_\mu^D u_\mu^{D'}} \tag{3.31}$$

and Eq. (3.29) can be written as (see also Eq. (4.4) in [8])

$$\begin{aligned}\langle \Phi_D|\,\Phi_{D'}\rangle &= \prod_{\mu>0} u_\mu^D u_\mu^{D'} \left[1 + \frac{v_\mu^D v_\mu^{D'}}{u_\mu^D u_\mu^{D'}}\right] \\ &= \prod_{\mu>0} \left(u_\mu^D u_\mu^{D'} + v_\mu^D v_\mu^{D'}\right)\end{aligned} \tag{3.32}$$

where, as noted in [4], the product spans a restricted set of quasiparticle states $\mu$ such that $v_\mu^D \neq 0$ (and $v_\mu^{D'} \neq 0$). The kernel overlap for our numerical example (Appendix B.5) is shown in Fig. 3.1.

We now turn to the Hamiltonian overlap, Eq. (3.7). We introduce the matrix $M^{D'}$ defined in Eq. (3.44) of [4],

$$M^{D'} = \tan\theta^{D'} \left(\tau^{DD'}\right)^\dagger \tan\theta^D \tau^{DD'}$$

which is diagonal like $M^D$ and has elements along the diagonal given by

$$M_{\mu\mu}^{D'} = \frac{v_\mu^D v_\mu^{D'}}{u_\mu^D u_\mu^{D'}} \tag{3.33}$$

Note that these are identical in our simple example to those of $M^D$ in Eq. (3.31). We can now calculate the matrix elements that make up the general-

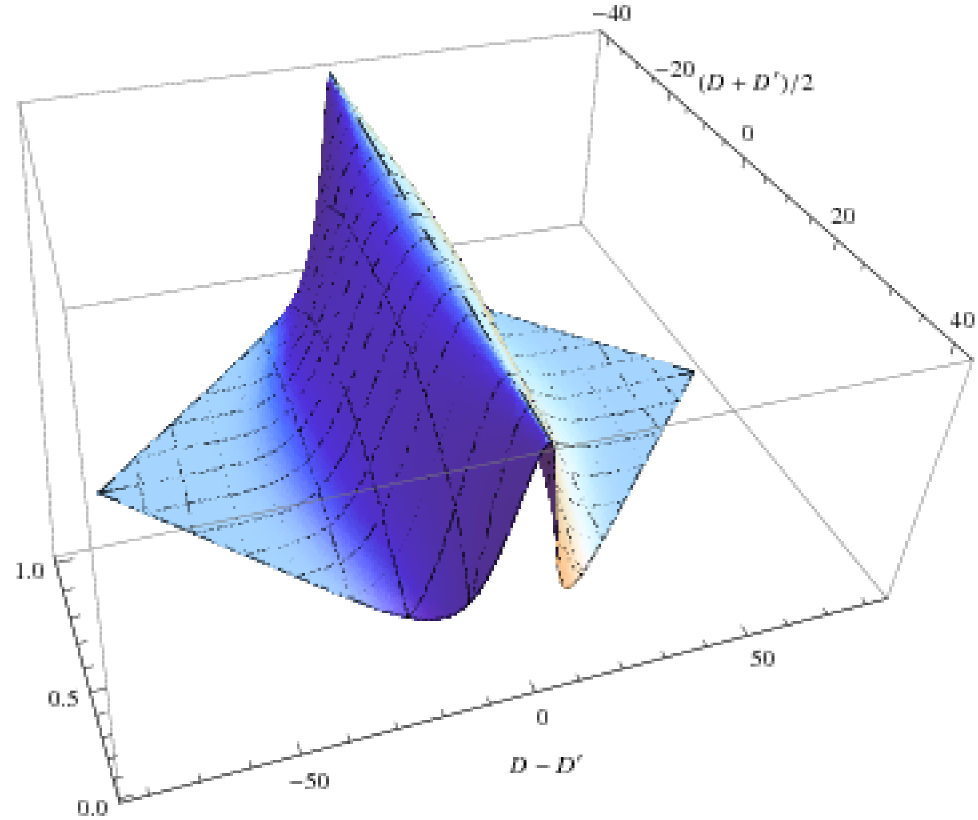


**Fig. 3.1** Kernel overlap function calculated using Eq. (3.32) and plotted as a function of the average deformation, $(D + D')/2$, and difference in deformations $D - D'$.

ized density matrix using Eqs. (3.46), (3.47), and (3.48) in [4],

$$\begin{aligned} S_{\nu\mu} &\equiv \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\nu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \middle| \Phi_{D'} \right\rangle} \\ &= \delta_{\mu\nu} \frac{v_\mu^D v_\mu^{D'}}{u_\mu^D u_\mu^{D'} + v_\mu^D v_\mu^{D'}} \end{aligned} \tag{3.34}$$

and

$$\begin{aligned} T_{\mu\bar{\nu}} &\equiv \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_{\bar{\nu}}^{D'\dagger} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \middle| \Phi_{D'} \right\rangle} \\ &= \delta_{\mu\nu} \frac{v_\mu^D u_\mu^{D'}}{u_\mu^D u_\mu^{D'} + v_\mu^D v_\mu^{D'}} \end{aligned} \tag{3.35}$$

and

$$\begin{aligned} Y_{\bar{\mu}\nu} &\equiv \frac{\left\langle \Phi_D \left| a_{\bar{\mu}}^{D'} a_{\nu}^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \\ &= \delta_{\mu\nu} \frac{u_\mu^D v_\mu^{D'}}{u_\mu^D u_\mu^{D'} + v_\mu^D v_\mu^{D'}} \end{aligned} \tag{3.36}$$

To evaluate the Hamiltonian overlap $\left\langle \Phi_D \left| \hat{H} \right| \Phi_{D'} \right\rangle$ with $\hat{H}$ given by Eq. (1.79), we make use of the extended Wick's theorem discussed in section 3.1 of [4] and obtain first for the spherical term

$$\begin{aligned} \left\langle \Phi_D \left| \hat{H}_0 \right| \Phi_{D'} \right\rangle &= \sum_\mu e_\mu^0 \left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle \\ &= 2 \left\langle \Phi_D \right| \Phi_{D'} \rangle \sum_{\mu>0} e_\mu^0 \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \end{aligned} \tag{3.37}$$

For the quadrupole term, $\hat{H}_Q$, we will need to calculate

$$\left\langle \Phi_D \left| \hat{H}_Q \right| \Phi_{D'} \right\rangle = -\frac{1}{2} \chi \sum_{\mu\nu} d_\mu \sigma_\mu d_\nu \sigma_\nu \left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} a_\nu^{D'\dagger} a_\nu^{D'} \right| \Phi_{D'} \right\rangle$$

Ignoring exchange terms and using [4] we find

$$\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} a_\nu^{D'\dagger} a_\nu^{D'} \right| \Phi_{D'} \right\rangle \approx \left\langle \Phi_D \right| \Phi_{D'} \rangle \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \frac{\left\langle \Phi_D \left| a_\nu^{D'\dagger} a_\nu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle}$$

and therefore

$$\left\langle \Phi_D \left| \hat{H}_Q \right| \Phi_{D'} \right\rangle \approx \quad -2\chi \left\langle \Phi_D \right| \Phi_{D'} \rangle \left[ \sum_{\mu>0} d_\mu \sigma_\mu \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \right]^2 \tag{3.38}$$

Finally, for the pairing term

$$\begin{aligned} \left\langle \Phi_D \left| \hat{H}_P \right| \Phi_{D'} \right\rangle &= -\frac{1}{2} G \sum_{\mu,\nu>0} \left[ \left\langle \Phi_D \left| a_\mu^{D'\dagger} a_{\bar{\mu}}^{D'\dagger} a_{\bar{\nu}}^{D'} a_\nu^{D'} \right| \Phi_{D'} \right\rangle \right. \\ &\quad \left. + \left\langle \Phi_D \left| a_{\bar{\mu}}^{D'} a_\mu^{D'} a_\nu^{D'\dagger} a_{\bar{\nu}}^{D'\dagger} \right| \Phi_{D'} \right\rangle \right] \\ &\approx -G \left\langle \Phi_D \right| \Phi_{D'} \rangle \left[ \sum_{\mu>0} \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_{\bar{\mu}}^{D'\dagger} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \right] \\ &\quad \times \left[ \sum_{\mu>0} \frac{\left\langle \Phi_D \left| a_{\bar{\mu}}^{D'} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \right| \Phi_{D'} \rangle} \right] \end{aligned} \tag{3.39}$$

Using Eqs. (3.34), (3.35), and (3.36)inside Eqs. (3.37), (3.38), and (3.39), we have all the necessary ingredients to calculate the Hamiltonian overlap

$$\left\langle \Phi_D \left| \hat{H} \right| \Phi_{D'} \right\rangle = \left\langle \Phi_D \left| \hat{H}_0 \right| \Phi_{D'} \right\rangle + \left\langle \Phi_D \left| \hat{H}_Q \right| \Phi_{D'} \right\rangle + \left\langle \Phi_D \left| \hat{H}_P \right| \Phi_{D'} \right\rangle \tag{3.40}$$

As a check, it is straightforward to verify that when $D = D'$ we recover the usual HB energy in Eq. (1.117). For our numerical example, the Hamiltonian overlap is shown in Fig. 3.2.

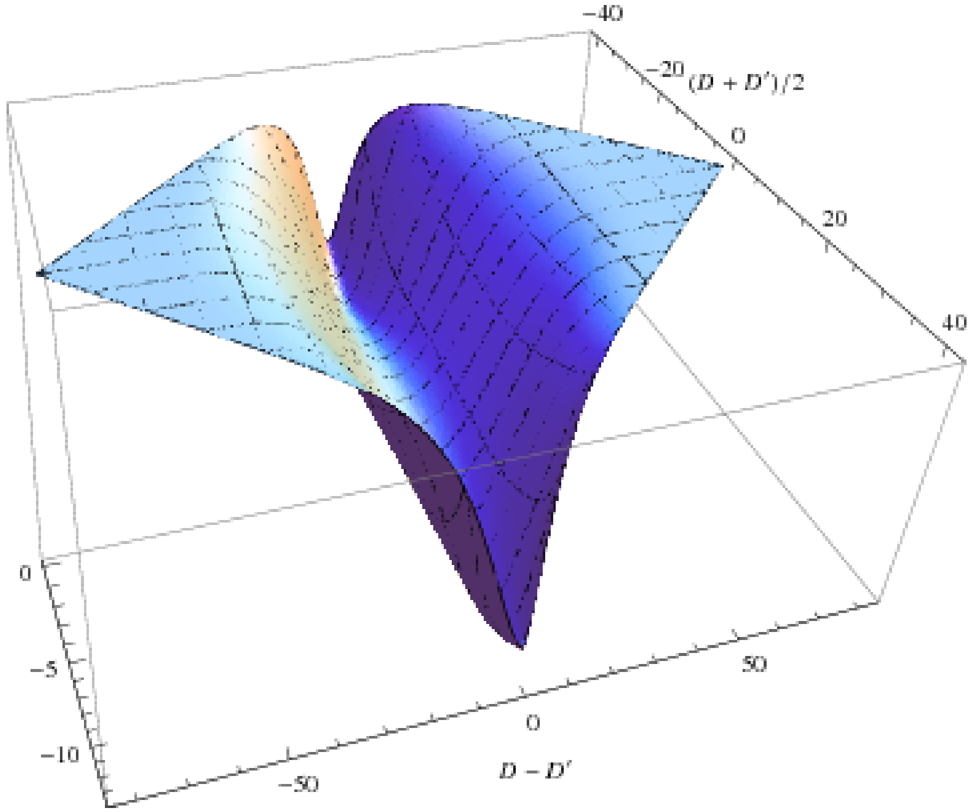


**Fig. 3.2** Hamiltonian overlap function calculated using Eq. (3.40) and plotted as a function of the average deformation, $(D + D')/2$, and difference in deformations $D - D'$.

It is also of interest to calculate the overlaps for the one-body operators used as constraints in the HB calculations, namely the number $\hat{N}$ and quadrupole $\hat{D}$ operators. The calculation is similar to the one performed for $\hat{H}_0$ above, and we find

$$\begin{aligned}\left\langle \Phi_D \left| \hat{N} \right| \Phi_{D'} \right\rangle &= 2 \left\langle \Phi_D \middle| \Phi_{D'} \right\rangle \sum_{\mu>0} \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \middle| \Phi_{D'} \right\rangle} \\ \left\langle \Phi_D \left| \hat{D} \right| \Phi_{D'} \right\rangle &= 2 \left\langle \Phi_D \middle| \Phi_{D'} \right\rangle \sum_{\mu>0} d_\mu \sigma_\mu \frac{\left\langle \Phi_D \left| a_\mu^{D'\dagger} a_\mu^{D'} \right| \Phi_{D'} \right\rangle}{\left\langle \Phi_D \middle| \Phi_{D'} \right\rangle}\end{aligned} \tag{3.41}$$

We plot these overlaps in Fig. 3.3.

### *3.1.3 Discrete-basis Hill-Wheeler method without projection*

The simplest way of solving the Hill-Wheeler equation, at least from a conceptual point of view, is to treat the problem on a discretized mesh of deformation values. The integral equation then reduces to a matrix diagonalization problem (section 10.2.2 in [9]). A standard approach [8, 10] is to first calculate the inverse square root of the kernel overlap matrix

$$\mathcal{N}^{-1/2}\left(D, D'\right) = \left\langle \Phi_D \middle| \Phi_{D'} \right\rangle^{-1/2}$$

transform the Hamiltonian overlap matrix

$$\tilde{\mathcal{H}}\left(D, D'\right) = \sum_{D'', D'''} \mathcal{N}^{-1/2}\left(D, D''\right) \left\langle \Phi_{D''} \left| \hat{H} \right| \Phi_{D'''} \right\rangle \mathcal{N}^{-1/2}\left(D''', D'\right)$$

and then obtain the collective energy spectrum $(E_k)$ at each deformation $D$ from the eigenvalue equation

$$\sum_{D'} \tilde{\mathcal{H}}\left(D, D'\right) g_k\left(D'\right) = E_k g_k\left(D\right) \tag{3.42}$$

The eigenvectors $g_k\left(D\right)$ are related to the weights $f_k\left(D\right)$ of the GCM wave function $\left|\Psi_k\right\rangle$, Eq. (3.9), through

$$f_k\left(D\right) = \sum_{D'} \mathcal{N}^{-1/2}\left(D, D'\right) g_k\left(D'\right)$$

where

$$\left|\Psi_k\right\rangle = \sum_D f_k\left(D\right) \left|\Phi_D\right\rangle$$

with $\left|\Phi_D\right\rangle$ the constrained HB solution at deformation $D$. The matrix element of any operator $\hat{O}$ between two GCM states is then given by

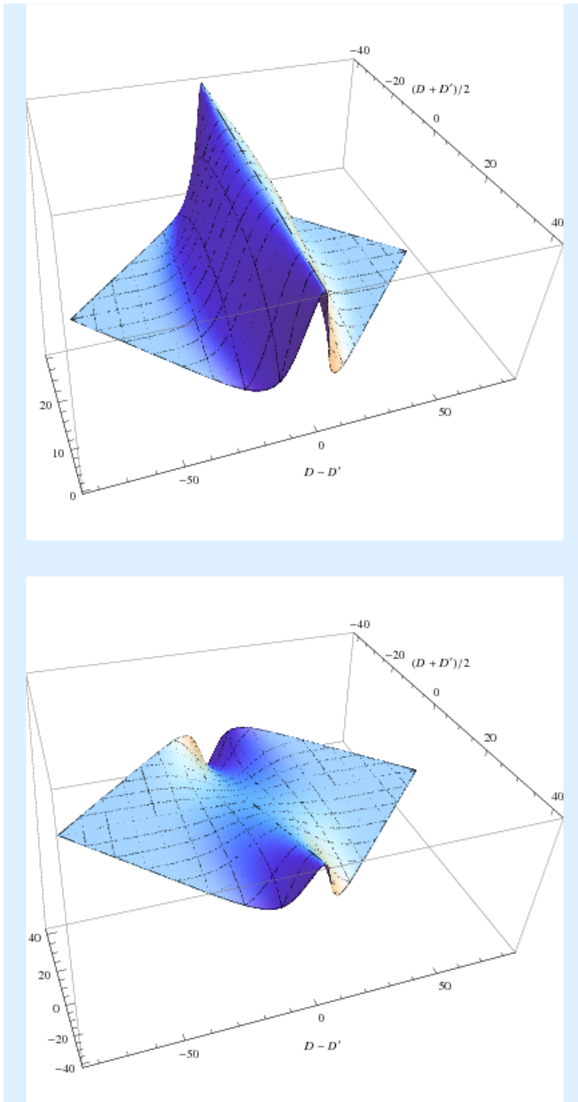


**Fig. 3.3** Overlaps of the constraint operators $\hat{N}$ (top panel) and $\hat{D}$ (bottom panel) given by Eq. (3.41) and plotted as a function of the average deformation, $(D+D')/2$, and difference in deformations $D-D'$.

$$\left\langle \Psi_k \left| \hat{O} \right| \Psi_l \right\rangle = \sum_{D,D'} g_k^* (D) \, \tilde{O} (D, D') \, g_l (D') \tag{3.43}$$

where

$$\tilde{O} (D, D') \equiv \sum_{D'',D'''} \mathcal{N}^{-1/2} (D, D'') \left\langle \Phi_{D''} \left| \hat{O} \right| \Phi_{D'''} \right\rangle \mathcal{N}^{-1/2} (D''', D') \tag{3.44}$$

The discretization of the continuous variables in the Hill-Wheeler equation does however introduce complications. In particular, it is well-known [8] that zero is an accumulation point for the eigenvalues of the norm overlap. Therefore, special care must be taken when calculating $\mathcal{N}^{-1/2} (D, D')$. In our numerical example (Appendix B.5), the inverse norm matrix, $\mathcal{N}^{-1}$ was first calculated by a singular value decomposition algorithm [11], which allows contributions with small eigenvalues (in our case, less than $10^{-6}$) to be ignored. Then for the square root very small but negative eigenvalues of $\mathcal{N}^{-1}$, which arise due to numerical errors, were also ignored. As a consequence, we find many GCM states with nearly zero energy $E_k$ obtained from Eq. (3.42), and nearly zero norm $\langle \Psi_k | \Psi_k \rangle$ given by Eq. (3.43). Discarding these spurious states, we are left with 21 levels for which we show the energy $E_k$, average particle number $\left\langle \Psi_k \left| \hat{N} \right| \Psi_l \right\rangle$, and average deformation $\left\langle \Psi_k \left| \hat{D} \right| \Psi_l \right\rangle$ of these levels in Fig. 3.4. The average particle number and deformation were calculated using Eqs. (3.43), (3.44), and (3.41).

Although the HB solution at each deformation is constrained to have the correct average particle number (28 in our case), there is no guarantee that the GCM state, which is a superposition of HB solutions, each with a distribution of particle numbers about the average will also have the correct particle number. This is apparent in the middle panel of Fig. 3.4 where the average particle number can be seen to fluctuate within $\approx \pm 2$ particles of the correct value 28.

### *3.1.4 Particle-number projected discrete Hill-Wheeler calculations*

In order to restore particle number conservation to the GCM states, we can project those states. The projection techniques are discussed in appendix C, and their application to the calculation of non-diagonal matrix elements needed in the GCM is discussed in appendix D. In this section we will adapt the general formalism in appendices C and D to the multi-$O(4)$ model, and calculate the GCM states and their properties with particle-number projection.

We start by calculating matrix elements of the spherical term in the Hamiltonian using the results in section D.4. As noted before, in the multi-$O(4)$

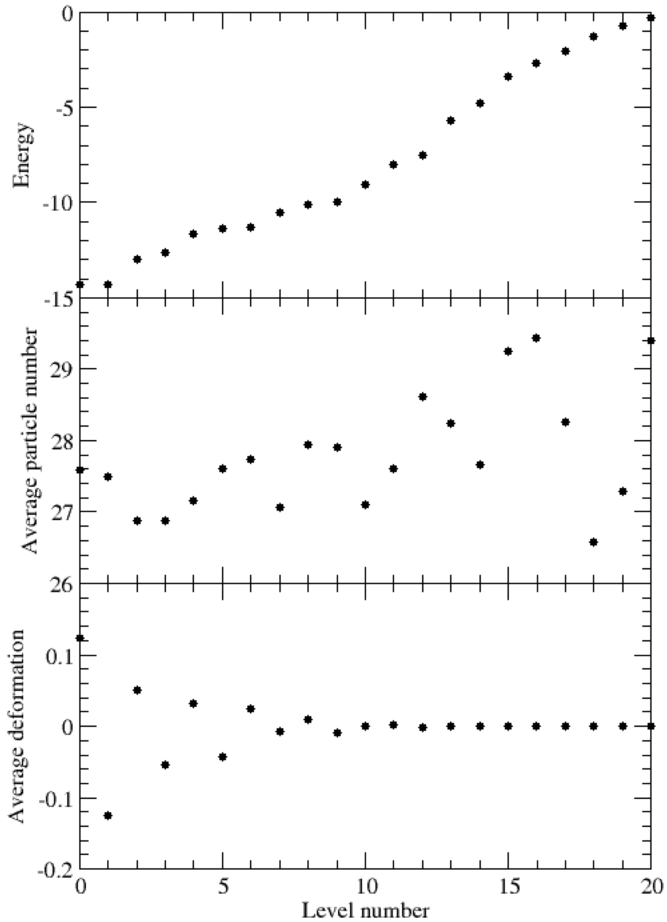


**Fig. 3.4** GCM level properties as a function of level index: level energy (top panel), average particle number (middle panel), and average deformation (bottom panel).

model the same single-particle basis is used at all deformations, and therefore the matrix $\tau^{qq'}$ defined in Eq. (D.2) is simply the identity matrix. Because of this, the matrices $M^q$ and $M^{q'}$ defined in Eqs. (D.19) and (D.34), respectively, are diagonal and their elements are given by Eqs. (3.31) and (3.33). From Eqs. (D.28), (D.29), (D.30), and (D.31) we then calculate the quantities

$$
\begin{aligned}
n(\xi) &= \prod_{\mu>0} \sqrt{1 + 2\cos(2\xi)\, M^{D}_{\mu\mu} + \left(M^{D}_{\mu\mu}\right)^2} \\
\Omega(\xi) &= \sum_{\mu>0} \tan^{-1}\left(1 + \cos(2\xi)\, M^{D}_{\mu\mu}, \sin(2\xi)\, M^{D}_{\mu\mu}\right)
\end{aligned}
\tag{3.45}
$$

which are needed in the calculation of overlaps of particle-number projected HFB states (Eq. (D.33)). Next, we adapt Eqs. (D.43) and (D.44) to the multi-$O(4)$ model, using the fact that the $S'$ matrix used in those equations, and defined in Eq. (D.42), is simply the identity matrix since $M^{q'}$ is already a diagonal matrix,

$$
\begin{aligned}
W'_{\beta\alpha}(\xi) &= \delta_{\alpha\beta} \frac{M^{D'}_{\alpha\alpha}\left[1 + M^{D'}_{\alpha\alpha}\cos(2\xi)\right]}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2} \\
Z'_{\beta\alpha}(\xi) &= -\delta_{\alpha\beta} \frac{\left(M^{D'}_{\alpha\alpha}\right)^2 \sin(2\xi)}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2}
\end{aligned}
\tag{3.46}
$$

These quantities enter into the computation of projected matrix elements of $a^{\dagger}a$ particle operator products. We can then use Eqs. (D.62) and (D.63) with $T^{q'}_{\alpha\beta} = \delta_{\alpha\beta} e^0_\alpha$ to calculate the contribution from the spherical term $\hat{H}_0$ in the Hamiltonian. This gives

$$
\begin{aligned}
W^{(0)}(\xi) &\equiv 2 \sum_{\alpha>0} e^0_\alpha W'_{\alpha\alpha}(\xi) \\
Z^{(0)}(\xi) &\equiv 2 \sum_{\alpha>0} e^0_\alpha Z'_{\alpha\alpha}(\xi)
\end{aligned}
\tag{3.47}
$$

The projected matrix element of $\hat{H}_0$ is then given by Eqs. (D.64) and (D.65). For the two-body part of the Hamiltonian, we first need to calculate a series of $W$ and $Z$ coefficients. We first consider the contribution from the quadrupole interaction. For this, we need to calculate $W'(\xi)$ and $Z'(\xi)$ given by Eqs. (D.66) and (D.67). For the multi-$O(4)$ model the quadrupole interaction matrix element simplifies to

$$
V^{D'}_{\alpha\beta\widetilde{\gamma\delta}} = -\chi \delta_{\alpha\gamma} \delta_{\beta\delta} d_\alpha \sigma_\alpha d_\beta \sigma_\beta
$$

and therefore

$$
\begin{aligned}
W'(\xi) &= -4\chi \sum_{\alpha,\beta>0} d_\alpha \sigma_\alpha d_\beta \sigma_\beta \left[W'_{\alpha\alpha}(\xi)\, W'_{\beta\beta}(\xi) - Z'_{\alpha\alpha}(\xi)\, Z'_{\beta\beta}(\xi)\right] \\
&= -4\chi \left\{ \left[\sum_{\alpha>0} d_\alpha \sigma_\alpha W'_{\alpha\alpha}(\xi)\right]^2 - \left[\sum_{\alpha>0} d_\alpha \sigma_\alpha Z'_{\alpha\alpha}(\xi)\right]^2 \right\}
\end{aligned}
\tag{3.48}
$$

and

$$\begin{aligned} Z'(\xi) &= -4\chi \sum_{\alpha,\beta>0} d_\alpha \sigma_\alpha d_\beta \sigma_\beta \left[W'_{\alpha\alpha}(\xi) Z'_{\beta\beta}(\xi) + Z'_{\alpha\alpha}(\xi) W'_{\beta\beta}(\xi)\right] \\ &= -8\chi \left[\sum_{\alpha>0} d_\alpha \sigma_\alpha W'_{\alpha\alpha}(\xi)\right] \left[\sum_{\alpha>0} d_\alpha \sigma_\alpha Z'_{\alpha\alpha}(\xi)\right] \end{aligned} \tag{3.49}$$

where the $W'_{\alpha\alpha}(\xi)$ and $Z'_{\alpha\alpha}(\xi)$ coefficients were already calculated explicitly in Eq. (3.46). Next, for the pairing contribution we need $W^{(\pm)}(\xi)$ and $Z^{(\pm)}(\xi)$ given by Eqs. (D.68) and (D.69), respectively. First we need to calculate the coefficients defined in Eqs. (D.53), (D.54), (D.58), and (D.59). We readily find for the multi-$O(4)$ model

$$\begin{aligned} W^{(-)}_{\beta\alpha}(\xi) &\equiv \delta_{\alpha\beta} \frac{\tan\theta^{D'}_\alpha \left[1 + M^{D'}_{\alpha\alpha}\cos(2\xi)\right]}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2} \\ Z^{(-)}_{\beta\alpha}(\xi) &\equiv -\delta_{\alpha\beta} \frac{\tan\theta^{D'}_\alpha M^{D'}_{\alpha\alpha}\sin(2\xi)}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2} \\ W^{(+)}_{\beta\alpha}(\xi) &\equiv \delta_{\alpha\beta} \frac{\tan\theta^{D}_\alpha \left[1 + M^{D'}_{\alpha\alpha}\cos(2\xi)\right]}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2} \\ Z^{(+)}_{\beta\alpha}(\xi) &\equiv -\delta_{\alpha\beta} \frac{\tan\theta^{D}_\alpha M^{D'}_{\alpha\alpha}\sin(2\xi)}{1 + 2M^{D'}_{\alpha\alpha}\cos(2\xi) + (M^{D'}_{\alpha\alpha})^2} \end{aligned}$$

For pairing in the multi-$O(4)$ model, the interaction matrix element simplifies to

$$V^{D'}_{\alpha\beta\widetilde{\gamma\delta}} = -4G\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\alpha>0}\delta_{\gamma>0}$$

and Eqs. (D.68) and (D.69) then give

$$\begin{aligned} W^{(\pm)}(\xi) &= -4G \sum_{\alpha,\gamma>0} \left[W^{(+)}_{\alpha\alpha}(\xi) W^{(-)}_{\gamma\gamma}(\xi) - Z^{(+)}_{\alpha\alpha}(\xi) Z^{(-)}_{\gamma\gamma}(\xi)\right] \\ &= -4G \left\{ \left[\sum_{\alpha>0} W^{(+)}_{\alpha\alpha}\right] \left[\sum_{\alpha>0} W^{(-)}_{\alpha\alpha}\right] - \left[\sum_{\alpha>0} Z^{(+)}_{\alpha\alpha}\right] \left[\sum_{\alpha>0} Z^{(-)}_{\alpha\alpha}\right] \right\} \end{aligned} \tag{3.50}$$

and

$$Z^{(\pm)}(\xi) = -4G \sum_{\alpha,\gamma>0} \left[ W^{(+)}_{\alpha\alpha}(\xi) Z^{(-)}_{\gamma\gamma}(\xi) + Z^{(+)}_{\alpha\alpha}(\xi) W^{(-)}_{\gamma\gamma}(\xi) \right]$$
$$= -4G \left\{ \left[ \sum_{\alpha>0} W^{(+)}_{\alpha\alpha} \right] \left[ \sum_{\alpha>0} Z^{(-)}_{\alpha\alpha} \right] + \left[ \sum_{\alpha>0} Z^{(+)}_{\alpha\alpha} \right] \left[ \sum_{\alpha>0} W^{(-)}_{\alpha\alpha} \right] \right\} \tag{3.51}$$

With these coefficients and for an even number of particles $N = 2p$, we can calculate numerically the number-projected norm overlap from Eq. (D.33) and using Eq. (3.45)

$$\left\langle \Phi^{(p)}_D \left| P^{(N)\dagger}_q P^{(N)}_{q'} \right| \Phi^{(p)}_{D'} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u^q_\mu u^{q'}_\mu \right) \int_0^\pi d\xi\, n(\xi) \cos\left[\Omega(\xi) - N\xi\right]$$

For the number-projected Hamiltonian overlap, we can use Eq. (D.71) to calculate numerically

$$\left\langle \Phi^{(p)}_D \left| P^{(N)\dagger}_q \hat{H} P^{(N)}_{q'} \right| \Phi^{(p)}_{D'} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u^q_\mu u^{q'}_\mu \right) \int_0^\pi d\xi\, n(\xi)\, n_H(\xi)$$
$$\times \cos\left[\Omega(\xi) + \Omega_H(\xi) - N\xi\right]$$

with $n_H(\xi)$ and $\Omega_H(\xi)$ defined by Eq. (D.70), and using the coefficients calculated in Eqs. (3.47), (3.48), (3.49), (3.50), and (3.51). The calculation of number-projected overlaps for the operators $\hat{N}$ and $\hat{D}$ can be derived in the same way as the one-body part of $\left\langle \Phi^{(p)}_D \left| P^{(N)\dagger}_q \hat{H} P^{(N)}_{q'} \right| \Phi^{(p)}_{D'} \right\rangle$ above, therefore we merely quote the results

$$\left\langle \Phi^{(p)}_D \left| P^{(N)\dagger}_q \hat{N} P^{(N)}_{q'} \right| \Phi^{(p)}_{D'} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u^q_\mu u^{q'}_\mu \right) \int_0^\pi d\xi\, n(\xi)\, n_N(\xi)$$
$$= \times \cos\left[\Omega(\xi) + \Omega_N(\xi) - (N-2)\xi\right]$$

where

$$n_N(\xi)\, e^{i\Omega_N(\xi)} = W^{(N)}(\xi) + iZ^{(N)}(\xi)$$

and

$$W^{(N)}(\xi) \equiv 2 \sum_{\alpha>0} W'_{\alpha\alpha}(\xi)$$
$$Z^{(N)}(\xi) \equiv 2 \sum_{\alpha>0} Z'_{\alpha\alpha}(\xi)$$

Similarly, for the deformation operator

$$\left\langle \Phi_D^{(p)} \left| P_q^{(N)\dagger} \hat{D} P_{q'}^{(N)} \right| \Phi_{D'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n(\xi) \, n_D(\xi) \times \cos\left[ \Omega(\xi) + \Omega_D(\xi) - (N-2)\xi \right]$$

where

$$n_D(\xi) \, e^{i\Omega_D(\xi)} = W^{(D)}(\xi) + iZ^{(D)}(\xi)$$

and

$$W^{(D)}(\xi) \equiv 2 \sum_{\alpha>0} d_\alpha \sigma_\alpha W'_{\alpha\alpha}(\xi)$$
$$Z^{(D)}(\xi) \equiv 2 \sum_{\alpha>0} d_\alpha \sigma_\alpha Z'_{\alpha\alpha}(\xi)$$

with the coefficients $W'_{\alpha\alpha}(\xi)$ and $Z'_{\alpha\alpha}(\xi)$ given by Eq. (3.46).

Once these number-projected overlaps have been calculated, the solution of the discrete Hill-Wheeler equation proceeds as in section 3.1.3. We compare in Fig. 3.5 the calculations with and without particle-number projection for the numerical example in appendix B.5. Not surprisingly, the effect of particle-number projection on the expectation values of the $\hat{N}$ and $\hat{D}$ operators is very significant. The particle number is now constant at $N = 28$ for all the GCM states, and the deformation is also constant at $D = 0$ for all the states. The effect of particle-number projection on the energy of the GCM states is small for the lowest levels ($\lesssim 0.1$ for the first 6 levels). The discrepancy in energy of the levels becomes larger for the higher-lying levels. It should be noted that the level energies are somewhat sensitive to the truncation level $\varepsilon$ chosen to exclude small eigenvalues (see discussion in section 3.1.3). The results in Fig. 3.5 were generated with $\varepsilon = 10^{-5}$. In Fig. 3.6 we show the low-lying spectrum of GCM states for different truncation levels. For $\varepsilon < 10^{-5}$ we find two spurious states (not shown in Fig. 3.6) at very low energies ($< -100$), which disappear for $\varepsilon \geq 10^{-5}$ . Although all the states plotted in Fig. 3.6 have remarkably stable energies as a function of $\varepsilon$, the higher ones show some variation near $\varepsilon = 10^{-1}$. For a discussion of numerical issues associated with the discretization of the Hill-Wheeler equation see, e.g., Chattopadhyay et al. [7].

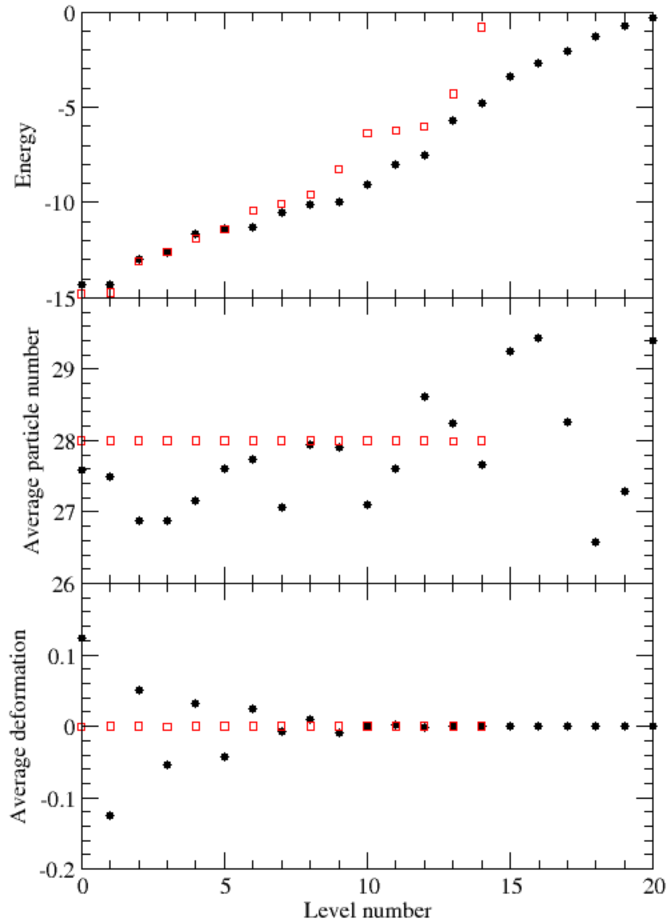


**Fig. 3.5** GCM level properties as a function of level index from the number-projected calculations (red squares) compared to the unprojected results shown in Fig. 3.4 (black disks). The quantities plotted are: level energy (top panel), average particle number (middle panel), and average deformation (bottom panel).

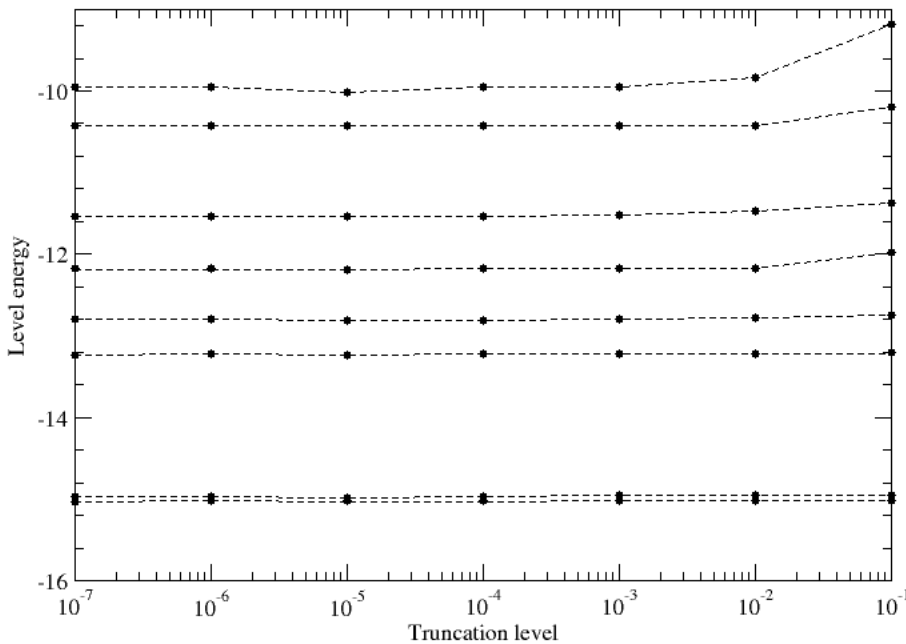


**Fig. 3.6** Variation of low-lying spectrum for the number-projected calculations as a function of truncation level $\varepsilon$ (see text).

## 3.2 A collective Schrödinger equation in the adiabatic limit

### *3.2.1 Reduction of the Hill-Wheeler equation to a Bohr-like Hamiltonian*

The numerical resolution of the HW equation either in the static forms (3.5)-(3.19) or the time-dependent forms (3.12)-(3.27) is far from being straightforward in applications to fission. In fact, one must compute beforehand all the values of the kernels $N(q, q')$ and $H(q, q')$, which clearly represents a tremendous amount of numerical work in the case of the fission of heavy nuclei where large single-particle configuration spaces and several generator coordinates have to be used. Whereas calculations of the overlap kernel values $N(q, q') = \langle \Phi_q | \Phi_{q'} \rangle$ are relatively easy, those of the Hamiltonian kernel

$H(q, q') = \langle \Phi_q | H | \Phi_{q'} \rangle$ are much heavier because of the complexity of the two-body effective interaction[2].

In view of this, most applications of the GCM in heavy nuclei make use of an approximation in which the HW integral equation is transformed into a Schrödinger-like second-order partial differential equation. As remarked in the introduction to this Chapter, this approximation also allows one to nicely connect the GCM description of fission to standard fission collective theories.

We will present in this Section the method of reduction based on the so-called Gaussian Overlap Approximation (GOA). An algorithm implementing this approach is given in Appendix A. This method is the most widely used technique for transforming the GCM equation into a partial differential equation. As mentioned at the beginning of this Chapter, the GOA approximation can be employed only when the states $|\Phi_q\rangle$ are invariant under time-reversal symmetry. Denoting by $T$ the (anti-unitary) time-reversal operator, the relations

$$T|\Phi_q\rangle = |\Phi_q\rangle \tag{3.52}$$

then imply that the kernels $N(q, q')$ and $H(q, q')$ are not only hermitian but real and symmetric.

Let us note that time-reversal symmetry can be assumed only when the $|\Phi_q\rangle$ are HFB vacua. This excludes the cases where the $|\Phi_q\rangle$ would contain quasi-particle excitations which would be necessary for treating odd or odd-odd nuclei and/or for describing possible excitations of the internal nucleus structure. Therefore the GCM approach based on constrained states obeying Eq. (3.52) can only be applied in the limit of adiabatic collective dynamics, in the sense that dissipation of the energy of collective motion into intrinsic excitations is excluded. This remark explains the term "adiabatic limit" in the title of this section.

Let us also note that adiabatic collective motion appears to be a realistic assumption in the case of the description of fission at relatively low energy presented in this book, essentially because the $|\Phi_q\rangle$ are HFB vacua that fully include pairing correlations. In fact, these correlations ensure that a pairing gap exists at all deformation $q$ and that there are no level crossings. As a consequence, excitation of the internal structure of the fissioning nucleus does not occur with high probability, at least provided the energy present in the fission mode is not too large.

Assuming the above time-reversal symmetry, the starting point of the GOA is the fact that the GCM kernels $N(q, q')$, $H(q, q')$ and $h(q, q')$ (Eqs. (3.6), (3.7), and (3.8), respectively) are sharply peaked functions of the differences $s_i = q_i - q'_i$ and slowly varying functions of the averages $\overline{q}_i = (q_i + q'_i)/2$. These features are apparent in figs. 3.1 and 3.2 of Section 3.1.2. where $N(q, q')$

---

[2] Let us mention that, when a density-dependent effective interaction is used – which is the case of the applications to fission presented in this book – the nature of the one-body density to insert in the effective interaction when calculating non-diagonal matrix elements $\langle \Phi_q | H | \Phi_{q'} \rangle$, $q \neq q'$ is unclear, and various prescriptions have been considered in the literature [12, 13].

and $H(q,q')$ are calculated in the multi-$O\,(4)$ model. Such a behavior has also been observed repeatedly in microscopic GCM approaches applied to collective phenomena in nuclei [8]. With this assumption it is reasonable to consider that the GCM kernels can be expanded up to second order in the $s_i$ variables with coefficients being slowly varying functions of the $\overline{q}_i$. Since the GCM kernels are symmetric, only even powers in the differences $s_i = q_i - q_i'$ appear and one obtains, taking as an example the energy kernel,

$$\begin{aligned} h(q,q') &\equiv h(\overline{q}+s/2, \overline{q}-s/2) \\ &= h_0(\overline{q}) + \frac{1}{2}\sum_{ij} \frac{s_i s_j}{4} \left[h_{ij}^{xx}(\overline{q}) - 2h_{ij}^{xy}(\overline{q}) + h_{ij}^{yy}(\overline{q})\right] \end{aligned} \tag{3.53}$$

with

$$\begin{aligned} &h_0(\overline{q}) = h(\overline{q},\overline{q}), \qquad h_{ij}^{xx}(\overline{q}) = \left.\frac{\partial^2 h(q,q')}{\partial q_i \partial q_j}\right|_{q=q'=\overline{q}} \\ &h_{ij}^{xy}(\overline{q}) = \left.\frac{\partial^2 h(q,q')}{\partial q_i \partial q_j'}\right|_{q=q'=\overline{q}}, \qquad h_{ij}^{yy}(\overline{q}) = \left.\frac{\partial^2 h(q,q')}{\partial q_i' \partial q_j'}\right|_{q=q'=\overline{q}} \end{aligned} \tag{3.54}$$

In (3.53), the summation indices $i$ and $j$ go from 1 to $n$, the number of generator coordinates. Since $h$ is symmetric, $h(q,q') = h(q',q)$, we find $h_{ij}^{xx}(\overline{q}) = h_{ij}^{yy}(\overline{q})$, and the expansion (3.53) becomes

$$h(q,q') = h_0(\overline{q}) + \frac{1}{2}\sum_{ij} s_i s_j \frac{h_{ij}^{xx}(\overline{q}) - h_{ij}^{xy}(\overline{q})}{2} \tag{3.55}$$

In the case of the norm kernel, the same type of expansion can be conveniently approximated by the Gaussian form

$$N(q,q') \equiv N(\overline{q}+s/2, \overline{q}-s/2) = \exp\left(-\frac{1}{2}\sum_{ij} g_{ij}(\overline{q})\, s_i s_j\right) \tag{3.56}$$

The advantage of this form is that it automatically incorporates the limiting cases $N(q,q) = 1$ and $N(q,q') \to 0$ when $|q_i|$ or $|q_i'|$ goes to infinity. Let us mention that an analysis of overlaps between differently deformed Slater determinants or HFB vacua shows that the Gaussian form (3.56) appears naturally when the number of occupied orbitals is large, i.e. in the case of heavy nuclei [2, 9].

The matrix $g$ is assumed to be symmetric, strictly positive, and a slowly varying function of $\overline{q}$. Expressions (3.56) and (3.55) embody the essential hypotheses of the GOA.

There are different ways of showing how the GOA allows one to reduce the GCM equation to a Schrödinger-like equation. The most widely known is explained in the book by Ring and Schuck [9]. We present here a slightly different method that starts from the reduced HW equation (3.19) or (3.27) and uses the properties of Gaussian functions to express the l.h.s. of (3.19) (or (3.27))

$$L(\xi) \equiv \int' \overline{H}(\xi,\xi')\,\overline{f}(\xi')\,d\xi' \tag{3.57}$$

as a second-order partial differential form. In order to do this, we assume that the matrix $g(\overline{q})$ can be treated as a constant. Since the widths $g_{ij}(\overline{q})$ have been already assumed to be slowly varying functions of $\overline{q}$, we will suppose that all developments involving differences like $s = q - q'$ are made in the vicinity of a fixed value of $\overline{q}$ which will be considered as a constant. The small deviations coming from slow variations as a function of $\overline{q}$ will be reintroduced in the end of this Section.

With this assumption and omitting the $\overline{q}$ dependence of the matrix $g$ we obtain the following expressions for the kernels $N^{1/2}$ and $N^{-1/2}$ defined in Eqs. (3.16) and (3.17):

$$N^{1/2}(q,\xi) = \left(\frac{2}{\pi}\right)^{n/4} G^{1/4} \exp\left(-\sum_{ij} g_{ij}(q_i-\xi_i)(q_j-\xi_j)\right) \tag{3.58}$$

$$N^{-1/2}(\xi,q) = \frac{G^{1/4}}{(2\pi)^{n/4}} \exp\left(-\frac{1}{4}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial\xi_i\partial\xi_j}\right)\delta^{(n)}(\xi-q) \tag{3.59}$$

with $G = \det g$, the determinant of the matrix $g$, $g^{-1}$ the inverse of $g$, and $\delta^{(n)}(\xi - q) = \prod_{i=1}^{n} \delta(\xi_i - q_i)$. The proof of (3.58) is straightforward (for example, by verifying that it satisfies Eq. (3.16)). Expression (3.59) can be easily found by first diagonalizing the (symmetric) matrix $g$, making a change a variables to the representation where $g$ is diagonal and then using the formula

$$\exp\left(-\frac{1}{4a}\frac{d^2}{dx^2}\right)e^{-ax^2} = \sqrt{\frac{\pi}{a}}\delta(x) \tag{3.60}$$

The latter formula can be proved by e.g. calculating the Fourier transform of the l.h.s. Expression (3.59) has the advantage of expressing $N^{-1/2}$ without introducing exponentials having positive arguments which would diverge at infinity.

From (3.18) the reduced Hamiltonian $\overline{H}(\xi,\xi')$ is

$$\overline{H}(\xi,\xi') = \int d^nq \int d^nq'\, N^{-1/2}(\xi,q)\,H(q,q')\,N^{-1/2}(\xi',q') \tag{3.61}$$

where we have taken into account that $N^{-1/2}(\xi, q)$ is real. Inserting (3.59), using the fact that we may replace in (3.59) the second derivative $\partial^2/(\partial\xi_i\partial\xi_j)$ by $\partial^2/(\partial q_i \partial q_j)$ and making integrations by parts, we obtain

$$\begin{aligned}\overline{H}(\xi, \xi') = \frac{G^{1/2}}{(2\pi)^{n/2}} \int d^n q \int d^n q' & \left[\exp\left(-\frac{1}{4}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial q_i \partial q_j}\right)\delta^{(n)}(\xi - q)\right] \\ & \times H(q, q') \left[\exp\left(-\frac{1}{4}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial q'_i \partial q'_j}\right)\delta^{(n)}(\xi' - q')\right] \\ = & \frac{G^{1/2}}{(2\pi)^{n/2}} \exp\left[-\frac{1}{4}\sum_{ij}(g^{-1})_{ij}\left(\frac{\partial^2}{\partial\xi_i\partial\xi_j} + \frac{\partial^2}{\partial\xi'_i\partial\xi'_j}\right)\right] H(\xi, \xi') \end{aligned} \tag{3.62}$$

We now make the change of variables $\overline{\xi} = (\xi + \xi')/2$, $\chi = \xi - \xi'$ and use the relation $H(\xi, \xi') = N(\xi, \xi')h(\xi, \xi')$ with $h(\xi, \xi')$ expanded up to second order in the differences $\chi_i$ as in (3.55)

$$h(\xi, \xi') \equiv h(\overline{\xi} + \chi/2, \overline{\xi} - \chi/2) = h_0(\overline{\xi}) + \frac{1}{2}\sum_{ij}\chi_i\chi_j h_{ij}(\overline{\xi}) \tag{3.63}$$

we obtain

$$\begin{aligned}\overline{H}(\xi, \xi') \equiv \overline{H}(\overline{\xi} + \chi/2, \overline{\xi} - \chi/2) = & \frac{G^{1/2}}{(2\pi)^{n/2}} \exp\left[-\frac{1}{2}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial\chi_i\partial\chi_j}\right] \\ & \times \left\{e^{-\frac{1}{2}\sum_{ij} g_{ij}\chi_i\chi_j}\left(\widetilde{h}_0(\overline{\xi}) + \frac{1}{2}\sum_{ij}\chi_i\chi_j\widetilde{h}_{ij}(\overline{\xi})\right)\right\} \end{aligned} \tag{3.64}$$

with

$$\widetilde{h}_0(\overline{\xi}) = \exp\left[-\frac{1}{8}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial\overline{\xi}_i\partial\overline{\xi}_j}\right] h_0(\overline{\xi}) \tag{3.65}$$

and a similar expression for $\widetilde{h}_{ij}$. In order to calculate the derivatives we use the generalization to $n$ dimensions of formula (3.60):

$$\exp\left[-\frac{1}{2}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial\chi_i\partial\chi_j}\right] e^{-\frac{1}{2}\sum_{ij} g_{ij}\chi_i\chi_j} = \frac{(2\pi)^{n/2}}{G^{1/2}}\delta^{(n)}(\chi) \tag{3.66}$$

This formula can be proved directly as in the one-dimensional case or by writing that $N^{-1/2}$, Eq. (3.59), is the inverse of $N^{1/2}$, Eq. (3.58). Expression (3.66) allows one to immediately calculate the coefficient of $\widetilde{h}_0(\overline{\xi})$ in (3.64). The second order term, which contains the additional product $\chi_i\chi_j$, can be calculated by taking the second derivative of (3.66) with respect to $\chi_k$ and $\chi_l$. This yields the other formula

$$\exp\left[-\frac{1}{2}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial\chi_i\partial\chi_j}\right]\chi_k\chi_l e^{-\frac{1}{2}\sum_{ij}g_{ij}\chi_i\chi_j} = \frac{(2\pi)^{n/2}}{G^{1/2}}$$
$$\times\left[(g^{-1})_{kl}\delta^{(n)}(\chi)+\sum_{ij}(g^{-1})_{ik}(g^{-1})_{jl}\frac{\partial^2}{\partial\chi_i\partial\chi_j}\delta^{(n)}(\chi)\right] \tag{3.67}$$

With (3.66) and (3.67), Eq. (3.64) thus becomes

$$\begin{aligned}\overline{H}(\xi,\xi') \equiv \overline{H}(\overline{\xi}+\chi/2,\overline{\xi}-\chi/2) &= \widetilde{h}_0(\overline{\xi})\delta^{(n)}(\chi)+\frac{1}{2}\sum_{ij}\widetilde{h}_{ij}(\overline{\xi})\\ &\times\left((g^{-1})_{ij}\delta^{(n)}(\chi)+\sum_{kl}(g^{-1})_{ik}(g^{-1})_{jl}\frac{\partial^2}{\partial\chi_k\partial\chi_l}\delta^{(n)}(\chi)\right)\\ &= a(\overline{\xi})\delta^{(n)}(\chi)+\frac{1}{2}\sum_{ij}b_{ij}(\overline{\xi})\frac{\partial^2}{\partial\chi_i\partial\chi_j}\delta^{(n)}(\chi)\end{aligned} \tag{3.68}$$

with

$$a(\overline{\xi}) = \widetilde{h}_0(\overline{\xi})+\frac{1}{2}\sum_{ij}(g^{-1})_{ij}\widetilde{h}_{ij}(\overline{\xi}) \tag{3.69}$$

$$b_{ij}(\overline{\xi}) = \sum_{kl}(g^{-1})_{ik}(g^{-1})_{jl}\widetilde{h}_{kl}(\overline{\xi}) \tag{3.70}$$

Let us now insert the expression (3.68) of $\overline{H}(\xi,\xi')$ into (3.57). We may ignore the prime on the integration symbol since the eigenvalues of $N(q,q')$ are Gaussians which are always non-zero except as $|\xi|\to\infty$ (see the explanation given after (3.18) in Section 3.1.1). Integrating by parts, we obtain

$$\begin{aligned}L(\xi) \equiv \int d\xi'\Bigg[a\left(\frac{\xi+\xi'}{2}\right)\delta^{(n)}(\xi-\xi')&\\ +\frac{1}{2}\sum_{ij}b_{ij}\left(\frac{\xi+\xi'}{2}\right)\frac{\partial^2}{\partial\xi'_i\partial\xi'_j}\delta^{(n)}(\xi'-\xi)\Bigg]\overline{f}(\xi')&\\ = a(\xi)\,\overline{f}(\xi)+\frac{1}{2}\sum_{ij}\frac{\partial^2}{\partial\xi'_i\partial\xi'_j}\left[b_{ij}\left(\frac{\xi+\xi'}{2}\right)\overline{f}(\xi')\right]\Bigg|_{\xi'=\xi}&\\ = \left(a(\xi)+\frac{1}{8}\sum_{ij}\frac{\partial^2 b_{ij}(\xi)}{\partial\xi_i\partial\xi_j}\right)\overline{f}(\xi)+\frac{1}{2}\sum_{ij}\left(\frac{\partial}{\partial\xi_i}b_{ij}(\xi)\frac{\partial}{\partial\xi_i}\right)\overline{f}(\xi)&\end{aligned} \tag{3.71}$$

This expression shows that the integral in the l.h.s. of the reduced HW equation (3.19) (and similarly in (3.27)) has been transformed into a second-order partial differential form. The second order differential operator acting on $\overline{f}(\xi)$ can therefore be interpreted as a quantum Hamiltonian. We may write it

$$\mathcal{H}\left(\xi, \partial/\partial\xi\right) = -\frac{\hbar^2}{2}\sum_{ij}\frac{\partial}{\partial\xi_i}B_{ij}(\xi)\frac{\partial}{\partial\xi_j} + \mathcal{V}(\xi) \tag{3.72}$$

where the partial derivatives act on all functions on their right, and with

$$B_{ij}(\xi) = -\frac{b_{ij}(\xi)}{\hbar^2} \tag{3.73}$$

$$\mathcal{V}(\xi) = a(\xi) + \frac{1}{8}\sum_{ij}\frac{\partial^2 b_{ij}(\xi)}{\partial\xi_i\partial\xi_j} \tag{3.74}$$

Thus, Eq. (3.19) is transformed into the stationary Schrödinger-like equation

$$\mathcal{H}\left(\xi, \partial/\partial\xi\right)\,\overline{f}(\xi) = E\overline{f}(\xi) \tag{3.75}$$

We notice that the limitation to second order in the differences $\xi_i - \xi_i'$ of the expansion of the energy kernel $h(\xi, \xi')$ is essential in order to produce a partial differential equation of second-order at most. If powers of order 4 or more had been included in the expansion of $h(\xi, \xi')$ the resulting partial differential equation would have contained derivatives of order 4 or more.

We also notice that the equation is written in the variables $\xi_i$ which label the eigenvalues of the norm kernel $N(q, q')$ (see Eq. (3.14) in Section 3.1.1). In principle, after solving the Schrödinger-like equation (3.75) (or the analogous time-dependent one involving $\overline{f}(\xi, t)$), one should get back to the GCM weight function $f(q)$ by inverting Eq. (3.20) in Section 3.1.1. From the latter equation

$$\begin{aligned} f(q) &= \int d^n\xi\,\overline{f}(\xi)\,N^{-1/2}(\xi, q) \\ &= \frac{G^{1/4}}{(2\pi)^{n/4}}\exp\left(-\frac{1}{4}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2}{\partial q_i\partial q_j}\right)\overline{f}(q) \end{aligned} \tag{3.76}$$

where we have used the expression (3.59) of $N^{-1/2}(\xi, \underline{q})$. We thus see that the variable $\xi$ has disappeared from the argument of $\overline{f}$, the variable $q$ reappearing in place of it. In view of this, we will henceforth replace everywhere the variable $\xi$ by the more usual notation $q$. We remark that, in doing so, the generator coordinates $q_i$ become full-fledged nucleus variables. We may call them the "collective coordinates" of the system. In the same spirit, we may call the Hamiltonian $\mathcal{H}\left(q, \partial/\partial q\right)$ the "collective Hamiltonian" of the system.

In (3.72) – rewritten with $q$ instead of $\xi$ – the matrix $B(q)$ can be interpreted as the inverse of an inertia. We will call this matrix the "inertia parameter" and keep the denomination "collective inertia" or "collective mass" for the inverse matrix $\mathcal{M} = B^{-1}$. We observe that $B(q)$ is coordinate-dependent (hence the denomination "Schrödinger-like" equation for Eq. (3.75)). In a similar fashion $\mathcal{V}(q)$ can be interpreted as a potential. We will call $\mathcal{V}(q)$ the "collective potential" of the system. With the GOA, the collective dynamics of the system therefore appear governed simply by the nucleus collective potential and collective inertia, as in standard models of collective motion. In a way, one could say that the GOA eventually provides a more transparent interpretation of collective dynamics than the full GCM approach.

The expression (3.74) of the collective potential $\mathcal{V}(q)$ can be further analyzed by using Eqs. (3.69), (3.70) and (3.65). From (3.65) we first have

$$\widetilde{h}_0(q) = h_0(q) - \frac{1}{8}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2 h_0(q)}{\partial q_i \partial q_j} + \dots \tag{3.77}$$

and a similar expression for $\widetilde{h}_{ij}(q)$. In accordance with the GOA, we will limit the expansion (3.77) to second order. On the other hand, from (3.63),

$$h_0(q) = h(q,q) = H(q,q) = \langle \Phi_q | H | \Phi_q \rangle = E_{HFB}(q) \tag{3.78}$$

where $E_{HFB}(q)$ is the HFB energy as a function of the deformation parameters $q_i$ i.e., the so-called "potential energy surface" of the nucleus. Using the relation (3.73) between $b_{ij}(q)$ and $B_{ij}(q)$, the definition (3.69) of $a(q)$ and the relation (3.70) to express $\widetilde{h}_{ij}(q)$ as a function of $b_{ij}(q)$, the expression (3.74) of $\mathcal{V}(q)$ finally becomes

$$\mathcal{V}(q) = E_{HFB}(q) - \varepsilon_0(q) \tag{3.79}$$

$$\varepsilon_0(q) = \frac{\hbar^2}{2}\sum_{ij} g_{ij} B_{ij}(q) + \frac{1}{8}\sum_{ij}(g^{-1})_{ij}\frac{\partial^2 E_{HFB}(q)}{\partial q_i \partial q_j} + \frac{\hbar^2}{8}\sum_{ij}\frac{\partial^2 B_{ij}(q)}{\partial q_i \partial q_j} \tag{3.80}$$

We see that the collective potential $\mathcal{V}(q)$ is equal to the HFB potential energy surface $E_{HFB}(q)$ minus a quantity $\varepsilon_0(q)$ which is usually called the "zero-point energy (ZPE) correction" associated with the collective motion. The first two components in (3.80) are the "kinetic zero-point energy correction" which is proportional to the inertia parameter and the "potential zero-point energy correction" which depends on the curvature of the potential energy surface $E_{HFB}(q)$. The third contribution representing the total curvature of the inertia parameter in collective space is usually neglected although it may be far from negligible. These corrections are of quantal nature. They mainly originate from the fluctuations of the collective coordinates $q_i$ in the constrained HFB states $|\Phi_q\rangle$ i.e. the $|\Phi_q\rangle$ are wave packets in the $q$ variable [14]. More precisely, with $q_i$ defined as the expectation value of the operator

$Q_i$ (see Eq. (3.2)) the fluctuations $\langle \Phi_q | (Q_i - q_i)(Q_j - q_j) | \Phi_q \rangle$ do not vanish in general.

Let us mention that, in our applications to fission a so-called "rotational ZPE" contribution is added to $\varepsilon_0(q)$. It is taken in the standard form $\langle \Phi_q | J^2 | \Phi_q \rangle / 2\mathcal{I}_x$ where $J$ is the angular momentum operator of the whole nucleus and $\mathcal{I}_x$ the moment of inertia around an axis perpendicular to the symmetry axis along which the stretching of the nucleus occurs.

An expression for the inertia parameter $B$ can be found from its expression (3.73) and the definitions (3.70) of $b_{ij}$ and (3.65) of $\widetilde{h}_{ij}(q)$. First, consistent with the GOA approximation, we will neglect the second-order derivatives of $h_{ij}(q)$. Therefore we will assume

$$\widetilde{h}_{ij}(q) \simeq h_{ij}(q) \tag{3.81}$$

As a consequence, from (3.70) and (3.73),

$$B_{ij} = -\frac{1}{\hbar^2} \sum_{kl} (g^{-1})_{ik} (g^{-1})_{jl} h_{kl}(q) \tag{3.82}$$

Now, the second-order expansion (3.63) of $h(q, q')$ and the definition $h(q, q') = H(q, q')/N(q, q')$ allow one to write

$$\begin{aligned} h_{kl}(\overline{q}) &= \left. \frac{\partial^2 h(\overline{q} + s/2, \overline{q} - s/2)}{\partial s_k \partial s_l} \right|_{s=0} \\ &= \left. \frac{\partial^2}{\partial s_k \partial s_l} \left[ H(\overline{q} + s/2, \overline{q} - s/2) e^{+\frac{1}{2} \sum_{ij} g_{ij} s_i s_j} \right] \right|_{s=0} \\ &= g_{kl} H(\overline{q}, \overline{q}) + \frac{1}{4} \left( \frac{\partial}{\partial q_k} - \frac{\partial}{\partial q'_k} \right) \left( \frac{\partial}{\partial q_l} - \frac{\partial}{\partial q'_l} \right) H(q, q') \Big|_{q=q'=\overline{q}} \end{aligned}$$

By defining the collective momentum operator

$$P_j = i\hbar \frac{\partial}{\partial q_i} \tag{3.83}$$

the Gaussian form (3.56) adopted for the norm kernel allows one to write

$$g_{ij} = \frac{1}{\hbar^2} \langle \Phi_q | P_i P_j | \Phi_q \rangle \tag{3.84}$$

As an illustration, we derive this last equation: using Eq. (3.56) with $s_j = q_j - q'_j$ one can write

$$\frac{\partial N(q, q')}{\partial q'_j} = N(q, q') \sum_i g_{ij}(\overline{q}) \, (q_i - q'_i)$$

$$\left.\frac{\partial^2 N(q,q')}{\partial q'_i \partial q'_j}\right|_{q'=q} = -g_{ij}(\overline{q})$$

With the definition $N(q,q') = \langle \Phi_q | \Phi_{q'} \rangle$, the above equation can be written

$$\begin{aligned} \langle \Phi_q | \frac{\partial^2}{\partial q_i \partial q_j} | \Phi_q \rangle &= \left.\frac{\partial^2 \langle \Phi_q | \Phi_{q'} \rangle}{\partial q'_i \partial q'_j}\right|_{q'=q} \\ &= -g_{ij}(\overline{q}) \end{aligned}$$

which gives Eq. (3.84) when the definition (3.83) of the $P_i$ is used. Similarly, the derivatives in the above expression of $h_{kl}$ can be replaced by $P$ operators. We thus obtain

$$\begin{aligned} h_{kl}(q) =& -\frac{1}{4\hbar^2} \langle \Phi_q | P_k P_l H + P_k H P_l + P_l H P_k + H P_k P_l | \Phi_q \rangle \\ &+ \frac{1}{\hbar^2} \langle \Phi_q | H | \Phi_q \rangle \langle \Phi_q | P_k P_l | \Phi_q \rangle \qquad (3.85) \\ \equiv& -\frac{1}{4\hbar^2} \langle \Phi_q | \left[ P_k, [P_l, H]_+ \right]_+ | \Phi_q \rangle_L \qquad (3.86) \end{aligned}$$

with $[A,B]_+ = AB + BA$. The index "L", which stands for "Linked", means that, in a diagrammatic picture of the matrix element (3.86), the unlinked diagrams – i.e. those containing two separate parts – must be omitted. Inserting this expression into (3.82) finally yields for the inertia parameter

$$B_{ij}(q) = \frac{1}{4\hbar^4} \sum_{kl} (g^{-1})_{ik} (g^{-1})_{jl} \langle \Phi_q | \left[ P_k, [P_l, H]_+ \right]_+ | \Phi_q \rangle_L \qquad (3.87)$$

In the case of $n = 1$ collective coordinate, the expressions (3.80) of $\varepsilon_0(q)$ – with the last term omitted – and (3.87) of $B$ coincide with those given in the book by Ring and Schuck [9], as can be easily checked by taking into account (3.84).

The previous developments have been made under the assumption that the overlap coefficients $g_{ij}$ are constant. In fact, it is not difficult to extend the formalism to the case where these coefficients depend on $q$. In order to show this, let us assume that we have diagonalized the – symmetric – matrix $g_{ij}(q)$ and performed a change of variables $q \to x$ such that

$$\sum_{ij} g_{ij} dq^i dq^j = \sum_k (dx^k)^2 \qquad (3.88)$$

Such a transformation is analogous to what is done in general relativity to define a local inertial system of coordinates from the curvilinear space-time coordinates [17]. In this latter case the $g_{ij}$ are the components of the space-time metric tensor of the Riemannian space whose squared line element is given by (3.88). As shown in [17], the transformation defined by (3.88) is always possible if the metric $g_{ij}$ is not singular.

In the above formula and in subsequent equations, we use the usual notation of differential geometry where upper indices indicate contravariant quantities (as the coordinates), lower indices indicate covariant quantities, and indices that appear twice, once as a subscript and once a superscript are summed over.

Since the metric tensor in the $x$ variables is constant – in fact unity – all the formula based on the GOA with constant overlap coefficients derived in this Section are valid when the $x$ variables are used. Now, in order to go back to the curvilinear variables $q$ one must perform two operations – in addition to the replacement of $x$ with $x(q)$ – (i) one must insert the Jacobian J$=\left\|\frac{\partial x}{\partial q}\right\|$ of the transformation $x \to q$ in the argument of integrals, and (ii) one must replace all derivatives $\partial/\partial x^k$ with covariant derivatives $\nabla_i$.

Concerning operation (i), we have from (3.88),

$$g_{ij} = \sum_k \frac{\partial x^k}{\partial q^i}\frac{\partial x^k}{\partial q^j}$$

from which it is easy to deduce (since the matrix $g_{ij}$ can be written as the product of the transposed Jacobian matrix with itself)

$$J = \sqrt{g} \tag{3.89}$$

with $g = \det(g_{ij})$. Consequently the normalization of the collective wave function $\overline{f}(q)$ must be changed to

$$\int d^n q \, \sqrt{g} \left|\overline{f}(q)\right|^2 = 1 \tag{3.90}$$

As to operation (ii), the covariant derivatives in the $q^i$ variables are defined as

$$\nabla_i S = \frac{\partial S}{\partial q^i} \qquad \text{for a scalar} \tag{3.91}$$

$$\nabla_i V^j = \frac{\partial V^j}{\partial q^i} + \left\{ \begin{matrix} j \\ i\,k \end{matrix} \right\} V^k \qquad \text{for a contravariant vector} \tag{3.92}$$

$$\nabla_i V_j = \frac{\partial V_j}{\partial q^i} - \left\{ \begin{matrix} k \\ i\,j \end{matrix} \right\} V_k \qquad \text{for a covariant vector} \tag{3.93}$$

where the

$$\left\{ \begin{matrix} k \\ i\,j \end{matrix} \right\} = \frac{1}{2} g^{kl} \left( \frac{\partial g_{li}}{\partial q^j} + \frac{\partial g_{lj}}{\partial q^i} - \frac{\partial g_{ij}}{\partial q^l} \right) \tag{3.94}$$

are Christoffel symbols defining the connection in the Riemannian space of the $q^i$. The replacement of ordinary derivatives by covariant ones in Eq.

(3.72) – with $q$ in place of $\xi$ – affects only the kinetic energy part of the collective Hamiltonian $\mathcal{H}(q, \partial/\partial q)$. When applying this part of the collective Hamiltonian to the collective wave function $\overline{f}(q)$, one must replace

$$T\overline{f} \equiv -\frac{\hbar^2}{2}\frac{\partial}{\partial q^i}B_{ij}(q)\frac{\partial \overline{f}}{\partial q^j} \tag{3.95}$$

with

$$\widetilde{T}\overline{f} = -\frac{\hbar^2}{2}\sum_{ij}\nabla_i B^{ij}(q)\nabla_j \overline{f} \tag{3.96}$$

Since $\overline{f}$ is a coordinate scalar, we have from (3.91), $\nabla_j \overline{f} = \partial\overline{f}/\partial q^j$, and since $B^{ij}\nabla_j \overline{f}$ is a contravariant vector, we get from (3.92)

$$\nabla_i B^{ij}(q)\nabla_j \overline{f} = \frac{\partial}{\partial q^i}B^{ij}(q)\frac{\partial \overline{f}}{\partial q^j} + \left\{ \begin{matrix} i \\ i\,k \end{matrix} \right\} B^{kj}(q)\frac{\partial \overline{f}}{\partial q^j} \tag{3.97}$$

But from (3.94), $\left\{ \begin{matrix} i \\ i\,k \end{matrix} \right\} = \frac{1}{\sqrt{g}}\frac{\partial\sqrt{g}}{\partial q^k}$ [17] and (3.97) becomes

$$\begin{aligned} \nabla_i B^{ij}(q)\nabla_j \overline{f} =& \frac{1}{\sqrt{g}}\left[\sqrt{g}\frac{\partial}{\partial q^i}B^{ij}(q)\frac{\partial \overline{f}}{\partial q^j} + \frac{\partial\sqrt{g}}{\partial q^k}B^{kj}(q)\frac{\partial \overline{f}}{\partial q^j}\right] \\ =& \frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\sqrt{g}\,B^{ij}(q)\frac{\partial \overline{f}}{\partial q^j} \end{aligned} \tag{3.98}$$

We therefore obtain the result that, when $g_{ij}(q)$ is not a constant, the Schrödinger-like equation (3.75) must be written

$$\widetilde{\mathcal{H}}\,(q, \partial/\partial q)\;\overline{f}(q) = E\overline{f}(q) \tag{3.99}$$

with

$$\widetilde{\mathcal{H}}\,(q, \partial/\partial q) = -\frac{\hbar^2}{2}\frac{1}{\sqrt{g}}\frac{\partial}{\partial q^i}\sqrt{g}\,B^{ij}(q)\frac{\partial}{\partial q^j} + \mathcal{V}(q) \tag{3.100}$$

and $\overline{f}(q)$ normalized as in (3.90).

Let us remark that one can revert to standard normalization (without the $\sqrt{g}$) by defining the new wave function

$$\overline{\overline{f}}(q) = g^{1/4}\overline{f}(q) \tag{3.101}$$

It is easy to show that the new wave function $\overline{\overline{f}}$ must obey the new equation

$$\widetilde{\widetilde{\mathcal{H}}}\,(q, \partial/\partial q)\;\overline{\overline{f}}(q) = E\overline{\overline{f}}(q) \tag{3.102}$$

with

$$\widetilde{\widetilde{\mathcal{H}}}\,(q,\partial/\partial q) = -\frac{\hbar^2}{2} g^{-1/4} \frac{\partial}{\partial q^i} \sqrt{g}\, B^{ij}(q) \frac{\partial}{\partial q^j} g^{-1/4} + \mathcal{V}(q) \tag{3.103}$$

and $\overline{\overline{f}}(q)$ normalized in the standard way

$$\int d^n q \left| \overline{\overline{f}}(q) \right|^2 = 1 \tag{3.104}$$

The expression (3.103) has been claimed a long time ago to be the correct quantum-mechanical Hamiltonian form in curvilinear coordinates [18].

Of course, similar equations are obtained in the time-dependent case by replacing $E$ with $i\hbar\partial/\partial t$ in (3.99) and (3.102) and introducing the extra time argument $t$ in $\overline{f}$ and $\overline{\overline{f}}$.

It is important to note that the above reduction of the GCM integral equation to a Schrödinger-like leads to a collective Hamiltonian which is directly written in quantized form. In particular, we have nowhere needed to resort to a method of quantizing a classical collective Hamiltonian. This is a remarkable result since quantization techniques such as Pauli quantization [19] are known to contain ambiguities [9]. In the present approach, changes in the order of the factors in the kinetic energy of $\mathcal{H}$ could be made at will, provided consistent supplementary contributions are added to the potential energy $\mathcal{V}(q)$.

For example, the form (3.103) of the collective Hamiltonian to be employed with a collective wave function $\overline{\overline{f}}(q)$ normalized in the standard way (see Eq. (3.104)) can be transformed back to the standard form (3.72) (with $\xi$ replaced by $q$) by adding to $\mathcal{V}(q)$ the additional contribution

$$V_K(q) = \frac{\hbar^2}{8g^{1/4}} \frac{\partial}{\partial q^i} \left[ B^{ij} g^{-3/4} \frac{\partial g}{\partial q^j} \right] \tag{3.105}$$

that is

$$\widetilde{\widetilde{\mathcal{H}}}\,(q,\partial/\partial q) = -\frac{\hbar^2}{2} \sum_{ij} \frac{\partial}{\partial q^i} B^{ij}(q) \frac{\partial}{\partial q^j} + \mathcal{V}(q) + V_K(q) \tag{3.106}$$

The proof of the equivalence between the forms (3.103) and (3.106) of $\widetilde{\widetilde{\mathcal{H}}}\,(q,\partial/\partial q)$ is straightforward although tedious.
Let us mention that, like the ZPE contribution given by the last term in Eq. (3.80), the additional potential $V_K(q)$ is often neglected in actual calculations with the argument that such contributions depend on second derivatives or on products of first derivatives which should be small if the reduction of the HW equations to a Schrödinger-like equation, i.e. the truncation of the Hamiltonian kernel to second order in its non-locality, is justified.

Finally, let us mention that the overlap coefficients $g_{ij}$ may be easily obtained from the expression (3.84). A heavier but seemingly more reliable method would be to compute numerically the norm kernel $N(q, q')$ as a function of $\overline{q} = (q + q')/2$ and $s = q - q'$ and to apply a least squared fit to a Gaussian form $\exp\left(-\frac{1}{2}\sum_{ij} g_{ij}(\overline{q}) s_i s_j\right)$. However, in the case of heavy even-even nuclei, one expects that $N(q', q')$ is very close to a Gaussian, so that the two methods should yield almost identical results.

### 3.2.2 Calculation of the inertia tensor

The inertia tensor $B_{ij}$ which appears in the collective Hamiltonian in the form (3.100) or (3.106) is given by Eq. (3.87). We will call this expression the "GCM inertia tensor" $B_{\mathrm{GCM}}$ and its inverse, $\mathcal{M}_{\mathrm{GCM}} = B_{\mathrm{GCM}}^{-1}$, the "GCM mass tensor". According to the developments of the previous Section, it is this expression of the inertia that in principle should be used in the collective Hamiltonian $\widetilde{\mathcal{H}}(q, \partial/\partial q)$. However, it has been observed for a long time that this formula does not seem to give the right collective inertia namely, the mass tensor $\mathcal{M}_{\mathrm{GCM}}$ obtained from Eq. (3.87) is significantly too small [15, 29, 30]. For instance, when the GCM is applied to the translation mode, the mass given by (3.87) is typically 75% of the nucleus mass $\mathcal{M}_A = Am$ [31, 32, 33]. Also, comparisons of nuclear spectra calculated with the collective Hamiltonian (3.106) and the GCM inertia tensor with experimental data in soft nuclei reach the same conclusion [34, 35, 29].

This anomalous behavior of the GCM inertia has been extensively discussed in the literature, see e.g. Ref. [36, 37, 38, 39]. For recent discussions about this problem, see also [40, 41, 3]. It is now recognized that such a deficiency originates from the fact that the GCM creates collective dynamics out of a static path $\{|\Phi_q\rangle\}$ whereas the true dynamic path must involve collective momenta $p_i$ conjugate to the collective variables $q_i$ [32, 38, 39]. In other words, the GCM ansatz is too restrictive a definition of physical states.

There has been a number of proposals aiming at correcting this inadequacy of the GCM approach. Most of them consists in extending the GCM theory by e.g. (i) introducing momenta $p_i$ in addition to the usual generator coordinates $q_i$ [38, 39], (ii) improving the GCM collective path either by performing a full variation including the many-body states $|\Phi_q\rangle$ besides the weight functions $f(q)$ [42, 15, 16], or by determining the constraining operators $Q_i$ in a self-consistent way [43], (iii) modifying the GCM ansatz itself [37]. Although such extensions are potentially able to correct the GCM collective inertia, as has been proved by looking at the particular case of translations [32, 33], they considerably increase the complexity of the GCM approach and they seem to have never been employed in practical applications.

In view of this, a consensus seems to have been reached in the physics community, that one should simply replace the GCM mass tensor $\mathcal{M}_{\mathrm{GCM}}$ with a expression that allows one to take into account the time-odd components of the self-consistent mean field that are not present in the usual inertia [39, 40, 30, 41], and that the best way to do this is to adopt the inertia $\mathcal{M}_{\mathrm{ATDHFB}}$ derived from the Adiabatic Time Dependent Hartree-Fock-Bogoliubov (ATDHFB) formalism. The latter approach is the extension incorporating pairing correlations of the Adiabatic Time Dependent Hartree-Fock (ATDHF) theory initially developed in the '70 for describing collective motion using the Time Dependent Hartree-Fock in the limit of small collective velocities [44, 45, 38, 36, 46, 47, 48, 39, 49, 50, 51, 52].

There are several reasons for choosing the ATDHFB inertia in place of the GCM one, (i) it is based on deeper physical principles [41], (ii) it automatically includes the time-odd components of the self-consistent mean field [40, 30], (iii) a GCM theory using a pair of conjugate parameters $(q, p)$ leads to a quantized form of ATDHF [39]. (iv) it produces the correct mass of the system in the case of translation [30]. Concerning the fission process, it is well known that the magnitude of the collective inertia strongly influences the collective dynamics along the fission path. In this respect, several authors have reached the conclusion that the GCM approach using the ATDHFB form of the collective inertia tensor provides the best framework to tackle the problem of nuclear dynamics at low fission energies [34, 29, 53, 54, 40, 41].

In what follows, we shall derive the expression of the ATDHF inertia $\mathcal{M}_{\mathrm{ATDHFB}}$ using the well-known property that it represents the dynamical response of the system to a change in deformation [15, 38, 36, 46, 39, 51, 41]. More precisely, the nucleus will be submitted to small momenta $p_i$ measured by displacement operators $P_i$, and the inertia of the system will be obtained by the HFB linear response tools developed in Chapter 2.

We derive in the following explicit expressions for the Gaussian overlap parameters $g_{ij}$, the GCM mass tensor $\mathcal{M}_{\mathrm{GCM}}$ and the ATDHFB mass tensor $\mathcal{M}_{\mathrm{ATDHFB}}$. The corresponding formulas allow one to compute these quantities directly from the results of constrained HFB calculations. However, as will be seen, the evaluation of these quantities is cumbersome as it requires to calculate the huge QRPA matrix $M(q)$ governing the response of the HFB mean fields to an external perturbation, and then to invert it. In view of this, it has become customary to employ approximate schemes (see, e.g., [47, 48, 16, 29, 55, 56, 40, 41]), the most widely used being the so-called "cranking" approximation [57, 58, 59, 60, 61, 62]. In this approximation, the residual interaction responsible for the rearrangement of the HFB fields under the influence of the collective momenta is neglected. Then the QRPA matrix becomes diagonal and can be trivially inverted.

This approximation introduces an element of theoretical uncertainty in the determination of the collective inertia since it amounts to neglect the time-odd interaction terms in the ATDHFB approach which are necessary to obtain the correct mass in the case of translations. Still, the ATDHFB inertia appears more realistic in applications than the GCM inertia even when the "cranking" approximation is used [35]. Nonetheless, work has been undertaken recently in order to devise methods of going beyond this approximation and estimate its real impact on the calculation of the nuclear collective inertia. More detail about the "cranking" approximation and its consequences on the values of calculated collective inertia tensors are given at the end of this Section.

As a prerequisite for the derivations of collective masses, we will need the matrix elements of the generators $P_j$ for translations along the $q_j$ variables in collective space. They are defined by the expression

$$|\Phi_{q+\delta q_j}\rangle = e^{-i/\hbar\,\delta q_j P_j}|\Phi_q\rangle \tag{3.107}$$

with the notation

$$q + \delta q_j = (q_1, \ldots, q_{j-1},\, q_j + \delta q_j,\, q_{j+1}, \ldots, q_n)$$

It is easy to see that this definition is consistent with Eq. (3.83):

$$P_j|\Phi_q\rangle = i\hbar \lim_{\delta q_j \to 0} \frac{|\Phi_{q+\delta q_j}\rangle - |\Phi_q\rangle}{\delta q_j} = i\hbar \frac{\partial}{\partial q_j}|\Phi_q\rangle \tag{3.108}$$

This equation implies that, when acting upon a state $|\Phi_q\rangle$, two operators $P_i$ and $P_j$ commute:

$$P_i P_j|\Phi_q\rangle = P_j P_i|\Phi_q\rangle \tag{3.109}$$

The relation (3.107) shows that $P_j$ may be taken as a one-body hermitian operator and that it must be odd under time-reversal since both $|\Phi_{q+\delta q_j}\rangle$ and $|\Phi_q\rangle$ are assumed to be time-reversal invariant. In view of these properties, $P_j$ may considered as a collective momentum operator in the $q_j$ direction. Let us mention that this operator is a function of the collective variables $q$.

We shall also need an explicit expression for the one-body constraining operators $Q_i$ in the quasiparticle basis associated to $|\Phi_q\rangle$. Starting from the particle representation of $Q_i$

$$Q_i = \sum_{mn} \left(Q_i^0\right)_{mn} a_m^\dagger a_n,$$

where $Q_i^0$ is a Hermitian matrix, we can rewrite it as

$$Q_i = \frac{1}{2}\mathrm{Tr}Q_i^0 + \frac{1}{2}\sum_{mn} \left( a_m^\dagger \;\, a_m \right) \begin{pmatrix} \left(Q_i^0\right)_{mn} & 0 \\ 0 & -\left(Q_i^0\right)^*_{mn} \end{pmatrix} \begin{pmatrix} a_n \\ a_n^\dagger \end{pmatrix}$$

Inserting the inverse Bogoliubov transformation,

$$\begin{pmatrix} a_n \\ a_n^\dagger \end{pmatrix} = \sum_\mu \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}_{n\mu} \begin{pmatrix} \eta_\mu \\ \eta_\mu^\dagger \end{pmatrix}$$

(see Eq. (1.3)) into it, we get

$$Q_i = \frac{1}{2}\mathrm{Tr}Q_i^0 + \frac{1}{2}\sum_{\mu\nu} \left( \eta_\mu^\dagger \; \eta_\mu \right) \begin{pmatrix} Q_i^{11} & -Q_i^{21^*} \\ Q_i^{21} & -Q_i^{11^*} \end{pmatrix}_{\mu\nu} \begin{pmatrix} \eta_\nu \\ \eta_\nu^\dagger \end{pmatrix} \tag{3.110}$$

with

$$\begin{aligned} Q_i^{11} &= U^\dagger Q_i^0 U - V^\dagger Q_i^{0^*} V = \left(Q_i^{11}\right)^\dagger \\ Q_i^{21} &= V^T Q_i^0 U - U^T Q_i^{0^*} V = -\left(Q_i^{21}\right)^T \end{aligned} \tag{3.111}$$

Eq. (3.110) can be written explicitly

$$\begin{aligned} Q_i =& \frac{1}{2}\mathrm{Tr}Q_i^0 + \frac{1}{2}\sum_{\mu\nu} \left[ (Q_i^{11})_{\mu\nu}\eta_\mu^\dagger\eta_\nu + (Q_i^{21})_{\mu\nu}\eta_\mu\eta_\nu \right. \\ & \qquad \left. -(Q_i^{21})^*_{\mu\nu}\eta_\mu^\dagger\eta_\nu^\dagger - (Q_i^{11})^*_{\mu\nu}\eta_\mu\eta_\nu^\dagger \right] \\ =& \frac{1}{2}\mathrm{Tr}Q_i^0 - \frac{1}{2}\mathrm{Tr}Q_i^{11} + \sum_{\mu\nu}(Q_i^{11})_{\mu\nu}\eta_\mu^\dagger\eta_\nu \\ & \qquad + \frac{1}{2}\sum_{\mu\nu} \left[ (Q_i^{21})_{\mu\nu}\eta_\mu\eta_\nu - (Q_i^{21})^*_{\mu\nu}\eta_\mu^\dagger\eta_\nu^\dagger \right] \end{aligned}$$

Now the constraint condition

$$\langle \Phi_q | Q_i | \Phi_q \rangle = q_i \tag{3.112}$$

shows that the difference between the two traces is equal to $q_i$. Hence,

$$Q_i = q_i + \sum_{\mu\nu}(Q_i^{11})_{\mu\nu}\eta_\mu^\dagger\eta_\nu + \frac{1}{2}\sum_{\mu\nu} \left[ (Q_i^{21})_{\mu\nu}\eta_\mu\eta_\nu - (Q_i^{21})^*_{\mu\nu}\eta_\mu^\dagger\eta_\nu^\dagger \right] \tag{3.113}$$

Because of the symmetry properties (3.111) of the matrices $Q_i^{11}$ and $Q_i^{21}$, the operator $Q_i$ appears to be hermitian as usually assumed.

Finally, the following formula

$$\langle \Phi_q | \left[ P_m, \left[ P_n, Q_i \right] \right] | \Phi_q \rangle = 0, \qquad \forall m, n, i \tag{3.114}$$

will be useful for the derivation of the GCM inertia. In order to prove it, we consider the equality analogous to (3.112)

$$\langle \Phi_{q+\delta q_m+\delta q_n} | Q_i | \Phi_{q+\delta q_m+\delta q_n} \rangle = q_i + \delta_{i,m}\,\delta q_m + \delta_{i,n}\,\delta q_n \tag{3.115}$$

From (3.108), with $P = \delta q_m P_m + \delta q_n P_n$, the l.h.s. is, up to second order in the $\delta q_k$,

$$\begin{aligned} \langle \Phi_q | e^{i/\hbar P} Q_i e^{-i/\hbar P} | \Phi_q \rangle =& \langle \Phi_q | Q_i + \frac{i}{\hbar}\left[ P, Q_i \right] - \frac{1}{2\hbar^2}\left[ P, \left[ P, Q_i \right] \right] | \Phi_q \rangle \\ =& q_i + \frac{i}{\hbar}\langle \Phi_q | \left[ P, Q_i \right] | \Phi_q \rangle - \frac{1}{2\hbar^2}\langle \Phi_q | \left[ P, \left[ P, Q_i \right] \right] | \Phi_q \rangle \end{aligned}$$

Equating the linear terms in $\delta q_k$ and the quadratic ones on both sides of Eq. (3.115) yields two equations

$$\begin{aligned}
&\frac{i}{\hbar}\delta q_m \langle \Phi_q|\,[P_m,Q_i]\,|\Phi_q\rangle + \frac{i}{\hbar}\delta q_n \langle \Phi_q|\,[P_n,Q_i]\,|\Phi_q\rangle = \delta_{i,m}\,\delta q_m + \delta_{i,n}\,\delta q_n \\
&\delta q_m^2 \langle \Phi_q|\,[P_m,[P_m,Q_i]]\,|\Phi_q\rangle + \delta q_m \delta q_n \langle \Phi_q|\,[P_m,[P_n,Q_i]] + [P_n,[P_m,Q_i]]\,|\Phi_q\rangle \\
&+ \delta q_n^2 \langle \Phi_q|\,[P_n,[P_n,Q_i]]\,|\Phi_q\rangle = 0
\end{aligned}$$

Since $\delta q_m$ and $\delta q_n$ are arbitrary numbers, that may be zero or equal to each other, the first relation is true only if

$$\langle \Phi_q|\,[P_m,Q_i]\,|\Phi_q\rangle = -i\hbar\delta_{i,m}, \qquad \forall m,i \tag{3.116}$$

and the second one implies the two relations

$$\begin{aligned}
&\langle \Phi_q|\,[P_m,[P_m,Q_i]]\,|\Phi_q\rangle = 0, \qquad \forall m,i \\
&\langle \Phi_q|\,[P_m,[P_n,Q_i]] + [P_n,[P_m,Q_i]]\,|\Phi_q\rangle = 0, \qquad \forall m,n,i
\end{aligned} \tag{3.117}$$

But, since $P_m P_n|\Phi_q\rangle = P_n P_m|\Phi_q\rangle$ and $\langle \Phi_q|P_m P_n = \langle \Phi_q|P_n P_m$, the two double commutators in the last equation are equal, as it is easy to check, which proves Eq. (3.114).

Let us note that the Eq. (3.116) is reminiscent of the usual quantum commutation relations between momenta and space variables. However, we see that, in the case of collective coordinates, these commutation relations hold only on average within the state $|\Phi_q\rangle$. The same is true for Eq. (3.114).

#### 3.2.2.1 Matrix elements of the $P_j$

According to a general theorem (see e.g. Appendix E in the book by Ring and Schuck [9]), two normalized HFB vacua $|\Phi_0\rangle$ and $|\Phi_1\rangle$ can always be related by a unitary transformation as

$$|\Phi_1\rangle = e^{iT}|\Phi_0\rangle$$

with

$$T = \frac{1}{2}\sum_{\mu\nu}\left(S_{\mu\nu}\eta_\mu\eta_\nu - S^*_{\mu\nu}\eta^\dagger_\mu\eta^\dagger_\nu\right) = T^\dagger$$

where the matrix $S$ is antisymmetric, $S^T = -S$, and the $\eta_\mu$ annihilate the vacuum $|\Phi_0\rangle$, i.e. $\eta_\mu|\Phi_0\rangle = 0$. Therefore, in view of Eq. (3.107), with the $\eta_\mu$ associated to the HFB state $|\Phi_q\rangle$, we may express the operator $P_j$ as

$$\begin{aligned} P_j =& \frac{1}{2} \sum_{\mu\nu} \left[ (P_j^{21})_{\mu\nu} \eta_\mu \eta_\nu - (P_j^{21})^*_{\mu\nu} \eta^\dagger_\mu \eta^\dagger_\nu \right], \qquad \left(P_j^{21}\right)^T = -P_j^{21} \\ =& \frac{1}{2} \left( \eta^\dagger \; \eta \right) \mathcal{P}_j \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \end{aligned} \tag{3.118}$$

where $P_j^{21}$ is an antisymmetric matrix and $\mathcal{P}_j$ the hermitian block matrix

$$\mathcal{P}_j = \begin{pmatrix} 0 & -P_j^{21^*} \\ P_j^{21} & 0 \end{pmatrix} = \mathcal{P}_j^\dagger \tag{3.119}$$

Since, as mentioned above, the $P_j$ are functions of the deformation $q$, so are the matrices $P_j^{21}$ and $\mathcal{P}_j$. In order to simplify the notations, we will not write explicitly such dependences on $q$ except in special cases.

The explicit form of $P_j$ in Eq. (3.118) allows one to derive the commutation relations

$$\Big[\eta_\lambda, P_j\Big] = -\sum_\mu (P_j^{21})^*_{\lambda\mu} \eta^\dagger_\mu, \qquad \Big[\eta^\dagger_\lambda, P_j\Big] = \sum_\mu (P_j^{21})_{\lambda\mu} \eta_\mu \tag{3.120}$$

which can be rewritten in the condensed forms

$$\left[ \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix}, P_j \right] = \mathcal{P}_j \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix}, \qquad \left[ \left( \eta^\dagger \; \eta \right), P_j \right] = -\left( \eta^\dagger \; \eta \right) \mathcal{P}_j \tag{3.121}$$

In order to find the matrix $P_j^{21}$, we have to express the relation between the two HFB vacua $|\Phi_{q+\delta q_j}\rangle$ and $|\Phi_q\rangle$. To this aim, let us recall that the HFB state $|\Phi_q\rangle$ is obtained by minimizing the functional (here, as in Section 1.5, we put a plus sign before the Lagrange multipliers)

$$\mathcal{F}(q) = \langle \Phi_q | \mathcal{H}(q) | \Phi_q \rangle \quad \text{with} \quad \mathcal{H}(q) = H + \sum_{i=1}^N \lambda_i(q)\, Q_i \tag{3.122}$$

where the Lagrange multipliers $\lambda_i(q)$ are determined such that the constraints

$$\langle \Phi_q | Q_i | \Phi_q \rangle = q_i, \qquad i = 1, \ldots, N \tag{3.123}$$

are satisfied. In the same way, the HFB state $|\Phi_{q+\delta q_j}\rangle$ is obtained by minimizing the functional

$$\mathcal{F}(q+\delta q_j) = \langle \Phi_q | \mathcal{H}(q+\delta q_j) | \Phi_q \rangle \quad \text{with} \quad \mathcal{H}(q+\delta q_j) = H + \sum_{i=1}^N \lambda_i(q+\delta q_j)\, Q_i \tag{3.124}$$

where the Lagrange multipliers $\lambda_i(q+\delta q_j)$ are determined such that the constraints

$$\langle \Phi_{q+\delta q_j} | Q_i | \Phi_{q+\delta q_j} \rangle = q_i + \delta_{i,j} \delta q_j, \qquad i = 1, \ldots, N \tag{3.125}$$

are satisfied. The HFB generalized density matrix $R(q+\delta q_j)$ obtained by minimizing (3.124) differs from the one, $R(q)$, obtained by minimizing (3.122) because of the additional field

$$\sum_{i=1}^{N}\Big(\lambda_i(q+\delta q_j)-\lambda_i(q)\Big)Q_i \sim \delta q_j \sum_{i=1}^{N}\frac{\partial \lambda_i(q)}{\partial q_j}Q_i$$

where we have assumed that $\delta q_j$ is a small quantity. The effect of this additional field can be found by applying the results of Sections 2.4 and 1.5. Up to first order in $\delta\lambda_j$, in the HFB representation that diagonalizes $R(q)$, we can write from (1.20)

$$R(q)=\begin{pmatrix}0 & 0\\ 0 & I\end{pmatrix}, \qquad R(q+\delta q_j)=\begin{pmatrix}0 & 0\\ 0 & I\end{pmatrix}+\begin{pmatrix}0 & -R^{21^*}\\ R^{21} & 0\end{pmatrix} \tag{3.126}$$

with, using the result (1.70),

$$\begin{pmatrix}R^{21}\\ R^{21^*}\end{pmatrix}=-\delta q_j\sum_{i=1}^{N}\frac{\partial\lambda_i(q)}{\partial q_j}[M(q)]^{-1}\begin{pmatrix}Q_i^{21}\\ Q_i^{21^*}\end{pmatrix} \tag{3.127}$$

In this equation, $Q_i^{21}$ is one of the submatrices that enter the quasiparticle representation of the operator $Q_i$, see Eqs. (3.110)-(3.112), and $M(q)$ is the QRPA matrix defined in Section 2.4 as $\begin{pmatrix}W & Z\\ Z^\dagger & W^*\end{pmatrix}$. We have explicitly made clear that this QRPA matrix depends on $q$. This is so because the variations envisaged here are not made around the HFB ground state as in Section 2.4, but around the constrained HFB state $|\Phi_q\rangle$. Hence, the second-order variations leading to the definition of the QRPA matrix are not those of the ground state energy, but those of the functional $\mathcal{F}(q)$ defined in (3.122). As a consequence, in the expressions (1.50) of the matrices $W$ and $Z$ as double commutators, one will have to replace the Hamiltonian $H$ with the constrained Hamiltonian $\mathcal{H}(q)$ (or Routhian) defined in Eq. (3.122), and these matrices will become dependent on $q$.

We have assumed in (3.127) that the matrix $M(q)$ can be inverted. Let us first note that this matrix governs the stability of the HFB solution $|\Phi_q\rangle$. Therefore its eigenvalues should be non negative, otherwise the state $|\Phi_q\rangle$ would not represent a minimum of the Routhian $\mathcal{H}(q)$. However, this matrix usually possesses zero eigenvalues associated with collective directions corresponding to symmetries of the Routhian $\mathcal{H}(q)$ which are broken by the vacuum $|\Phi_q\rangle$, such as translation and rotation invariances or particle number conservations. These collective directions are spurious in the sense that they do not describe proper small amplitude collective deformations of the nuclear structure. Therefore they should be projected out from the collective space used for treating small amplitude displacements of the deformation variables, as is the case here. This can be done by excluding from this collective space the eigenvectors of $M(q)$ associated with zero eigenvalues (see e.g., [74]). Once this operation is performed, the matrix $M(q)$ possesses only strictly positive eigenvalues and can be inverted.

Now, from the HFB formalism in Section 2.1, the generalized density matrix $R(q+\delta q_j)$ can also be written

$$R(q+\delta q_j) = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - \langle \Phi_{q+\delta q_j} | \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) | \Phi_{q+\delta q_j} \rangle \tag{3.128}$$

Using Eq. (3.107), the expectation value in the r.h.s. can be written up to first order in $\delta q_j$ as

$$\begin{aligned} &\langle \Phi_q | e^{i/\hbar\, \delta q_j P_j} \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) e^{-i/\hbar\, \delta q_j P_j} | \Phi_q \rangle \\ =&\langle \Phi_q | \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) | \Phi_q \rangle - \frac{i}{\hbar} \delta q_j \langle \Phi_q | \left[ \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right), P_j \right] | \Phi_q \rangle \end{aligned}$$

Since

$$\langle \Phi_q | \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) | \Phi_q \rangle = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - R(q) \tag{3.129}$$

the first term is $\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - R(q)$ and the second one is, making use of the commutation relations (3.121),

$$\begin{aligned} &-\frac{i}{\hbar} \delta q_j \langle \Phi_q | \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left[ \left( \eta^\dagger \ \eta \right), P_j \right] + \left[ \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix}, P_j \right] \left( \eta^\dagger \ \eta \right) | \Phi_q \rangle \\ =&-\frac{i}{\hbar} \delta q_j \langle \Phi_q | - \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) \mathcal{P}_j + \mathcal{P}_j \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) | \Phi_q \rangle \\ =&-\frac{i}{\hbar} \delta q_j \left[ \mathcal{P}_j, \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - R(q) \right] = \frac{i}{\hbar} \delta q_j \left[ \mathcal{P}_j, R(q) \right] \end{aligned}$$

Therefore

$$\langle \Phi_{q+\delta q_j} | \begin{pmatrix} \eta \\ \eta^\dagger \end{pmatrix} \left( \eta^\dagger \ \eta \right) | \Phi_{q+\delta q_j} \rangle = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} - R(q) + \frac{i}{\hbar} \delta q_j \left[ \mathcal{P}_j, R(q) \right]$$

and (3.128) becomes

$$R(q+\delta q_j) = R(q) - \frac{i}{\hbar} \delta q_j \left[ \mathcal{P}_j, R(q) \right]$$

The commutator can be calculated using the expressions of $\mathcal{P}_j$ and $R(q)$ given by Eqs. (3.119) and (3.126), which gives

$$R(q+\delta q_j) = R(q) + \frac{i}{\hbar} \delta q_j \begin{pmatrix} 0 & P_j^{21^*} \\ P_j^{21} & 0 \end{pmatrix} \tag{3.130}$$

Comparing this relation with the second Eq. (3.126), we thus obtain

$$P_j^{21} = -\frac{i\hbar}{\delta q_j} R^{21} \tag{3.131}$$

Consequently, using the expression (3.127) of $\begin{pmatrix} R^{21} \\ R^{21^*} \end{pmatrix}$, the matrix $P_j^{21}$ is given by the equation

$$\begin{aligned} \begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix} &= -\frac{i\hbar}{\delta q_j} \begin{pmatrix} R^{21} \\ -R^{21^*} \end{pmatrix} = -\frac{i\hbar}{\delta q_j} \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \begin{pmatrix} R^{21} \\ R^{21^*} \end{pmatrix} \\ &= i\hbar \sum_{i=1}^{N} \frac{\partial \lambda_i(q)}{\partial q_j} \tau M^{-1}(q) \begin{pmatrix} Q_i^{21} \\ Q_i^{21^*} \end{pmatrix} \end{aligned} \tag{3.132}$$

where we have defined the matrix

$$\tau = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \tag{3.133}$$

There remains to express the derivatives $\partial\lambda_i(q)/\partial q_j$. They can be deduced from Eq. (1.78) of Section 2.5 by identifying $\delta q_j$ with $\delta f_{(j)}^{(n)}$. With the definition of the matrix $T_{l,m}$ given in (1.76) which translates here into

$$T_{l,m} = \frac{1}{2} \begin{pmatrix} Q_l^{21^\dagger} & Q_l^{21^T} \end{pmatrix} M^{-1}(q) \begin{pmatrix} Q_m^{21} \\ Q_m^{21^*} \end{pmatrix} \tag{3.134}$$

where the matrices $Q_m^{21}$ are considered here as column vectors of elements $(Q_m^{21})_{\mu\nu}$, we obtain from Eq. (1.78), $\dfrac{\partial \lambda_i(q)}{\partial q_j} = -\left[T^{-1}\right]_{i,j}$. We define here more general quantities than (3.134),

$$\left[T_{(-\alpha)}\right]_{l,m} = \frac{1}{2} \begin{pmatrix} Q_l^{21^\dagger} & Q_l^{21^T} \end{pmatrix} [M(q)]^{-\alpha} \begin{pmatrix} Q_m^{21} \\ Q_m^{21^*} \end{pmatrix} \tag{3.135}$$

which will be useful in subsequent developments. These quantities may be called “moments” of order $(-\alpha)$ of the matrix $M(q)$ with respect to the constraining operators $Q_l$ and $Q_m$. We observe that the matrix $T_{(-\alpha)}$ is hermitian. Moreover, since according to the above discussion the matrix $M(q)$ is positive definite once the zero eigenvalues associated to spurious collective directions have been removed, so are the matrices $[M(q)]^{-\alpha}$ for any $\alpha$. It is then easy to show by expressing $M(q)$ in the representation where this matrix is diagonal that $T_{(-\alpha)}$ is also positive definite. In addition, it can be shown that, when the HFB states $|\Phi_q\rangle$ are invariant under time-reversal, all the matrices involved in the expansion of time-even operators onto the quasiparticle basis $(\eta, \eta^\dagger)$ associated with $|\Phi_q\rangle$ are real whereas the matrices associated with time-odd operators are purely imaginary. Since all the developments made in Section 4.2 assume time-reversal invariance, we may then assume that the matrices $Q_i^{21}$, $M(q)$, $T_{(-\alpha)}$, etc. are real and that the matrices $P_j^{21}$ are purely imaginary – although we shall often keep conjugation signs for real matrix elements for the sake of clarity. As a consequence, the matrix $T_{(-\alpha)}$ defined above can be considered as real, symmetric, positive definite and therefore invertible.

Coming back to Eq. (1.78), since $T \equiv T_{(-1)}$, we then may write it

$$\frac{\partial \lambda_i(q)}{\partial q_j} = -\left[T_{(-1)}\right]^{-1}_{i,j} \tag{3.136}$$

Inserting this expression into Eq. (3.132) finally yields the expression of the matrix $P_j^{21}$ as

$$\begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix} = -\, i\hbar \sum_{i=1}^{N} \left[T_{(-1)}\right]^{-1}_{i,j} \tau M^{-1}(q) \begin{pmatrix} Q_i^{21} \\ Q_i^{21^*} \end{pmatrix} \tag{3.137}$$

#### 3.2.2.2 Expression of $g_{ij}$

According to Eq. (3.84), the Gaussian overlap parameters $g_{ij}$ are given by

$$\hbar^2 g_{ij} = \langle \Phi_q | P_i P_j | \Phi_q \rangle \tag{3.138}$$

Using the expression (3.118) of the $P_i$, the calculation of the r.h.s. is straightforward. We obtain

$$\begin{aligned} \langle \Phi_q | P_i P_j | \Phi_q \rangle &= \sum_{\mu\nu\lambda\sigma} \left\langle \Phi_q \left| \frac{1}{2} (P_i^{21})_{\mu\nu} \eta_\mu \eta_\nu - \frac{1}{2} (P_j^{21})^*_{\lambda\sigma} \eta^\dagger_\lambda \eta^\dagger_\sigma \right| \Phi_q \right\rangle \\ &= -\, \frac{1}{4} \sum_{\mu\nu\lambda\sigma} (P_i^{21})_{\mu\nu} (P_j^{21})^*_{\lambda\sigma} \left( \delta_{\nu\lambda}\delta_{\mu\sigma} - \delta_{\nu\sigma}\delta_{\mu\lambda} \right) \\ &= \frac{1}{2} \sum_{\mu\nu} (P_i^{21})_{\mu\nu} (P_j^{21})^*_{\mu\nu} \end{aligned} \tag{3.139}$$

Since from Eq. (3.109) $P_i$ can be interchanged with $P_j$ when $P_i P_j$ is applied to $|\Phi_q\rangle$, the last expression can be symmetrized, which gives

$$\begin{aligned}\langle\Phi_q|P_iP_j|\Phi_q\rangle =&\frac{1}{4}\sum_{\mu\nu}\left((P_i^{21})^*_{\mu\nu}(P_j^{21})_{\mu\nu}+(P_i^{21})_{\mu\nu}(P_j^{21})^*_{\mu\nu}\right)\\ =&\frac{1}{4}\sum_{\mu\nu}\left((P_i^{21})^*_{\nu\mu}(P_j^{21})_{\nu\mu}+(P_i^{21})_{\mu\nu}(P_j^{21})^*_{\mu\nu}\right)\\ =&\frac{1}{4}\begin{pmatrix}P_i^{21^\dagger} & P_i^{21^T}\end{pmatrix}\begin{pmatrix}P_j^{21}\\ P_j^{21^*}\end{pmatrix}\end{aligned}$$

where, as before, the matrices $P_j^{21}$ are considered as column vectors of elements $(P_j^{21})_{\mu\nu}$. Inserting the expression (3.137) of $\begin{pmatrix}P_j^{21}\\ P_j^{21^*}\end{pmatrix}$ and using the fact that the QRPA matrix $M(q)$ is hermitian we thus obtain

$$\begin{aligned}\hbar^2 g_{ij} = \frac{\hbar^2}{4}\sum_{k,l=1}^{N}&\begin{pmatrix}Q_k^{21^\dagger} & Q_k^{21^T}\end{pmatrix} M^{-1}(q)\;\tau\left(\left[T_{(-1)}\right]^{-1}_{k,i}\right)^*\\ &\times\left[T_{(-1)}\right]^{-1}_{l,j}\,\tau\, M^{-1}(q)\begin{pmatrix}Q_l^{21}\\ Q_l^{21^*}\end{pmatrix}\end{aligned}$$

which finally gives

$$g_{ij} = \frac{1}{2}\sum_{k,l=1}^{N}\left[T_{(-1)}\right]^{-1}_{i,k}\left[T_{(-2)}\right]_{k,l}\left[T_{(-1)}\right]^{-1}_{l,j} \tag{3.140}$$

where we have used the property $\tau^2 = I$, the hermiticity of the matrix $T_{(-1)}$ and the definition (3.135) of $\left[T_{(-2)}\right]_{k,l}$. In matrix notation, denoting by $[g]$ the matrix whose elements are the $g_{ij}$ (in order to avoid confusion with the determinant $g$ of $[g]$ introduced previously), the above equation reads

$$[g] = \frac{1}{2}\left[T_{(-1)}\right]^{-1}\left[T_{(-2)}\right]\left[T_{(-1)}\right]^{-1} \tag{3.141}$$

Let us note that since, as remarked in Section 4.2.2.1, the matrices $T_{(-\alpha)}$ are real, symmetric, positive definite and invertible, the matrix $[g]$ possesses the same properties, as it should.

From (3.141), the elements $g^{ij}$ of the inverse matrix $[g]^{-1}$ are

$$g^{ij} \equiv [g]^{-1}_{ij} = 2\sum_{k,l=1}^{N}\left[T_{(-1)}\right]_{i,k}\left[T_{(-2)}\right]^{-1}_{k,l}\left[T_{(-1)}\right]_{l,j} \tag{3.142}$$

#### 3.2.2.3 Expression of the GCM inertia tensor

The GCM inertia tensor is given by Eq. (3.87) of Section 4.2 as

$$B_{ij}(q) = \frac{1}{4\hbar^4} \sum_{kl} g^{ik} \ \langle \Phi_q | \left[ P_k, [P_l, H]_+ \right]_+ | \Phi_q \rangle_L \ g^{jl} \tag{3.87}$$

where $g^{ik}$ denotes the elements of the inverse of the matrix of the Gaussian overlap parameters $g_{ij}$ calculated in the previous Section, see Eq. (3.142), and the linked matrix element is defined by Eqs. (3.85)-(3.86) as

$$\begin{aligned} \langle \Phi_q | \left[ P_k, [P_l, H]_+ \right]_+ | \Phi_q \rangle_L = & \langle \Phi_q | \left[ P_k, [P_l, H]_+ \right]_+ | \Phi_q \rangle \\ & - 4 \langle \Phi_q | H | \Phi_q \rangle \langle \Phi_q | P_k P_l | \Phi_q \rangle \end{aligned}$$

with $[A, B]_+ = AB + BA$. In order to calculate the linked matrix element, it will be convenient to make appear, in place of the Hamiltonian $H$, the constrained Hamiltonian $\mathcal{H}(q) = H + \sum_{i=1}^{N} \lambda_i(q)\, Q_i$ defined in Eq. (3.122). In fact, as will be seen, replacing $H$ with $\mathcal{H}(q)$ will allow us to express the linked matrix element in terms of the QRPA matrix $M(q)$ that governs small amplitude collective motion around the HFB state $|\Phi_q\rangle$.

We shall denote the above linked matrix element by $L_{kl}[H]$ i.e.,

$$\begin{aligned} L_{kl}[H] = & \langle \Phi_q | P_k P_l H + P_k H P_l + P_l H P_k + H P_l P_k | \Phi_q \rangle \\ & - 4 \langle \Phi_q | H | \Phi_q \rangle \langle \Phi_q | P_k P_l | \Phi_q \rangle \end{aligned} \tag{3.143}$$

Also, the commutation properties following from Eq. (3.109), $P_k P_l |\Phi_q\rangle = P_l P_k |\Phi_q\rangle$ and $\langle \Phi_q | P_k P_l = \langle \Phi_q | P_l P_k$, will be used repeatedly in what follows without being always recalled. We have

$$L_{kl}[H] = L_{kl}[\mathcal{H}(q)] - \sum_{i=1}^{N} \lambda_i(q)\, L_{kl}[Q_i] \tag{3.144}$$

We first show that, for a one-body hermitian constraining operators $Q_i$ whose general expression is given by (3.113) the corresponding linked matrix elements vanish, i.e.

$$\begin{aligned} L_{kl}[Q_i] \equiv & \langle \Phi_q | P_k P_l Q_i + P_k Q_i P_l + P_l Q_i P_k + Q_i P_l P_k | \Phi_q \rangle \\ & - 4 \langle \Phi_q | Q_i | \Phi_q \rangle \langle \Phi_q | P_k P_l | \Phi_q \rangle = 0 \end{aligned} \tag{3.145}$$

In order to prove this, we use in a first step the expression (3.118) of the $P_j$ to calculate $\langle \Phi_q | P_k P_l Q_i | \Phi_q \rangle$ and its complex conjugate $\langle \Phi_q | Q_i P_l P_k | \Phi_q \rangle$. We have

$$\begin{aligned}
P_l P_k|\Phi_q\rangle =& -\frac{1}{4}\sum_{\mu\nu\lambda\sigma}\left((P_l^{21})_{\mu\nu}\eta_\mu\eta_\nu - (P_l^{21})^*_{\mu\nu}\eta^\dagger_\mu\eta^\dagger_\nu\right)(P_k^{21})^*_{\lambda\sigma}\eta^\dagger_\lambda\eta^\dagger_\sigma|\Phi_q\rangle \\
=& -\frac{1}{4}\sum_{\mu\nu\lambda\sigma}\Big\{(P_l^{21})_{\mu\nu}(P_k^{21})^*_{\lambda\sigma}\left(\delta_{\lambda\nu}\delta_{\sigma\mu}-\delta_{\lambda\mu}\delta_{\sigma\nu}\right) \\
&\qquad -(P_l^{21})^*_{\mu\nu}(P_k^{21})^*_{\lambda\sigma}\eta^\dagger_\mu\eta^\dagger_\nu\eta^\dagger_\lambda\eta^\dagger_\sigma\Big\}|\Phi_q\rangle \\
=&\frac{1}{2}\sum_{\mu\nu}(P_l^{21})_{\mu\nu}(P_k^{21})^*_{\mu\nu}|\Phi_q\rangle + \frac{1}{4}\sum_{\mu\nu\lambda\sigma}(P_l^{21})^*_{\mu\nu}(P_k^{21})^*_{\lambda\sigma}\eta^\dagger_\mu\eta^\dagger_\nu\eta^\dagger_\lambda\eta^\dagger_\sigma|\Phi_q\rangle \\
=&\langle\Phi_q|P_lP_k|\Phi_q\rangle\ |\Phi_q\rangle + \frac{1}{4}\sum_{\mu\nu\lambda\sigma}(P_l^{21})^*_{\mu\nu}(P_k^{21})^*_{\lambda\sigma}\eta^\dagger_\mu\eta^\dagger_\nu\eta^\dagger_\lambda\eta^\dagger_\sigma|\Phi_q\rangle
\end{aligned} \tag{3.146}$$

where, in the last line, we have used Eq. (3.139). When applying $\langle\Phi_q|Q_i$ on the left, only the first term gives a non-zero contribution since, from Eq. (3.113), $Q_i$ contains products of no more than two annihilation operators $\eta$. Consequently, using the commuting property of $P_k$ and $P_l$ mentioned above, we get

$$\langle\Phi_q|Q_iP_lP_k|\Phi_q\rangle = \langle\Phi_q|P_kP_lQ_i|\Phi_q\rangle = \langle\Phi_q|P_lP_k|\Phi_q\rangle\langle\Phi_q|Q_i|\Phi_q\rangle \tag{3.147}$$

The quantity $L_{kl}[Q_i]$ defined in (3.145) therefore is

$$L_{kl}[Q_i] = \langle\Phi_q|P_kQ_iP_l + P_lQ_iP_k|\Phi_q\rangle - 2\langle\Phi_q|Q_i|\Phi_q\rangle\langle\Phi_q|P_kP_l|\Phi_q\rangle$$

By reusing (3.147), this equation can also be written

$$\begin{aligned}
L_{kl}[Q_i] =&\langle\Phi_q|P_kQ_iP_l + P_lQ_iP_k|\Phi_q\rangle - \langle\Phi_q|P_kP_lQ_i + Q_iP_lP_k|\Phi_q\rangle \\
=& -\langle\Phi_q|\,[P_k,[P_l,Q_i]]\,|\Phi_q\rangle
\end{aligned}$$

Formula (3.114) proved previously then leads to the result (3.145), i.e. $L_{kl}[Q_i]=0$.

There remains to express the quantity $L_{kl}[\mathcal{H}(q)]$ in Eq. ((3.144)). To this aim, we first calculate $\langle\Phi_q|\mathcal{H}(q)P_lP_k|\Phi_q\rangle = \langle\Phi_q|\mathcal{H}(q)P_kP_l|\Phi_q\rangle$. Using (3.146), we get

$$\begin{aligned}
\langle\Phi_q|\mathcal{H}(q)P_lP_k|\Phi_q\rangle =&\langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\langle\Phi_q|P_kP_l|\Phi_q\rangle \\
&+\frac{1}{4}\sum_{\mu\nu\lambda\sigma}(P_k^{21})^*_{\mu\nu}(P_l^{21})^*_{\lambda\sigma}\langle\Phi_q|\mathcal{H}(q)\eta^\dagger_\mu\eta^\dagger_\nu\eta^\dagger_\lambda\eta^\dagger_\sigma|\Phi_q\rangle
\end{aligned}$$

According to Eq. (1.51), the matrix element in the second line is equal to four times the element $Z_{(\mu\nu),(\lambda\sigma)}$ of the submatrix $Z$ of the QRPA matrix $M(q)$. Hence,

$$\begin{aligned}\langle\Phi_q|\mathcal{H}(q)P_lP_k|\Phi_q\rangle =& \langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\langle\Phi_q|P_kP_l|\Phi_q\rangle \\ &+ \sum_{\mu\nu\lambda\sigma}(P_k^{21})^*_{\mu\nu}Z_{(\mu\nu),(\lambda\sigma)}(P_l^{21})^*_{\lambda\sigma}\end{aligned} \tag{3.148}$$

The complex conjugate of this equation gives the term $\langle\Phi_q|P_kP_l\mathcal{H}(q)|\Phi_q\rangle$ as

$$\begin{aligned}\langle\Phi_q|P_kP_l\mathcal{H}(q)|\Phi_q\rangle =& \langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\langle\Phi_q|P_kP_l|\Phi_q\rangle \\ &+ \sum_{\mu\nu\lambda\sigma}(P_k^{21})_{\mu\nu}Z^*_{(\mu\nu),(\lambda\sigma)}(P_l^{21})_{\lambda\sigma}\end{aligned} \tag{3.149}$$

We now calculate $\langle\Phi_q|P_k\mathcal{H}(q)P_l|\Phi_q\rangle$ using the expression (3.118) of the $P_j$. We get

$$\langle\Phi_q|P_k\mathcal{H}(q)P_l|\Phi_q\rangle = -\frac{1}{4}\sum_{\mu\nu\lambda\sigma}(P_k^{21})_{\mu\nu}\langle\Phi_q|\eta_\mu\eta_\nu\mathcal{H}(q)\eta_\lambda^\dagger\eta_\sigma^\dagger|\Phi_q\rangle(P_l^{21})^*_{\lambda\sigma}$$

According to Eq. (1.51), the matrix element can be expressed as a function of the element $W^*_{(\mu\nu),(\lambda\sigma)}$ of the submatrix $W$ of the QRPA matrix $M(q)$. We obtain

$$\begin{aligned}\langle\Phi_q|P_k\mathcal{H}(q)P_l|\Phi_q\rangle = \sum_{\mu\nu\lambda\sigma}(P_k^{21})_{\mu\nu}\Big\{&W^*_{(\mu\nu),(\lambda\sigma)} \\ &-\frac{1}{4}\left(\delta_{\lambda\nu}\delta_{\sigma\mu}-\delta_{\lambda\mu}\delta_{\sigma\nu}\right)\langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\Big\}(P_l^{21})^*_{\lambda\sigma}\end{aligned}$$

The contribution of the sum over the $\delta$ terms in the brace is

$$\begin{aligned}-\frac{1}{4}\sum_{\lambda\sigma}\left((P_k^{21})_{\sigma\lambda}-(P_k^{21})_{\lambda\sigma}\right)(P_l^{21})^*_{\lambda\sigma} =& \frac{1}{2}\sum_{\lambda\sigma}(P_k^{21})_{\lambda\sigma}P_l^{21})^*_{\lambda\sigma} \\ =& \langle\Phi_q|P_kP_l|\Phi_q\rangle\end{aligned}$$

where Eq. (3.139) has been used in the last line. Therefore

$$\begin{aligned}\langle\Phi_q|P_k\mathcal{H}(q)P_l|\Phi_q\rangle =& \sum_{\mu\nu\lambda\sigma}(P_k^{21})_{\mu\nu}W^*_{(\mu\nu),(\lambda\sigma)}(P_l^{21})^*_{\lambda\sigma} \\ &+ \langle\Phi_q|P_kP_l|\Phi_q\rangle\langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\end{aligned} \tag{3.150}$$

Taking the complex conjugate yields

$$\begin{aligned}\langle\Phi_q|P_l\mathcal{H}(q)P_k|\Phi_q\rangle =& \sum_{\mu\nu\lambda\sigma}(P_k^{21})^*_{\mu\nu}W_{(\mu\nu),(\lambda\sigma)}(P_l^{21})_{\lambda\sigma} \\ &+ \langle\Phi_q|P_kP_l|\Phi_q\rangle\langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle\end{aligned} \tag{3.151}$$

Collecting Eqs. (3.148)-(3.151), we thus get

$$
\begin{aligned}
L_{kl}[\mathcal{H}(q)] &= \sum_{\mu\nu\lambda\sigma} \left( (P_k^{21})^*_{\mu\nu} \; (P_k^{21})_{\mu\nu} \right) \begin{pmatrix} W & Z \\ Z^* & W^* \end{pmatrix}_{(\mu\nu),(\lambda\sigma)} \begin{pmatrix} (P_l^{21})_{\lambda\sigma} \\ (P_l^{21})^*_{\lambda\sigma} \end{pmatrix} \\
&= \left( (P_k^{21})^\dagger \; (P_k^{21})^T \right) M(q) \begin{pmatrix} P_l^{21} \\ P_l^{21^*} \end{pmatrix}
\end{aligned}
$$

where we have identified the QRPA matrix $M(q)$ of (1.52) and, as previously, the matrices $P_l^{21}$ are considered as column vectors of elements $(P_l^{21})_{\mu\nu}$. There remains to insert the expression (3.137) of the vectors $\begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix}$. Taking into account the hermiticity of the QRPA matrix $M(q)$ we obtain

$$
\begin{aligned}
L_{kl}[\mathcal{H}(q)] = \hbar^2 \sum_{mn=1}^{N} & \left( Q_m^{21^\dagger} \; Q_m^{21^T} \right) M^{-1}(q) \; \tau \left[ T_{(-1)} \right]^{-1^*}_{m,k} \\
& \times M(q) \left[ T_{(-1)} \right]^{-1}_{n,l} \tau M^{-1}(q) \begin{pmatrix} Q_n^{21} \\ Q_n^{21^*} \end{pmatrix}
\end{aligned}
$$

We define a modified QRPA moment of order $(-1)$ with the formula

$$
\left[ \widetilde{T}_{(-1)} \right]_{m,n} = \frac{1}{2} \left( Q_m^{21^\dagger} \; Q_m^{21^T} \right) M^{-1}(q) \, \tau \, M(q) \, \tau \, M^{-1}(q) \begin{pmatrix} Q_n^{21} \\ Q_n^{21^*} \end{pmatrix} \tag{3.152}
$$

The matrix $\widetilde{T}_{(-1)}$ is hermitian as the matrix $T_{(-\alpha)}$ of Eq. (3.135).
With the definition (3.152) we find

$$
L_{kl}[\mathcal{H}(q)] = 2\hbar^2 \sum_{mn=1}^{N} \left[ T_{(-1)} \right]^{-1}_{k,m} \left[ \widetilde{T}_{(-1)} \right]_{m,n} \left[ T_{(-1)} \right]^{-1}_{n,l}
$$

Finally, from Eq. (3.87), with the expression (3.142) of $g^{ij}$, the GCM inertia tensor are the elements of the $N \times N$ matrix

$$
B_{\mathrm{GCM}}(q) = \frac{2}{\hbar^2} T_{(-1)} \left[ T_{(-2)} \right]^{-1} \left[ \widetilde{T}_{(-1)} \right] \left[ T_{(-2)} \right]^{-1} T_{(-1)} \tag{3.153}
$$

and its inverse, the GCM mass tensor, is given by

$$
\mathcal{M}_{\mathrm{GCM}}(q) = \frac{\hbar^2}{2} \left[ T_{(-1)} \right]^{-1} T_{(-2)} \left[ \widetilde{T}_{(-1)} \right]^{-1} T_{(-2)} \left[ T_{(-1)} \right]^{-1} \tag{3.154}
$$

According to the remarks made at the end of Section 4.2.2.2, all the matrices entering the above expressions can be assumed to be real. Therefore the above inertia and mass tensors are real symmetric matrices as they should.

#### 3.2.2.4 Expression of the ATDHFB mass tensor

As mentioned in the introduction to this Section, we derive the expression of the ATDHF inertia $\mathcal{M}_{\mathrm{ATDHFB}}$ by using the well-known property that it can be obtained from the HFB response of the system to small momenta $p_i$ measured by the displacement operators $P_i$ defined in (3.118). More precisely, the collective inertia will be deduced from the increase in HFB energy – in the form of collective kinetic energy – produced by these small collective momenta.

According to this technique, we look for the solutions $|\Phi_{qp}\rangle$ of the HFB equations obtained by minimizing the functional (here, as in Section 1.5, we put a plus sign before the Lagrange multipliers)

$$\begin{aligned}\mathcal{F}(q,p) =&\langle\Phi_{qp}|H + \sum_{i=1}^{N}\lambda_i(q,p)\,Q_i + \sum_{i=1}^{N}\mu_i(q,p)\,P_i|\Phi_{qp}\rangle \\ \equiv&\langle\Phi_{qp}|\mathcal{H}(q,p)|\Phi_{qp}\rangle\end{aligned} \tag{3.155}$$

where the Routhian $\mathcal{H}(q,p)$ is defined by this equation and the Lagrange multipliers $\lambda_i(q,p)$ and $\mu_i(q,p)$ are determined such that the constraints

$$\begin{cases}\langle\Phi_{qp}|Q_i|\Phi_{qp}\rangle = q_i \\ \langle\Phi_{qp}|P_i|\Phi_{qp}\rangle = p_i\end{cases} \qquad i = 1,\ldots,N \tag{3.156}$$

are satisfied. Here the momenta $p_i$ are assumed to be small. For $p_i = 0$, the functional (3.155) reduces to the functional

$$\mathcal{F}(q) = \langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle \quad \text{with} \quad \mathcal{H}(q) = H + \sum_{i=1}^{N}\lambda_i(q)\,Q_i \tag{3.122}$$

defined in Section 4.2.2.1 whose minimization yields the static HFB states $|\Phi_q\rangle$. We therefore make the identification $\lambda_i(q, p = 0) \equiv \lambda_i(q)$ and we must have $\mu_i(q,p)$ of the same order as the $p_i$ with $\mu_i(q, p = 0) = 0$. Using the above notations, the Routhian $\mathcal{H}(q,p)$ defining the functional $\mathcal{F}(q,p)$ can then be expanded up to first order in the $p_i$ as

$$\begin{aligned}\mathcal{H}(q,p) =&\mathcal{H}(q) + \sum_{i,j=1}^{N}\left[\left.\frac{\partial\lambda_i(q,p)}{\partial p_j}\right|_{p=0} Q_i + \left.\frac{\partial\mu_i(q,p)}{\partial p_j}\right|_{p=0} P_i\right] p_j \\ \equiv=&\mathcal{H}(q) + \sum_{i,j=1}^{N}(a_{ij}\,Q_i + b_{ij}\,P_i)\,p_j\end{aligned} \tag{3.157}$$

where the coefficients $a_{ij}$ and $b_{ij}$ are defined by the above equation.

According to the general theorem mentioned at the beginning of Section 4.2.2.1, the HFB state $|\Phi_{qp}\rangle$ can be related to the HFB state $|\Phi_q\rangle$ by means of a unitary transformation as (absorbing the $i$ in the exponential into the operator $L$)

$$|\Phi_{qp}\rangle = e^{L}|\Phi_q\rangle \tag{3.158}$$

with $L$ a one-body antihermitian operator of the form

$$L = \frac{1}{2}\sum_{\mu\nu}\left(K_{\mu\nu}\eta_\mu\eta_\nu + K^*_{\mu\nu}\eta^\dagger_\mu\eta^\dagger_\nu\right) = -L^\dagger \tag{3.159}$$

where the matrix $K$ is antisymmetric, $K^T = -K$, and the $\eta_\mu$ annihilate the HFB vacuum $|\Phi_q\rangle$, i.e. $\eta_\mu|\Phi_q\rangle = 0$. We expect that the operator $L$ and the matrix $K$ are of the same order as the $p_i$.

Now, a way to express the stationarity of the functional $\mathcal{F}(q,p)$ in HFB theory follows from the general theorem mentioned above. Any variation of the state $|\Phi_{qp}\rangle$ can be written $e^S|\Phi_{qp}\rangle$ with $S$ a one-body antihermitian operator of the same form (3.159) as $L$ and the corresponding variation of the functional $\mathcal{F}(q,p)$ is

$$\begin{aligned}\mathcal{F}(q,p) + \delta\mathcal{F}(q,p) =& \langle\Phi_{qp}|e^{-S}\mathcal{H}(q,p)e^{S}|\Phi_{qp}\rangle\\ =& \mathcal{F}(q,p) + \langle\Phi_{qp}|\left[\mathcal{H}(q,p),S\right]|\Phi_{qp}\rangle + \ldots\end{aligned}$$

Therefore the stationarity of $\mathcal{F}(q,p)$ for the HFB state $|\Phi_{qp}\rangle$ is equivalent to the condition

$$\langle\Phi_{qp}|\left[\mathcal{H}(q,p),S\right]|\Phi_{qp}\rangle = 0, \qquad \forall S \tag{3.160}$$

Using (3.158) and (3.157), this condition reads

$$\langle\Phi_q|e^{-L}\left[\mathcal{H}(q) + \sum_{i,j=1}^{N}\left(a_{ij}\,Q_i + b_{ij}\,P_i\right)p_j,\; S\right]e^{L}|\Phi_q\rangle = 0, \qquad \forall S$$

that is, keeping only the terms up to first order in $p_j$ and $L$,

$$\begin{aligned}&\langle\Phi_q|\left[\mathcal{H}(q) + \sum_{i,j=1}^{N}\left(a_{ij}\,Q_i + b_{ij}\,P_i\right)p_j,\; S\right]|\Phi_q\rangle\\ &+\langle\Phi_q|\left[\left[\mathcal{H}(q),\; S\right],L\right]|\Phi_q\rangle = 0, \qquad \forall S\end{aligned}$$

The stationarity of the functional $\mathcal{F}(q)$ that yields the stationary states $|\Phi_q\rangle$ implies, in an analogous fashion as (3.160), $\langle\Phi_q|\left[\mathcal{H}(q),S\right]|\Phi_q\rangle = 0$ for any $S$. Therefore the above equation gives

$$\sum_{i,j=1}^{N}\langle\Phi_q|\left[\left(a_{ij}\,Q_i + b_{ij}\,P_i\right),\,S\right]|\Phi_q\rangle p_j + \langle\Phi_q|\left[\left[\mathcal{H}(q),\;S\right],L\right]|\Phi_q\rangle = 0, \quad \forall S$$

Now, because $S$ is of the form (3.159), and since the matrix elements in front of the operators $\eta_\mu \eta_\nu$ and $\eta_\mu^\dagger \eta_\nu^\dagger$ are arbitrary, this equation is equivalent to the pair of equations

$$\begin{cases} \sum_{i,j=1}^{N} \langle \Phi_q | \left[ (a_{ij}\, Q_i + b_{ij}\, P_i)\,, \eta_\mu^\dagger \eta_\nu^\dagger \right] |\Phi_q\rangle p_j + \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu^\dagger \eta_\nu^\dagger \right], L \right] |\Phi_q\rangle = 0 \\ \sum_{i,j=1}^{N} \langle \Phi_q | \left[ (a_{ij}\, Q_i + b_{ij}\, P_i)\,, \eta_\mu \eta_\nu \right] |\Phi_q\rangle p_j + \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu \eta_\nu \right], L \right] |\Phi_q\rangle = 0 \end{cases} \tag{3.161}$$

for any $\mu, \nu$. The first terms in both equations are easily expressed from the commutation relations

$$\begin{aligned} \langle \Phi_q | \left[ Q_i, \eta_\mu^\dagger \eta_\nu^\dagger \right] |\Phi_q\rangle &= -(Q_i^{21})_{\mu\nu}, \quad \langle \Phi_q | \left[ P_i, \eta_\mu^\dagger \eta_\nu^\dagger \right] |\Phi_q\rangle = -(P_i^{21})_{\mu\nu} \\ \langle \Phi_q | \left[ Q_i, \eta_\mu \eta_\nu \right] |\Phi_q\rangle &= -(Q_i^{21})^*_{\mu\nu}, \quad \langle \Phi_q | \left[ P_i, \eta_\mu \eta_\nu \right] |\Phi_q\rangle = -(P_i^{21})^*_{\mu\nu} \end{aligned} \tag{3.162}$$

which follow in a straightforward way from the definitions (3.113) and (3.118) of the operators $Q_i$ and $P_i$ and the fact that the matrices $Q_i^{21}$ and $P_i^{21}$ are antisymmetric. The first terms in Eqs. (3.161) thus yield

$$- \sum_{i,j=1}^{N} \left( a_{ij}\, (Q_i^{21})_{\mu\nu} + b_{ij}\, (P_i^{21})_{\mu\nu} \right) p_j$$

and its complex conjugate, respectively (note that the coefficients $a_{ij}$ and $b_{ij}$ are real numbers). As to the second terms in Eqs. (3.161), upon inserting the expression (3.159) of $L$, they can be expressed as

$$\begin{cases} \frac{1}{2} \sum_{\lambda\sigma} \Big( \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu^\dagger \eta_\nu^\dagger \right], \eta_\lambda \eta_\sigma \right] |\Phi_q\rangle K_{\lambda\sigma} \\ \qquad + \langle \Phi_q | \Big[ \left[ \mathcal{H}(q), \eta_\mu^\dagger \eta_\nu^\dagger \right], \eta_\lambda^\dagger \eta_\sigma^\dagger \Big] |\Phi_q\rangle K^*_{\lambda\sigma} \Big) = 0 \\ \frac{1}{2} \sum_{\lambda\sigma} \Big( \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu \eta_\nu \right], \eta_\lambda \eta_\sigma \right] |\Phi_q\rangle K_{\lambda\sigma} \\ \qquad + \langle \Phi_q | \Big[ \left[ \mathcal{H}(q), \eta_\mu \eta_\nu \right], \eta_\lambda^\dagger \eta_\sigma^\dagger \Big] |\Phi_q\rangle K^*_{\lambda\sigma} \Big) = 0 \end{cases}$$

that is, using the expressions (1.50) of the submatrices $W$ and $Z$ entering the matrix $M(q)$ associated with the stability of the Routhian $\mathcal{H}(q)$ (see. Section 2.3),

$$\begin{cases} 2 \sum_{\lambda\sigma} \Big( W_{(\mu\nu),(\lambda\sigma)} K_{\lambda\sigma} + Z_{(\mu\nu),(\lambda\sigma)} K^*_{\lambda\sigma} \Big) = 0 \\ 2 \sum_{\lambda\sigma} \Big( Z^*_{(\mu\nu),(\lambda\sigma)} K_{\lambda\sigma} + W^*_{(\mu\nu),(\lambda\sigma)} K^*_{\lambda\sigma} \Big) = 0 \end{cases}$$

Consequently, introducing the matrix $M(q) = \begin{pmatrix} W & Z \\ Z^* & W^* \end{pmatrix}$ as in (1.52), the two equations (3.161) can be written in the matrix form

$$2M(q)\begin{pmatrix} K \\ K^* \end{pmatrix} = \sum_{i,j=1}^{N}\left[a_{ij}\begin{pmatrix} Q_i^{21} \\ Q_i^{21^*} \end{pmatrix} + b_{ij}\begin{pmatrix} P_i^{21} \\ P_i^{21^*} \end{pmatrix}\right] p_j$$

where, as usual, the matrices $K$, $Q_i^{21}$ and $P_i^{21}$ are column vectors of elements $K_{\mu\nu}$, $(Q_i^{21})_{\mu\nu}$ and $(P_i^{21})_{\mu\nu}$, respectively. This equation therefore gives the matrix elements $K_{\mu\nu}$ entering the operator $L$ in the form

$$\begin{pmatrix} K \\ K^* \end{pmatrix} = \frac{1}{2}M^{-1}(q)\sum_{i,j=1}^{N}\left[a_{ij}\begin{pmatrix} Q_i^{21} \\ Q_i^{21^*} \end{pmatrix} + b_{ij}\begin{pmatrix} P_i^{21} \\ P_i^{21^*} \end{pmatrix}\right] p_j \tag{3.163}$$

There remains to find the coefficients $a_{ij}$ and $b_{ij}$ that is, the variations of the Lagrange multipliers $\lambda_i$ and $\mu_i$ under the influence of the imposed collective momenta $p_i$. These variations of course follow from the constraint conditions (3.156). Expressing the state $|\Phi_{qp}\rangle$ as in (3.158) these conditions give, up to first order in $L$,

$$\begin{cases} \langle\Phi_q|e^{-L}Q_i e^L|\Phi_q\rangle \sim \langle\Phi_q|Q_i|\Phi_q\rangle + \langle\Phi_q|\,[Q_i, L]\,|\Phi_q\rangle = q_i \\ \langle\Phi_q|e^{-L}P_i e^L|\Phi_q\rangle \sim \langle\Phi_q|P_i|\Phi_q\rangle + \langle\Phi_q|\,[P_i, L]\,|\Phi_q\rangle = p_i \end{cases}$$

for $i = 1, \ldots, N$. Since $|\Phi_q\rangle$ is a static HFB state such that $\langle\Phi_q|Q_i|\Phi_q\rangle = q_i$, $\langle\Phi_q|P_i|\Phi_q\rangle = 0$, the above two conditions become

$$\langle\Phi_q|\,[Q_i, L]\,|\Phi_q\rangle = 0, \qquad \langle\Phi_q|\,[P_i, L]\,|\Phi_q\rangle = p_i, \qquad i = 1, \ldots, N \tag{3.164}$$

Inserting the form (3.159) of $L$ and using the commutation relations (3.162), these conditions yield

$$\begin{cases} -\dfrac{1}{2}\displaystyle\sum_{\mu\nu}\left((Q_i^{21})^*_{\mu\nu}K_{\mu\nu} + (Q_i^{21})_{\mu\nu}K^*_{\mu\nu}\right) = 0 \\ -\dfrac{1}{2}\displaystyle\sum_{\mu\nu}\left((P_i^{21})^*_{\mu\nu}K_{\mu\nu} + (P_i^{21})_{\mu\nu}K^*_{\mu\nu}\right) = p_i \end{cases}$$

that is, in matrix form,

$$\begin{cases} \begin{pmatrix} Q_i^{21^\dagger} & Q_i^{21^T} \end{pmatrix}\begin{pmatrix} K \\ K^* \end{pmatrix} = 0 \\ \begin{pmatrix} P_i^{21^\dagger} & P_i^{21^T} \end{pmatrix}\begin{pmatrix} K \\ K^* \end{pmatrix} = -2p_i \end{cases}$$

By using the expression (3.163) of $\begin{pmatrix} K \\ K^* \end{pmatrix}$ we thus obtain two equations

$$\begin{cases} \sum_{j,k=1}^{N} \left( \left[T_{(-1)}\right]_{i,j} a_{jk} + \left[T^{QP}_{(-1)}\right]_{i,j} b_{jk} \right) p_k = 0 \\ \sum_{j,k=1}^{N} \left( \left[T^{PQ}_{(-1)}\right]_{i,j} a_{jk} + \left[T^{PP}_{(-1)}\right]_{i,j} b_{jk} \right) p_k = -2p_i \end{cases} \tag{3.165}$$

where we have used the definition (3.135) of $\left[T_{(-1)}\right]_{i,j}$ and introduced the new moments

$$\begin{aligned} \left[T^{QP}_{(-1)}\right]_{i,j} &= \frac{1}{2} \left( Q_i^{21^\dagger} \; Q_i^{21^T} \right) M^{-1}(q) \begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix} \\ \left[T^{PQ}_{(-1)}\right]_{i,j} &= \frac{1}{2} \left( P_i^{21^\dagger} \; P_i^{21^T} \right) M^{-1}(q) \begin{pmatrix} Q_j^{21} \\ Q_j^{21^*} \end{pmatrix} \\ \left[T^{PP}_{(-1)}\right]_{i,j} &= \frac{1}{2} \left( P_i^{21^\dagger} \; P_i^{21^T} \right) M^{-1}(q) \begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix} \end{aligned} \tag{3.166}$$

The quantities $a_{jk}$ and $b_{jk}$ are therefore the solutions of the linear system (3.165). Fortunately, this linear system considerably simplifies since the "mixed" moment matrices $T^{QP}_{(-1)}$ and $T^{PQ}_{(-1)}$ vanish. In order to prove this, let us remark that, since $|\Phi_q\rangle$ is a static HFB state, we have $\langle \Phi_q | P_i | \Phi_q \rangle = 0$. This relation is also true at the neighboring deformation $q + \delta q_j$ that is, $\langle \Phi_{q+\delta q_j} | P_i | \Phi_{q+\delta q_j} \rangle = 0$. Using the expression (3.118) of $P_i$, this condition reads

$$0 = \frac{1}{2} \sum_{\mu\nu} \left[ (P_i^{21})_{\mu\nu} \; \kappa_{\mu\nu}(q + \delta q_j) + (P_i^{21})^*_{\mu\nu} \; \kappa^*_{\mu\nu}(q + \delta q_j) \right]$$

where $\kappa_{\mu\nu}(q + \delta q_j) = \langle \Phi_{q+\delta q_j} | \eta_\mu \eta_\nu | \Phi_{q+\delta q_j} \rangle$ is the pairing tensor associated with the state $|\Phi_{q+\delta q_j}\rangle$. Defining in the usual way the corresponding generalized density matrix as $R(q + \delta q_j) = \begin{pmatrix} \rho(q + \delta q_j) & -\kappa(q + \delta q_j) \\ \kappa^*(q + \delta q_j) & I - \rho^*(q + \delta q_j) \end{pmatrix}$, it is easy to see that the above expression can be written

$$0 = \frac{1}{2} \sum_{\mu\nu} \mathrm{Tr} \left[ (\mathcal{P}_i)_{\mu\nu} \, R_{\nu\mu}(q + \delta q_j) \right] \equiv \frac{1}{2} \mathrm{Tr} \left[ \mathcal{P}_i \, R(q + \delta q_j) \right]$$

where $\mathcal{P}_i = \begin{pmatrix} 0 & -P_i^{21^*} \\ P_i^{21} & 0 \end{pmatrix}$ is the supermatrix defined in (3.119). Now expanding the matrix $R(q + \delta q_j)$ up to first order in $\delta q_j$ as in (3.126), $R(q + \delta q_j) = R(q) + \begin{pmatrix} 0 & -R^{21^*} \\ R^{21} & 0 \end{pmatrix}$, the above equation gives

$$0 = \frac{1}{2}\mathrm{Tr}\left[\mathcal{P}_i\, R(q)\right] + \frac{1}{2}\mathrm{Tr}\left[\begin{pmatrix} 0 & -P_i^{21^*} \\ P_i^{21} & 0 \end{pmatrix}\begin{pmatrix} 0 & -R^{21^*} \\ R^{21} & 0 \end{pmatrix}\right]$$

The first term in the r.h.s. vanishes since it is equal to $\langle \Phi_q | P_i | \Phi_q \rangle = 0$ and we obtain

$$\begin{aligned} 0 =& \frac{1}{2}\sum_{\mu\nu}\left[\left(-P_i^{21}\right)^*_{\mu\nu} R^{21}_{\nu\mu} + \left(-P_i^{21}\right)_{\mu\nu} R^{21^*}_{\nu\mu}\right] \\ =& \frac{1}{2}\sum_{\mu\nu}\left[\left(P_i^{21}\right)^*_{\mu\nu} R^{21}_{\mu\nu} + \left(P_i^{21}\right)_{\mu\nu} R^{21^*}_{\mu\nu}\right] = \frac{1}{2}\begin{pmatrix} P_i^{21^\dagger} & P_i^{21^T} \end{pmatrix}\begin{pmatrix} R^{21} \\ R^{21^*} \end{pmatrix} \end{aligned}$$

where, in the matrix product on the right, the matrices $R^{21}$ and $P_i^{21}$ are column vectors of elements $R^{21}_{\mu\nu}$ and $(P_i^{21})_{\mu\nu}$, respectively. We now use the expression (3.127) of $\begin{pmatrix} R^{21} \\ R^{21^*} \end{pmatrix}$ that we derived in Section 4.2.2.1 together with the value (3.136) of $\partial\lambda_i(q)/\partial q_j$, that is

$$\begin{pmatrix} R^{21} \\ R^{21^*} \end{pmatrix} = \delta q_j \sum_{k=1}^{N}\left[T_{(-1)}\right]^{-1}_{k,j}\left[M(q)\right]^{-1}\begin{pmatrix} Q_k^{21} \\ Q_k^{21^*} \end{pmatrix}$$

With the definition of the matrix $T^{PQ}_{(-1)}$ given in Eq. (3.166), we thus obtain

$$0 = \frac{1}{2}\delta q_j \sum_{k=1}^{N}\left[T_{(-1)}\right]^{-1}_{k,j}\left[T^{PQ}_{(-1)}\right]_{i,k} = \frac{1}{2}\delta q_j\left[T^{PQ}_{(-1)}\left[T_{(-1)}\right]^{-1}\right]_{i,j}$$

As this relation should hold for any values of $i$ and $j$ and any $\delta q_j$, we find that the matrix $T^{PQ}_{(-1)}\left[T_{(-1)}\right]^{-1}$ must vanish. Therefore, by multiplying on the right by $T_{(-1)}$, we get $T^{PQ}_{(-1)} = 0$. Since from Eq. (3.166), $T^{QP}_{(-1)} = \left[T^{PQ}_{(-1)}\right]^\dagger$, this latter matrix also vanishes. In view of this result, the linear system (3.165) reduces to

$$\begin{cases} \displaystyle\sum_{j,k=1}^{N}\left[T_{(-1)}\right]_{i,j} a_{jk} p_k = 0 \\ \displaystyle\sum_{j,k=1}^{N}\left[T^{PP}_{(-1)}\right]_{i,j} b_{jk} p_k = -2p_i \end{cases}$$

Since this relations must hold for any value of $i$, we obtain, assuming that the matrices $T_{(-1)}$ and $T^{PP}_{(-1)}$ can be inverted

$$\begin{cases} \displaystyle\sum_{k=1}^{N} a_{jk} p_k \equiv \sum_{k=1}^{N} \left.\frac{\partial \lambda_j(q,p)}{\partial p_k}\right|_{p=0} p_k = 0 \\ \displaystyle\sum_{k=1}^{N} b_{jk} p_k \equiv \sum_{k=1}^{N} \left.\frac{\partial \mu_j(q,p)}{\partial p_k}\right|_{p=0} p_k = -2\sum_{i=1}^{N} \left[T^{PP}_{(-1)}\right]^{-1}_{j,i} p_i \end{cases} \tag{3.167}$$

that is, since only first order values of the $p_k$ have been considered,

$$\begin{cases} \lambda_j(q,p) = \lambda_j(q) \\ \displaystyle\mu_j(q,p) = -2\sum_{i=1}^{N} \left[T^{PP}_{(-1)}\right]^{-1}_{j,i} p_i \end{cases} \tag{3.168}$$

Consequently, adding constraints on small collective momenta in the HFB equations do not change, to first order, the values of the Lagrange multipliers $\lambda_i$ that impose the deformation parameters $q_i$, and the Lagrange multipliers $\mu_i$ that impose the deformation momenta $p_i$ are linear combinations of the $p_i$.

Inserting the results (3.167) in Eq. (3.163), the expression of the matrix $K$ entering the "velocity" transformation $e^L$ that defines the state $|\Phi_{qp}\rangle$ becomes

$$\begin{pmatrix} K \\ K^* \end{pmatrix} = -\sum_{i,j=1}^{N} \left[T^{PP}_{(-1)}\right]^{-1}_{i,j} p_j M^{-1}(q) \begin{pmatrix} P_i^{21} \\ P_i^{21^*} \end{pmatrix} \tag{3.169}$$

In order tho find the collective inertia, we now calculate the total HFB energy $E(q,p) \equiv \langle\Phi_{qp}|H|\Phi_{qp}\rangle$ of the nucleus when the small collective momenta $p_i$ are present. In order to make the QRPA matrix $M(q)$ appear in the result, we will first replace the Hamiltonian $H$ with the Routhian $\mathcal{H}(q) = H + \sum_{i=1}^{N} \lambda_i Q_i$ defined in (3.122). Then, expressing the state $|\Phi_{qp}\rangle$ as in Eq. (3.158), we have successively

$$\begin{aligned} E(q,p) =& \langle\Phi_{qp}|\mathcal{H}(q) - \sum_{i=1}^{N} \lambda_i Q_i |\Phi_{qp}\rangle = \langle\Phi_q|e^{-L}\mathcal{H}(q)e^{L}|\Phi_q\rangle - \sum_{i=1}^{N} \lambda_i q_i \\ =& \langle\Phi_q|\mathcal{H}(q)|\Phi_q\rangle - \sum_{i=1}^{N} \lambda_i q_i + \langle\Phi_q| \left[\mathcal{H}(q), L\right] |\Phi_q\rangle \\ &+ \frac{1}{2}\langle\Phi_q| \left[\left[\mathcal{H}(q), L\right], L\right] |\Phi_q\rangle + \ldots \\ =& E(q,0) + \langle\Phi_q| \left[\mathcal{H}(q), L\right] |\Phi_q\rangle + \frac{1}{2}\langle\Phi_q| \left[\left[\mathcal{H}(q), L\right], L\right] |\Phi_q\rangle + \ldots \end{aligned}$$

The term of first order in $L$ vanishes because of the HFB condition mentioned previously, i.e. $\langle\Phi_q| \left[\mathcal{H}(q), S\right] |\Phi_q\rangle = 0$ for any one-body operator $S$. The second order term can be calculated by using the expression (3.159) of the operator $L$ and the expressions (1.50) of the submatrices $W$ and $Z$

defining the matrix $M(q) = \begin{pmatrix} W & Z \\ Z^* & W^* \end{pmatrix}$ associated with the stability of the Routhian $\mathcal{H}(q)$ (see. Section 2.3). We thus obtain up to second order in $L$

$$
\begin{aligned}
E(q,p) = E(q,0) + \frac{1}{8} \sum_{\mu\nu\lambda\sigma} \Big\{ & K_{\mu\nu} \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu \eta_\nu \right], \eta_\lambda \eta_\sigma \right] | \Phi_q \rangle K_{\lambda\sigma} \\
& + K_{\mu\nu} \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu \eta_\nu \right], \eta_\lambda^\dagger \eta_\sigma^\dagger \right] | \Phi_q \rangle K^*_{\lambda\sigma} \\
& + K^*_{\mu\nu} \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu^\dagger \eta_\nu^\dagger \right], \eta_\lambda \eta_\sigma \right] | \Phi_q \rangle K_{\lambda\sigma} \\
& + K^*_{\mu\nu} \langle \Phi_q | \left[ \left[ \mathcal{H}(q), \eta_\mu^\dagger \eta_\nu^\dagger \right], \eta_\lambda^\dagger \eta_\sigma^\dagger \right] | \Phi_q \rangle K^*_{\lambda\sigma} \Big\} \\
= E(q,0) + \frac{1}{2} \sum_{\mu\nu\lambda\sigma} \Big\{ & K_{\mu\nu} Z^*_{(\mu\nu),(\lambda\sigma)} K_{\lambda\sigma} + K_{\mu\nu} W^*_{(\mu\nu),(\lambda\sigma)} K^*_{\lambda\sigma} \\
& + K^*_{\mu\nu} W_{(\mu\nu),(\lambda\sigma)} K_{\lambda\sigma} + K^*_{\mu\nu} Z_{(\mu\nu),(\lambda\sigma)} K^*_{\lambda\sigma} \Big\}
\end{aligned}
$$

In matrix form, considering the matrices and $K$ and $K^*$ as column vectors of elements $K_{\mu\nu}$ and $K^*_{\mu\nu}$, this equation can be written

$$
E(q,p) = E(q,0) + \frac{1}{2} \left( K^\dagger \; K^T \right) M(q) \begin{pmatrix} K \\ K^* \end{pmatrix}
$$

Finally, inserting the expression (3.169) of the column matrix $\begin{pmatrix} K \\ K^* \end{pmatrix}$ into this equation, we get

$$
E(q,p) = E(q,0) + \sum_{jk} \left[ T^{PP}_{(-1)} \right]^{-1}_{j,k} p_j p_k
$$

where we have made use of the definition of the matrix $T^{PP}_{(-1)}$ given in (3.166). From the ATDHFB semi-classical expression

$$
E(q,p) = E(q,0) + \frac{1}{2} \sum_{jk} \left[ \mathcal{M}_{\mathrm{ATDHFB}} \right]^{-1}_{jk} p_j p_k \tag{3.170}
$$

we then deduce

$$
\left[ \mathcal{M}_{\mathrm{ATDHFB}} \right]_{jk} = \frac{1}{2} \left[ T^{PP}_{(-1)} \right]_{jk} \equiv \frac{1}{4} \left( P_j^{21^\dagger} \; P_j^{21^T} \right) M^{-1}(q) \begin{pmatrix} P_k^{21} \\ P_k^{21^*} \end{pmatrix} \tag{3.171}
$$

It is usual to express this mass tensor in terms of moments of the QRPA matrix between matrix elements of the constraining operators $Q_i$ rather than between those of the displacement operators $P_i$. To this aim we insert the expression (3.137) of $\begin{pmatrix} P_j^{21} \\ P_j^{21^*} \end{pmatrix}$ into the definition of $\left[ T^{PP}_{(-1)} \right]_{i,j}$ given in Eq.

(3.166). We obtain

$$\left[T^{PP}_{(-1)}\right]_{i,j} = \hbar^2 \sum_{mn=1}^{N} \left[T_{(-1)}\right]^{-1}_{i,m} \left[\widetilde{T}_{(-3)}\right]_{m,n} \left[T_{(-1)}\right]^{-1}_{n,j}$$

where we have defined a modified QRPA moment of order $(-3)$ containing $\tau$ matrices as the moment $\left[\widetilde{T}_{(-1)}\right]_{m,n}$ defined previously (see Eq. (3.152)):

$$\left[\widetilde{T}_{(-3)}\right]_{m,n} = \frac{1}{2} \begin{pmatrix} Q^{21^\dagger}_m & Q^{21^T}_m \end{pmatrix} M^{-1}(q)\tau M^{-1}(q)\tau M^{-1}(q) \begin{pmatrix} Q^{21}_n \\ Q^{21^*}_n \end{pmatrix} \tag{3.172}$$

We thus obtain the following usual expression of the ATDHF mass tensor as

$$\mathcal{M}_{\mathrm{ATDHFB}}(q) = \frac{\hbar^2}{2} \left[T_{(-1)}\right]^{-1} \widetilde{T}_{(-3)} \left[T_{(-1)}\right]^{-1} \tag{3.173}$$

We observe that the expression of this mass tensor is quite different from the one of the GCM mass tensor given in Eq. (3.154).

To end this section, let us note that the relationship (3.168) between the Lagrange multipliers $\mu_i$ and the momenta $p_i$ given by Eq. (3.168) can be rewritten using Eq. (3.171),

$$\mu_i(q,p) = -\sum_{j=1}^{N} \left[\mathcal{M}_{\mathrm{ATDHFB}}\right]^{-1}_{i,j} p_j$$

and that this relation is consistent with the usual expression derived in Lagrange multiplier theory [9] (with a plus sign before the Lagrange multipliers)

$$\mu_i = -\frac{\partial E(q,p)}{\partial p_i}$$

These equations show that the Lagrange multipliers $\mu_i$ can be interpreted as the opposite of collective velocities.

#### 3.2.2.5 The so-called "cranking" approximation

As mentioned in the introduction of Section 4.2.2, the "cranking" approximation[3] consists of neglecting in the QRPA matrix $M(q)$ the residual interaction responsible for the rearrangement of the HFB fields. With this approxima-

[3] The denomination "cranking" comes from a model proposed by Inglis to describe rotations in deformed nuclei, the cranking model [63, 57], which gives for the nuclear moment an expression of the same form as the one of the ATDHF collective inertia when the "cranking" approximation is used.

tion, the elements of the submatrices $W$ and $Z$ given in Section 2.3 then reduce to

$$W_{(\mu\nu),(\lambda\sigma)} = (\varepsilon_\mu + \varepsilon_\nu)\delta_{\mu,\lambda}\delta_{\nu,\sigma}$$
$$Z_{(\mu\nu),(\lambda\sigma)} = 0$$

where the $\varepsilon_\mu$ are the quasiparticle energies associated with the HFB state $|\Phi_q\rangle$, and the matrix $M(q)$ becomes diagonal

$$[M(q)]_{(\mu\nu),(\lambda\sigma)} = \delta_{\mu,\lambda}\delta_{\nu,\sigma} \begin{pmatrix} \varepsilon_\mu + \varepsilon_\nu & 0 \\ 0 & \varepsilon_\mu + \varepsilon_\nu \end{pmatrix} \tag{3.174}$$

Therefore, it can be inverted in a trivial way. As a consequence, the moments of the QRPA matrix defined in Eqs. (3.135), (3.152) and (3.172) take the much simpler forms

$$\left[T^{\mathrm{CR}}_{(-\alpha)}\right]_{l,m} = \frac{1}{2}\sum_{\mu\nu} \frac{\left(Q^{21}_l\right)^*_{\mu\nu}\left(Q^{21}_m\right)_{\mu\nu} + \left(Q^{21}_l\right)_{\mu\nu}\left(Q^{21}_m\right)^*_{\mu\nu}}{(\varepsilon_\mu + \varepsilon_\nu)\alpha}$$
$$\left[\widetilde{T}^{\mathrm{CR}}_{(-1)}\right]_{l,m} = \left[T^{\mathrm{CR}}_{(-1)}\right]_{l,m}$$
$$\left[\widetilde{T}^{\mathrm{CR}}_{(-3)}\right]_{l,m} = \left[T^{\mathrm{CR}}_{(-3)}\right]_{l,m}$$

where the superscript "CR" means "cranking". The last two relations follow from the facts that the now diagonal matrices $M(q)$ and $M^{-1}(q)$ commute with the matrix $\tau = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ and that $\tau^2$ is equal to the identity matrix. The expressions of the GCM and ATDHFB mass tensors given by Eqs. (3.154) and (3.173) thus become

$$\begin{aligned} \mathcal{M}^{\mathrm{CR}}_{\mathrm{GCM}}(q) &= \frac{\hbar^2}{2}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} T^{\mathrm{CR}}_{(-2)}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} T^{\mathrm{CR}}_{(-2)}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} \\ \mathcal{M}^{\mathrm{CR}}_{\mathrm{ATDHFB}}(q) &= \frac{\hbar^2}{2}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} T^{\mathrm{CR}}_{(-3)}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} \end{aligned} \tag{3.175}$$

and the expression (3.141) of the matrix $[g]$ of Gaussian overlap parameters is formally unchanged:

$$[g]^{\mathrm{CR}} = \frac{1}{2}\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1}\left[T^{\mathrm{CR}}_{(-2)}\right]\left[T^{\mathrm{CR}}_{(-1)}\right]^{-1} \tag{3.176}$$

According to some authors the collective masses (either GCM or ATDHF) calculated with the "cranking" approximation are too small [49, 64]. However, other authors, relying on tests calculations using solvable models, claim that "cranking" masses do deviate from full ATDHF ones but offer in most cases rather acceptable values [65, 16].

The most thorough comparisons between the different expressions of the nuclear inertia are those made in the case of collective rotations. The equivalent for rotations of the ATDHFB mass is the Thouless-Valatin moment of inertia [66] and the corresponding "cranking" approximation is given by the Inglis-Belyaev moment of inertia [57, 58]. For rotations about the $x$ axis, the Thouless-Valatin moment of inertia $\mathcal{I}_x^{\mathrm{TV}}$ is obtained from the ATDHFB formula (3.171) by replacing both displacement operators $P_j$ and $P_k$ by the angular momentum component $J_x$, and the corresponding Inglis-Belyaev moment of inertia $\mathcal{I}_x^{\mathrm{IB}}$ by further replacing the QRPA matrix $M(q)$ by its diagonal form (3.174). In fact, in all studies, the Thouless-Valatin moment of inertia is not calculated from the standard formula – which is too difficult – but derived numerically from HFB calculations in a rotating frame (also called "Cranked HFB calculations") where time-reversal symmetry is broken [67, 68, 69, 70, 71, 72]. It is then found that the moment of inertia $\mathcal{I}_x^{\mathrm{IB}}$ calculated with the "cranking approximation" is too small by a factor ranging from 1.2 to 1.4 [49, 29, 73]. One may then expect that the "cranking" approximation introduces discrepancies of this order of magnitude in the ATDHFB inertia mass tensor for collective deformations .

In view of this, attempts have been made to go beyond the "cranking" approximation in the calculation of the ATDHFB inertia mass tensor. In Ref. [64], effects coming from the static rearrangement of the average and pairing fields have been included. As a result, large increases in the values of the "cranking" masses for quadrupole deformations were found. However, effects coming from the time-odd components of these fields were not taken into account and one may wonder if including them would not smooth out the large oscillations which were found without them. In Ref. [30] a method of calculating the ATDHFB inertia tensor (or the Thouless-Valatin moment of inertia) via the inversion of the full QRPA matrix $M(q)$ has been proposed. This method is based on the fact that the interaction terms entering the QRPA matrix $M(q)$ are usually much smaller than the diagonal part which is taken into account in the "cranking" approximation. It is then shown that the inverse matrix $M^{-1}(q)$ can be expressed as a fast-converging perturbative expansion that allows one to introduce step by step all the time-odd rearrangement terms of the nuclear fields on top of the "cranking" expression. This kind of technique in the calculation of the inertia would undoubtedly be needed in the case of fission and will certainly be the subject of further investigations in the future.

To end this Section, let us remark that the nuclear collective inertia strongly depends on the magnitude of pairing correlations. Actually, the variations obtained by changing the intensity of pairing or the way pairing correlations are treated, e.g. using the BCS formalism instead of the HFB theory, may be larger than those resulting from the approximations adopted for their calculation. In a sense, ensuring that pairing is calculated as accurately as possible may be more important than the type of formula used to calculate the nuclear collective inertia.

## 3.3 The Schrödinger Collective Intrinsic Model

### 3.3.1 General formalism

In this section we discuss a generalization of the GCM that incorporates the coupling between collective and single-particle degrees of freedom known as the Schrödinger Collective Intrinsic Model (SCIM). This approach was introduced in [20], with prior efforts to describe the collective-intrinsic coupling dating back to the 1970's [21, 22, 23]. The derivation of the SCIM relies on the symmetric moment expansion method [24, 25]. We start from the symmetrized Hill-Wheeler equation in one dimension,

$$\int ds\, e^{is\hat{P}/2} \left[H\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right) - EN\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right)\right] e^{is\hat{P}/2} f\left(\bar{q}\right) = 0 \tag{3.177}$$

with

$$\hat{P} = i\frac{\partial}{\partial \bar{q}}$$

as in Eq. ((3.83)), but where we have set $\hbar = 1$ for convenience. We write for an arbitrary operator $\hat{O}\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right)$

$$\begin{aligned}\int ds\, e^{is\hat{P}/2} \hat{O}\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right) e^{is\hat{P}/2} = &\sum_{n=0}^{\infty} \frac{1}{2^n n!} \sum_{k=0}^{n} \binom{n}{k} \left(\frac{is}{2}\hat{P}\right)^{n-k} \\ &\times \left[i^n \int ds\, s^n \hat{O}\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right)\right] \left(\frac{is}{2}\hat{P}\right)^{k}\end{aligned} \tag{3.178}$$

We now introduce the more compact notation in Eq. (5) of [20]

$$\hat{O}^{(n)}\left(\bar{q}\right) \equiv i^n \int_{-\infty}^{+\infty} ds\, s^n \hat{O}\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right) \tag{3.179}$$

and the notation of Eq. (6) in [20] for Symmetric Ordered Products of Operators (SOPO),

$$\left[\hat{O}^{(n)}\left(\bar{q}\right)\hat{P}\right]^{(n)} \equiv \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} \hat{P}^{n-k} \hat{O}^{(n)}\left(\bar{q}\right) \hat{P}^{k} \tag{3.180}$$

With this new notation, Eq. (3.177) becomes

$$\sum_{n=0}^{\infty} \frac{1}{n!} \left\{ \left[H^{(n)}\left(\bar{q}\right)\hat{P}\right]^{(n)} - E\left[N^{(n)}\left(\bar{q}\right)\hat{P}\right]^{(n)} \right\} f\left(\bar{q}\right) = 0 \tag{3.181}$$

Note that the definition in Eq. (3.180) involves derivatives (i.e. instances of $\hat{P}$) of all orders up to and including $n$. To obtain a local Schrödinger-like equation from Eq. (3.181) we need to invert the overlap kernel,

$$\hat{N}(\bar{q}) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[ N^{(n)}(\bar{q}) \hat{P} \right]^{(n)} \tag{3.182}$$

We therefore define $\hat{N}^{1/2}(\bar{q})$ through[4]

$$\hat{N}(\bar{q}) = \left[ \hat{N}^{1/2}(\bar{q}) \right]^{\dagger} \hat{N}^{1/2}(\bar{q}) \tag{3.183}$$

and introduce the collective wave functions $g(\bar{q})$ where

$$g(\bar{q}) = \hat{N}^{1/2}(\bar{q}) f(\bar{q}) \tag{3.184}$$

We assume that we can also define the inverse operator $\hat{N}^{-1/2}(\bar{q})$. Then Eq. (3.181) takes the form

$$\left\{ \left[ \hat{N}^{-1/2}(\bar{q}) \right]^{\dagger} \sum_{n=0}^{\infty} \frac{1}{n!} \left[ H^{(n)}(\bar{q}) \hat{P} \right]^{(n)} \hat{N}^{-1/2}(\bar{q}) - E \right\} g(\bar{q}) = 0 \tag{3.185}$$

We now take a closer look at the overlap kernel and the operators derived from it. It is useful to write Eq. (3.182) as

$$\begin{aligned} \hat{N}(\bar{q}) &= N^{(0)}(\bar{q}) + \sum_{n=1}^{\infty} \frac{1}{n!} \left[ N^{(n)}(\bar{q}) \hat{P} \right]^{(n)} \\ &= \sqrt{N^{(0)}(\bar{q})} \left\{ I + \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \sum_{n=1}^{\infty} \frac{1}{n!} \left[ N^{(n)}(\bar{q}) \hat{P} \right]^{(n)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \right\} \sqrt{N^{(0)}(\bar{q})} \end{aligned} \tag{3.186}$$

where, in the case of a single degree of freedom, $N^{(0)}(\bar{q})$ is a c-number given by Eq. (3.179). When we consider additional collective and intrinsic degrees of freedom $N^{(0)}(\bar{q})$ will become a matrix. We define

$$\hat{u}(\bar{q}) \equiv \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \sum_{n=1}^{\infty} \frac{1}{n!} \left[ N^{(n)}(\bar{q}) \hat{P} \right]^{(n)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \tag{3.187}$$

and

$$\hat{J}(\bar{q}) \equiv I + \hat{u}(\bar{q}) \tag{3.188}$$

In analogy with Eq. (3.183) we write

$$\hat{J}(\bar{q}) = \left[ \hat{J}^{1/2}(\bar{q}) \right]^{\dagger} \hat{J}^{1/2}(\bar{q}) \tag{3.189}$$

[4] as noted in [20], this is not a proper square root since we take the adjoint on the left.

and make the identifications that follow from Eqs. (3.183) and (3.186),

$$\hat{N}^{1/2}(\bar{q}) = \hat{J}^{1/2}(\bar{q})\sqrt{N^{(0)}(\bar{q})} \tag{3.190}$$

$$\left[\hat{N}^{1/2}(\bar{q})\right]^{\dagger} = \sqrt{N^{(0)}(\bar{q})}\left[\hat{J}^{1/2}(\bar{q})\right]^{\dagger} \tag{3.191}$$

and assume that we can construct the inverse operator

$$\hat{J}_{-1/2}(\bar{q}) \equiv \hat{J}^{-1/2}(\bar{q})$$

which allows us to invert Eq. ((3.190)),

$$\hat{N}^{-1/2}(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\hat{J}_{-1/2}(\bar{q}) \tag{3.192}$$

and Eq. ((3.191)),

$$\left[\hat{N}^{-1/2}(\bar{q})\right]^{\dagger} = \left[\hat{J}_{-1/2}(\bar{q})\right]^{\dagger}\frac{1}{\sqrt{N^{(0)}(\bar{q})}} \tag{3.193}$$

In particular, thanks to Eqs. (3.188) and (3.189) we have

$$\left[\hat{J}_{-1/2}(\bar{q})\right]^{\dagger}\left[I + \hat{u}(\bar{q})\right]\hat{J}_{-1/2}(\bar{q}) = I \tag{3.194}$$

This is the basic identity we will use to determine $\hat{J}_{-1/2}(\bar{q})$. In principle, if we can solve Eq. (3.194) and get $\hat{J}_{-1/2}(\bar{q})$, we can then insert Eqs. ((3.192)) and ((3.193)) into Eq. (3.185) which becomes

$$\{\mathscr{H}(\bar{q}) - E\}\, g(\bar{q}) = 0 \tag{3.195}$$

where

$$\begin{aligned}\mathscr{H}(\bar{q}) &\equiv \left[\hat{N}^{-1/2}(\bar{q})\right]^{\dagger}\sum_{n=0}^{\infty}\frac{1}{n!}\left[H^{(n)}(\bar{q})\,\hat{P}\right]^{(n)}\hat{N}^{-1/2}(\bar{q}) \\ &= \left[\hat{J}_{-1/2}(\bar{q})\right]^{\dagger}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\sum_{n=0}^{\infty}\frac{1}{n!}\left[H^{(n)}(\bar{q})\,\hat{P}\right]^{(n)}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\hat{J}_{-1/2}(\bar{q})\end{aligned} \tag{3.196}$$

Since it is shown in [20] that symmetric ordered products of operators are Hermitian, it is clear that $\mathscr{H}(\bar{q})$ is also Hermitian. In practice, we will truncate the series in Eqs. (3.194) and (3.195) at $n = 2$. In the next sections, we will derive an explicit expression for $\hat{J}_{-1/2}(\bar{q})$ in order to calculate $\mathscr{H}(\bar{q})$ in Eq. (3.196). The algebra needed to work with SOPO's can be found in the appendices of [20] and in appendix (E) of this book.

### 3.3.2 Calculation of $\hat{J}_{-1/2}(\bar{q})$ in the one-dimensional case

For illustration purposes, we consider first the one-dimensional case, where $N^{(n)}(\bar{q})$ can be expressed as a c-number rather than a matrix. We will extend the results presented here to the multi-dimensional case in section (3.3.3.1).

#### 3.3.2.1 Series expansion for $\hat{J}(\bar{q})$

We return to the definition of $J$ in Eq. (3.188), which to second order in the SOPO gives

$$\begin{aligned}\hat{J}(\bar{q}) &= 1 + \hat{u}(\bar{q}) \\ &= 1 + \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \frac{1}{2} \left[ N^{(2)}(\bar{q}) \hat{P} \right]^{(2)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\end{aligned}$$

Note that in the one-dimensional case the $n = 1$ term in Eq. ((3.187)) vanishes (see, e.g., appendix C.1 in [20]). Using Eq. (A6) in [20], this can be written as (here as well the $C^{(1)}$ coefficient vanishes in the one-dimensional case)

$$\begin{aligned}\hat{J}(\bar{q}) &= 1 - \frac{1}{2} C^{(2)} \left( N^{(2)}(\bar{q}), N^{(0)}(\bar{q}) \right) + \frac{1}{2} \left[ \bar{N}^{(2)}(\bar{q}) \hat{P} \right]^{(2)} \\ &\equiv 1 + \alpha_{(0)}(\bar{q}) + \frac{1}{2} \left[ \bar{N}^{(2)}(\bar{q}) \hat{P} \right]^{(2)}\end{aligned}$$

with

$$\alpha_{(0)}(\bar{q}) \equiv -\frac{1}{2} C^{(2)} \left( N^{(2)}(\bar{q}), N^{(0)}(\bar{q}) \right)$$

and

$$\begin{aligned}C^{(2)} \left( N^{(2)}, N^{(0)} \right) \equiv \frac{1}{4} \Bigg[ &\left( \frac{1}{\sqrt{N^{(0)}}} \right)'' N^{(2)} \frac{1}{\sqrt{N^{(0)}}} + 2 \left( \frac{1}{\sqrt{N^{(0)}}} \right)' N^{(2)} \left( \frac{1}{\sqrt{N^{(0)}}} \right)' \\ &+ \frac{1}{\sqrt{N^{(0)}}} N^{(2)} \left( \frac{1}{\sqrt{N^{(0)}}} \right)'' \Bigg]\end{aligned}$$

and

$$\bar{N}^{(2)} \equiv \frac{1}{\sqrt{N^{(0)}}} N^{(2)} \frac{1}{\sqrt{N^{(0)}}}$$

If $\alpha_{(0)}(\bar{q})$ is small compared to 1, we will neglect it. Otherwise we write

$$\hat{J}(\bar{q}) = \sqrt{1+\alpha_{(0)}(\bar{q})}\left\{1+\frac{1}{\sqrt{1+\alpha_{(0)}(\bar{q})}}\frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\hat{P}\right]^{(2)}\frac{1}{\sqrt{1+\alpha_{(0)}(\bar{q})}}\right\}\sqrt{1+\alpha_{(0)}(\bar{q})}$$

we define

$$A_{(0)}(\bar{q}) \equiv 1+\alpha_{(0)}(\bar{q})$$

and use Eq. (A6) in [20] again to write

$$\hat{J}(\bar{q}) = \sqrt{A_{(0)}(\bar{q})}\left\{1+\alpha_{(1)}(\bar{q})+\frac{1}{2}\left[\bar{\bar{N}}^{(2)}(\bar{q})\hat{P}\right]^{(2)}\right\}\sqrt{A_{(0)}(\bar{q})}$$

where

$$\alpha_{(1)}(\bar{q}) = -\frac{1}{2}C^{(2)}\left(N^{(2)}(\bar{q}), A_{(0)}(\bar{q})\right)$$

and

$$\bar{\bar{N}}^{(2)} = \frac{1}{\sqrt{A_{(0)}}}\bar{N}^{(2)}\frac{1}{\sqrt{A_{(0)}}}$$

In effect, we can write

$$\frac{1}{\sqrt{A_{(0)}(\bar{q})}}\hat{J}(\bar{q})\frac{1}{\sqrt{A_{(0)}(\bar{q})}} = 1+\alpha_{(1)}(\bar{q})+\frac{1}{2}\left[\bar{\bar{N}}^{(2)}(\bar{q})\hat{P}\right]^{(2)}$$

Then, in Eq. (3.189) we can substitute

$$\left[\hat{J}^{1/2}(\bar{q})\right]^{\dagger} \to \frac{1}{\sqrt{A_{(0)}(\bar{q})}}\left[\hat{J}^{1/2}(\bar{q})\right]^{\dagger}$$
$$\hat{J}^{1/2}(\bar{q}) \to \hat{J}^{1/2}(\bar{q})\frac{1}{\sqrt{A_{(0)}(\bar{q})}}$$

and in Eqs. (3.190) and (3.191) we see that the $1/\sqrt{A_{(0)}(\bar{q})}$ can simply be absorbed into the coefficients $\sqrt{N^{(0)}(\bar{q})}$ thereby renormalizing $N^{(0)}(\bar{q})$,

$$N^{(0)}(\bar{q}) \to \frac{N^{(0)}(\bar{q})}{A_{(0)}(\bar{q})}$$

At this point, if $\alpha_{(1)}(\bar{q})$ is small we neglect it, otherwise we iterate the process to obtain $\alpha_{(2)}(\bar{q})$ renormalizing $N^{(0)}(\bar{q})$ again. Eventually, we will be able to write to a good approximation an expression of the form

$$\hat{J}(\bar{q}) = 1+\frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\hat{P}\right]^{(2)}$$

which implies (Eq. (3.188))

$$\hat{u}\left(\bar{q}\right)=\frac{1}{2}\left[\bar{N}^{(2)}\left(\bar{q}\right)\hat{P}\right]^{(2)} \tag{3.197}$$

#### 3.3.2.2 Series expansion for $\hat{J}_{\pm 1/2}\left(\bar{q}\right)$

In fact the quantity we need in Eq. (3.196) is $\hat{J}_{-1/2}\left(\bar{q}\right)$ which satisfies the basic identity in Eq. (3.194), and with Eq. ((3.197)) this becomes

$$\left[\hat{J}_{-1/2}\left(\bar{q}\right)\right]^{\dagger}\left[1+\frac{1}{2}\left[\bar{N}^{(2)}\left(\bar{q}\right)\hat{P}\right]^{(2)}\right]\hat{J}_{-1/2}\left(\bar{q}\right)=1 \tag{3.198}$$

Solving this problem is a non-trivial exercise. We will assume a solution of the form [20, 9]

$$\hat{J}_{-1/2}\left(\bar{q}\right)=A_{-1/2}\left(\bar{q}\right)+\left[B_{-1/2}\left(\bar{q}\right)\hat{P}\right]^{(2)}+\left[C_{-1/2}\left(\bar{q}\right)\hat{P}\right]^{(4)} \tag{3.199}$$

but inserting Eq. (3.199) into Eq. (3.198) still leads to very cumbersome formulas. To simplify the problem further, we will include only up to the first derivative of $\bar{N}^{(2)}\left(\bar{q}\right)$. We begin by investigating the operators

$$\hat{J}_{A,1/2}\left(\bar{q}\right)\equiv 1+\frac{1}{2}\hat{u}\left(\bar{q}\right)-\frac{1}{8}\hat{u}^{2}\left(\bar{q}\right)\approx\sqrt{1+\hat{u}\left(\bar{q}\right)} \tag{3.200}$$

and

$$\hat{J}_{A,-1/2}\left(\bar{q}\right)\equiv 1-\frac{1}{2}\hat{u}\left(\bar{q}\right)+\frac{3}{8}\hat{u}^{2}\left(\bar{q}\right)\approx\frac{1}{\sqrt{1+\hat{u}\left(\bar{q}\right)}} \tag{3.201}$$

as approximate expansions for $\hat{J}_{1/2}$ and $\hat{J}_{-1/2}$. The first task is to show that Eq. (3.200) can be put in the form of Eq. (3.199). The results are given in appendix C2 of [20] with the appropriate coefficients given for $\hat{J}_{A,1/2}\left(\bar{q}\right)$ in Eq. (C5) and for $\hat{J}_{A,-1/2}\left(\bar{q}\right)$ in Eq. (C6).

To obtain these results, we insert Eq. (3.197) into Eq. (3.200) to write

$$\hat{J}_{A,1/2}\left(\bar{q}\right)=1+\frac{1}{4}\left[\bar{N}^{(2)}\left(\bar{q}\right)\hat{P}\right]^{(2)}-\frac{1}{32}\left[\bar{N}^{(2)}\left(\bar{q}\right)\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}\left(\bar{q}\right)\hat{P}\right]^{(2)}$$

Then we use Eq. (A3) in [20] (see also appendix (.1.4) in this book) to write

$$\begin{aligned}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} &= \sum_{i=0}^{4}\frac{1}{2^i}\sum_{s=\max(0,i-2)}^{\min(2,i)}\binom{2}{s}\binom{2}{i-s}(-1)^{i-s}\\ &\quad\times\left[\left[\hat{P}^{i-s}\bar{N}^{(2)}(\bar{q})\right]\left[\hat{P}^{s}\bar{N}^{(2)}(\bar{q})\right]\hat{P}\right]^{(4-i)}\\ &= \sum_{i=0}^{2}\frac{1}{2^i}\sum_{s=0}^{i}\binom{2}{s}\binom{2}{i-s}(-1)^{i-s}\\ &\quad\times\left[\left[\hat{P}^{i-s}\bar{N}^{(2)}(\bar{q})\right]\left[\hat{P}^{s}\bar{N}^{(2)}(\bar{q})\right]\hat{P}\right]^{(4-i)}\end{aligned}$$

Since we neglect derivatives of $\bar{N}^{(2)}(\bar{q})$ of order higher than 1 we only keep the indices $(i,s)=(0,0)$, $(1,0)$, $(1,1)$, $(2,1)$. Explicitly, this gives

$$\begin{aligned}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} &= \left[\bar{N}^{(2)}(\bar{q})\,\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(4)}\\ &\quad+\frac{1}{2}2\,(-1)\left[\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]\left[\bar{N}^{(2)}(\bar{q})\right]\hat{P}\right]^{(3)}\\ &\quad+\frac{1}{2}2\left[\left[\bar{N}^{(2)}(\bar{q})\right]\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]\hat{P}\right]^{(3)}\\ &\quad+\frac{1}{4}2\times2\,(-1)\left[\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]\hat{P}\right]^{(2)}\end{aligned}$$

or

$$\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} = -\left[\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(2)}+\left[\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)}$$

Next, we use the linear property of SOPO's to group terms

$$\hat{J}_{A,1/2}(\bar{q}) = 1+\left[\left(\frac{1}{4}\bar{N}^{(2)}(\bar{q})+\frac{1}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\right)\hat{P}\right]^{(2)}+\left[-\frac{1}{32}\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)}$$

which gives $\hat{J}_{A,1/2}(\bar{q})$ in the form of Eq. ((3.199)). Similarly, for $\hat{J}_{A,-1/2}(\bar{q})$ we can use the previous results to obtain

$$\begin{aligned}\hat{J}_{A,-1/2}(\bar{q}) &= 1-\frac{1}{4}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}+\frac{3}{32}\hat{u}^2(\bar{q})\\ &= 1+\left[\left(-\frac{1}{4}\bar{N}^{(2)}(\bar{q})-\frac{3}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\right)\hat{P}\right]^{(2)}+\left[\frac{3}{32}\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)}\end{aligned}$$

Note that, to fourth-order SOPO's we can write

$$
\begin{aligned}
\hat{J}_{A,-1/2}(\bar{q})\,\hat{J}_{A,1/2}(\bar{q}) &= \left\{A_{-1/2} + \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\right\} \\
&\quad \times \left\{A_{1/2} + \left[B_{1/2}\hat{P}\right]^{(2)} + \left[C_{1/2}\hat{P}\right]^{(4)}\right\} \\
&\approx A_{-1/2}A_{1/2} + \left[\left(B_{-1/2}A_{1/2} + A_{-1/2}B_{1/2}\right)\hat{P}\right]^{(2)} \\
&\quad + \left[B_{-1/2}\hat{P}\right]^{(2)}\left[B_{1/2}\hat{P}\right]^{(2)} \\
&\quad + \left[\left(C_{-1/2}A_{1/2} + A_{-1/2}C_{1/2}\right)\hat{P}\right]^{(4)}
\end{aligned}
$$

where we have used the fact that $A_{\pm 1/2}$ is a constant. In our case,[5]

$$
\begin{aligned}
B_{-1/2} &= -\frac{1}{4}\bar{N}^{(2)}(\bar{q}) - \frac{3}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2 \\
B_{1/2} &= \frac{1}{4}\bar{N}^{(2)}(\bar{q}) + \frac{1}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2
\end{aligned}
$$

and

$$
\begin{aligned}
C_{-1/2} &= \frac{3}{32}\left[\bar{N}^{(2)}(\bar{q})\right]^2 \\
C_{1/2} &= -\frac{1}{32}\left[\bar{N}^{(2)}(\bar{q})\right]^2
\end{aligned}
$$

then, keeping only up to first-order derivatives of $\bar{N}^{(2)}(\bar{q})$ we write

$$
\left[B_{-1/2}\hat{P}\right]^{(2)}\left[B_{1/2}\hat{P}\right]^{(2)} = \frac{1}{16}\left[\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(2)} - \frac{1}{16}\left[\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)}
$$

Thus, more explicitly, we have

$$
\begin{aligned}
\hat{J}_{A,-1/2}(\bar{q})\,\hat{J}_{A,1/2}(\bar{q}) &\approx 1 + \left[\left(-\frac{2}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\right)\hat{P}\right]^{(2)} \\
&\quad + \left(\frac{1}{16}\left[\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(2)} - \frac{1}{16}\left[\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)}\right) \\
&\quad + \left[\left(\frac{3}{32} - \frac{1}{32}\right)\left[\bar{N}^{(2)}(\bar{q})\right]^2\hat{P}\right]^{(4)} \\
&= 1
\end{aligned}
$$

as expected if $\hat{J}_{A,-1/2}(\bar{q})$ and $\hat{J}_{A,1/2}(\bar{q})$ are meant to approximate $\hat{J}_{-1/2}(\bar{q})$ and $\hat{J}_{1/2}(\bar{q})$, respectively.

[5] The difference in sign from Eq. (C5) in [20] for $B_{-1/2}(\bar{q})$ and $B_{1/2}(\bar{q})$ is due to the fact that we use $\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2$ instead of $\left[\bar{N}^{(2)\prime}(\bar{q})\right]^2$, and there is a minus sign from an $i^2$ factor that appears when $\hat{P}$ is written as a differential operator.

#### 3.3.2.3 Verification of the basic identity for $\hat{J}_{-1/2}(\bar{q})$ (part I)

Next, we must verify that $\hat{J}_{A,-1/2}(\bar{q})$ and $\hat{J}_{A,1/2}(\bar{q})$ satisfy Eq. (3.198). We first derive this result making some simplifying assumptions that we will lift in the next section. We write Eq. (3.198) as

$$\left\{1+\left[B_{-1/2}\hat{P}\right]^{(2)}+\left[C_{-1/2}\hat{P}\right]^{(4)}\right\}^{\dagger}\left[1+\frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\right]$$
$$\times\left\{1+\left[B_{-1/2}\hat{P}\right]^{(2)}+\left[C_{-1/2}\hat{P}\right]^{(4)}\right\}=1$$

Keeping only up to fourth-order SOPO's, the left-hand side of the equation reduces to

$$\mathrm{LHS}=\left\{1+\left[B_{-1/2}\hat{P}\right]^{(2)}+\left[C_{-1/2}\hat{P}\right]^{(4)}\right\}^{\dagger}\left\{1+\left[B_{-1/2}\hat{P}\right]^{(2)}+\left[C_{-1/2}\hat{P}\right]^{(4)}\right.$$
$$\left.+\frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}+\frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)}\right\}$$

We then write (using appendix (.1.4))

$$\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)}=-\left[\left[\hat{P}\bar{N}^{(2)}\right]\left[\hat{P}B_{-1/2}\right]\hat{P}\right]^{(2)}+\left[\bar{N}^{(2)}B_{-1/2}\hat{P}\right]^{(4)}$$

At this stage, we make a simplifying assumption and keep only the term in $\bar{N}^{(2)}(\bar{q})$ inside $B_{-1/2}$ in the fourth-order SOPOs,

$$\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)}=\frac{1}{4}\left[\left[\hat{P}\bar{N}^{(2)}\right]^{2}\hat{P}\right]^{(2)}-\frac{1}{4}\left[\left[\bar{N}^{(2)}\right]^{2}\hat{P}\right]^{(4)}$$

Thus we have

$$\mathrm{LHS}=\left\{1+\left[B_{-1/2}\hat{P}\right]^{(2)}+\left[C_{-1/2}\hat{P}\right]^{(4)}\right\}^{\dagger}$$
$$\times\left\{1+\left[\left(B_{-1/2}+\frac{1}{2}\bar{N}^{(2)}+\frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^{2}\right)\hat{P}\right]^{(2)}\right.$$
$$\left.+\left[\left(C_{-1/2}-\frac{1}{8}\left[\bar{N}^{(2)}\right]^{2}\right)\hat{P}\right]^{(4)}\right\}$$

We can show that SOPO's are Hermitian (property (ii) in appendix A of [20]). Then to fourth-order SOPOs,

$$\begin{aligned}
\text{LHS} = 1 &+ \left[\left(B_{-1/2} + \frac{1}{2}\bar{N}^{(2)} + \frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(2)} + \left[\left(C_{-1/2} - \frac{1}{8}\left[\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(4)} \\
&+ \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[B_{-1/2}\hat{P}\right]^{(2)}\left[\left(B_{-1/2} + \frac{1}{2}\bar{N}^{(2)} + \frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(2)} \\
&+ \left[C_{-1/2}\hat{P}\right]^{(4)}
\end{aligned}$$

We simplify further

$$\begin{aligned}
&\left[B_{-1/2}\hat{P}\right]^{(2)}\left[\left(B_{-1/2} + \frac{1}{2}\bar{N}^{(2)} + \frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(2)} \\
&= -\left[\left[\hat{P}\left(-\frac{1}{4}\bar{N}^{(2)}\right)\right]\left[\hat{P}\left(\frac{1}{4}\bar{N}^{(2)}\right)\right]\hat{P}\right]^{(2)} \\
&\quad + \left[\left(-\frac{1}{4}\bar{N}^{(2)}\right)\left(\frac{1}{4}\bar{N}^{(2)}\right)\hat{P}\right]^{(4)}
\end{aligned}$$

and therefore

$$\begin{aligned}
\text{LHS} &= 1 + \left[\left(2B_{-1/2} + \frac{1}{2}\bar{N}^{(2)} + \frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^2 + \frac{1}{16}\left[\hat{P}\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(2)} \\
&\quad + \left[\left(2C_{-1/2} - \frac{1}{8}\left[\bar{N}^{(2)}\right]^2 - \frac{1}{16}\left[\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(4)} \\
&= 1 + \left[\left(-\frac{1}{2}\bar{N}^{(2)} - \frac{3}{16}\left[\hat{P}\bar{N}^{(2)}\right]^2 + \frac{1}{2}\bar{N}^{(2)}\right.\right. \\
&\quad \left.\left. + \frac{1}{8}\left[\hat{P}\bar{N}^{(2)}\right]^2 + \frac{1}{16}\left[\hat{P}\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(2)} \\
&\quad + \left[\left(\frac{3}{16}\left[\bar{N}^{(2)}\right]^2 - \frac{1}{8}\left[\bar{N}^{(2)}\right]^2 - \frac{1}{16}\left[\bar{N}^{(2)}\right]^2\right)\hat{P}\right]^{(4)}
\end{aligned}$$

which reduces to

$$\text{LHS} = 1$$

which verifies Eq. (3.198).

#### 3.3.2.4 Verification of the basic identity for $\hat{\boldsymbol{J}}_{-1/2}(\bar{\boldsymbol{q}})$ (part II)

In the previous section we ignored first-order derivatives of $\bar{N}^{(2)}$ in the fourth-order SOPO. The difficulty lies in the fact that we need to add contributions from higher-than-fourth order terms so that we should really write

$$C_{-1/2}(\bar{q}) \approx \frac{3}{32}\left[\bar{N}^{(2)}(\bar{q})\right]^2 \left(1 + a_1\xi(\bar{q}) + a_2\xi^2(\bar{q})\right)$$

where

$$\begin{aligned}\xi(\bar{q}) &\equiv \frac{\left[\frac{d}{d\bar{q}}\bar{N}^{(2)}(\bar{q})\right]^2}{\bar{N}^{(2)}(\bar{q})} \\ &= -\frac{\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2}{\bar{N}^{(2)}(\bar{q})}\end{aligned}$$

The coefficients $a_1$ and $a_2$ can be determined by explicitly including the contributions from higher-order SOPO's, but we will determine them by requiring that $\hat{J}_{A,-1/2}(\bar{q})$ satisfies Eq. (3.198). We can write

$$\begin{aligned}B_{-1/2}(\bar{q}) &= -\frac{1}{4}\bar{N}^{(2)}(\bar{q}) - \frac{3}{32}\left[\hat{P}\bar{N}^{(2)}(\bar{q})\right]^2 \\ &= -\frac{1}{4}\bar{N}^{(2)}(\bar{q})\left[1 - \frac{3}{8}\xi(\bar{q})\right]\end{aligned}$$

We then have for the left-hand side of Eq. (3.198)

$$\begin{aligned}\mathrm{LHS} &= \left\{1 + \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\right\}^{\dagger}\left[1 + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\right] \\ &\quad \times \left\{1 + \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\right\} \\ &= \left\{1 + \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\right\}\left\{1 + \left[B_{-1/2}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\right. \\ &\quad \left. + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)} + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)} + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[C_{-1/2}\hat{P}\right]^{(4)}\right\}\end{aligned}$$

For clarity, we break up the expanded expression into products of 0, 1, 2, and 3 SOPOs:

$$\mathrm{LHS}_0 = 1$$

and

$$\mathrm{LHS}_1 = 2\left[B_{-1/2}\hat{P}\right]^{(2)} + 2\left[C_{-1/2}\hat{P}\right]^{(4)} + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}$$

and

$$\begin{aligned}
\mathrm{LHS}_2 = {} & \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)} + \frac{1}{2}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[C_{-1/2}\hat{P}\right]^{(4)} \\
& + \left[B_{-1/2}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)} + \left[B_{-1/2}\hat{P}\right]^{(2)}\left[C_{-1/2}\hat{P}\right]^{(4)} \\
& + \frac{1}{2}\left[B_{-1/2}\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)} + \left[C_{-1/2}\hat{P}\right]^{(4)}\left[B_{-1/2}\hat{P}\right]^{(2)} \\
& + \left[C_{-1/2}\hat{P}\right]^{(4)}\left[C_{-1/2}\hat{P}\right]^{(4)} + \frac{1}{2}\left[C_{-1/2}\hat{P}\right]^{(4)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{LHS}_3 = {} & \frac{1}{2}\left[B_{-1/2}\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)} \\
& + \frac{1}{2}\left[B_{-1/2}\hat{P}\right]^{(2)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[C_{-1/2}\hat{P}\right]^{(4)} \\
& + \frac{1}{2}\left[C_{-1/2}\hat{P}\right]^{(4)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[B_{-1/2}\hat{P}\right]^{(2)} \\
& + \frac{1}{2}\left[C_{-1/2}\hat{P}\right]^{(4)}\left[\bar{N}^{(2)}\hat{P}\right]^{(2)}\left[C_{-1/2}\hat{P}\right]^{(4)}
\end{aligned}$$

with of course,

$$\mathrm{LHS} = \mathrm{LHS}_0 + \mathrm{LHS}_1 + \mathrm{LHS}_2 + \mathrm{LHS}_3$$

Next, we reduce $\mathrm{LHS}_2$ and $\mathrm{LHS}_3$ to linear combinations of individual SOPO's using Eqs. (.12) and (.14), respectively, keeping only SOPO's up to order 4, and neglecting derivatives of $\bar{N}^{(2)}(\bar{q})$ of second and higher order. Under those conditions, for an arbitrary function $f(\bar{q})$ we then get, up to the fourth-order derivative of $f(\bar{q})$,

$$\begin{aligned}
\mathrm{LHS}f(\bar{q}) = {} & f(\bar{q}) + \frac{3}{8}\left[\frac{d}{d\bar{q}}\bar{N}^{(2)}(\bar{q})\right]^3\left(a_1 + \frac{15}{8}\right)f^{(3)}(\bar{q}) \\
& + \frac{3}{16}\left[\frac{d}{d\bar{q}}\bar{N}^{(2)}(\bar{q})\right]^2\left\{\bar{N}^{(2)}(\bar{q})\left(a_1 + \frac{15}{8}\right)\right. \\
& \left. + \left[\frac{d}{d\bar{q}}\bar{N}^{(2)}(\bar{q})\right]^2\left(a_2 + \frac{1}{2}a_1 - \frac{45}{64}\right)\right\}f^{(4)}(\bar{q})
\end{aligned}$$

The coefficients of the first and second derivatives of $f(\bar{q})$ are already zero, and we can force the coefficients of the third and fourth derivatives to vanish as well by choosing

$$\begin{aligned}
a_1 &= -\frac{15}{8} \\
a_2 &= -\frac{105}{64}
\end{aligned}$$

With this choice, we have therefore satisfied Eq. (3.198), and given an explicit expression for $\hat{J}_{A,-1/2}(\bar{q})$.

## 3.3.3 A Schrödinger-like equation

### 3.3.3.1 General form of the Hamiltonian kernel

In the previous section, we have also obtained an explicit expression for the operator $\hat{J}_{-1/2}(\bar{q})$ in the one-dimensional case and are now ready to generalize it to any number of dimensions and revisit Eq. (3.196). To this end, we derive an expression for

$$\mathscr{H}(\bar{q}) \equiv \hat{J}_{-1/2}(\bar{q})\, H(\bar{q})\, \hat{J}_{-1/2}(\bar{q}) \tag{3.202}$$

where we assume the generic forms

$$\hat{J}_{-1/2}(\bar{q}) = \sum_{i=0}^{2} \left[ j_{(i)}(\bar{q})\, \hat{P} \right]^{(i)}$$
$$H(\bar{q}) = \sum_{i=0}^{2} \left[ h_{(i)}(\bar{q})\, \hat{P} \right]^{(i)}$$

We can expand Eq. (3.202) up to second-order SOPO's, using the rules for the composition of SOPO's in Eqs. (.12) and (.14), to obtain an expression of the form

$$\mathscr{H}(\bar{q}) = S(\bar{q}) + \left[ T(\bar{q})\, \hat{P} \right]^{(1)} + \left[ U(\bar{q})\, \hat{P} \right]^{(2)} \tag{3.203}$$

The calculation is straightforward in principle but cumbersome in practice, and leads to sums of very large numbers of terms for $S(\bar{q})$, $T(\bar{q})$, and $U(\bar{q})$. We give in appendix B a Mathematica script to calculate all these terms, but here we will only list the results for some special cases. For example, making similar restrictions as in [20], to wit

$$h_{(0)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 3$$
$$h_{(1)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 1$$
$$h_{(2)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 2$$

and

$$j_{(1)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 2$$
$$j_{(2)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 2$$

where we are using the notation

$$A^{(p)}(\bar{q}) \equiv i^p \frac{\partial^p}{\partial \bar{q}^p} A(\bar{q})$$

We obtain

$$\begin{aligned} S = h_{(0)} &+ \frac{1}{2}\left[j_{(1)}, h_{(0)}^{(1)}\right]_- + \frac{1}{8}\left[j_{(1)}, h_{(0)}^{(2)}, j_{(2)}^{(1)}\right]_- - \frac{1}{4}\left[j_{(2)}, h_{(0)}^{(2)}, j_{(1)}^{(1)}\right]_- \\ &+ \frac{1}{4}\left[j_{(1)}^{(1)}, h_{(0)}^{(1)}, j_{(2)}^{(1)}\right]_- + \frac{1}{4}\left[j_{(2)}, h_{(0)}^{(2)}\right]_+ - \frac{1}{4}\left[j_{(1)}, h_{(0)}^{(1)}, j_{(1)}^{(1)}\right]_+ \\ &- \frac{1}{4} j_{(1)} h_{(0)}^{(2)} j_{(1)} - \frac{1}{4} j_{(1)}^{(1)} h_{(0)} j_{(1)}^{(1)} + \frac{1}{4} j_{(2)}^{(1)} h_{(0)}^{(2)} j_{(2)}^{(1)} \end{aligned} \tag{3.204}$$

$$\begin{aligned} T = h_{(1)} &+ \frac{1}{2}\left[h_{(1)}, j_{(1)}^{(1)}\right]_- + \left[j_{(2)}, h_{(0)}^{(1)}\right]_- + \frac{1}{2}\left[j_{(1)}, h_{(0)}, j_{(1)}^{(1)}\right]_- \\ &- \frac{1}{4}\left[j_{(2)}, h_{(0)}^{(2)}, j_{(2)}^{(1)}\right]_- + \left[h_{(0)}, j_{(1)}\right]_+ - \frac{1}{2}\left[h_{(2)}^{(1)}, j_{(1)}^{(1)}\right]_+ - \frac{1}{2}\left[j_{(1)}, h_{(0)}^{(1)}, j_{(2)}^{(1)}\right]_+ \\ &- \frac{1}{4}\left[j_{(1)}, h_{(0)}^{(2)}, j_{(2)}\right]_+ - \frac{1}{2}\left[j_{(1)}^{(1)}, h_{(0)}, j_{(2)}^{(1)}\right]_+ - \frac{3}{4} j_{(1)}^{(1)} h_{(1)} j_{(1)}^{(1)} \end{aligned} \tag{3.205}$$

$$\begin{aligned} U = h_{(2)} &+ \frac{1}{2}\left[h_{(1)}, j_{(2)}^{(1)}\right]_- + \left[h_{(2)}, j_{(1)}^{(1)}\right]_- + \frac{1}{2}\left[j_{(1)}, h_{(2)}^{(1)}\right]_- \\ &+ \frac{1}{2}\left[j_{(1)}, h_{(0)}, j_{(2)}^{(1)}\right]_- + \left[j_{(1)}, h_{(1)}, j_{(1)}^{(1)}\right]_- - \frac{1}{2}\left[j_{(1)}, h_{(0)}^{(1)}, j_{(2)}\right]_- \\ &+ \left[j_{(2)}, h_{(0)}, j_{(1)}^{(1)}\right]_- + \left[j_{(1)}^{(1)}, h_{(2)}^{(1)}, j_{(2)}^{(1)}\right]_- + \left[h_{(0)}, j_{(2)}\right]_+ + \left[h_{(1)}, j_{(1)}\right]_+ \\ &- \left[h_{(2)}^{(1)}, j_{(2)}^{(1)}\right]_+ - \frac{1}{4}\left[j_{(1)}, h_{(2)}^{(1)}, j_{(1)}^{(1)}\right]_+ - \frac{1}{2}\left[j_{(2)}, h_{(0)}^{(1)}, j_{(2)}^{(1)}\right]_+ \\ &- \frac{5}{4}\left[j_{(1)}^{(1)}, h_{(1)}, j_{(2)}^{(1)}\right]_+ + j_{(1)} h_{(0)} j_{(1)} - \frac{1}{2} j_{(2)} h_{(0)}^{(2)} j_{(2)} \\ &- \frac{7}{4} j_{(1)}^{(1)} h_{(2)} j_{(1)}^{(1)} - j_{(2)}^{(1)} h_{(0)} j_{(2)}^{(1)} \end{aligned} \tag{3.206}$$

where we have used the compact notation

$$[A, B]_\pm \equiv AB \pm BA$$
$$[A, B, C]_\pm \equiv ABC \pm CBA$$

With this, we can for example recover the results in section 10.7.2 of [9]. Taking

$$\begin{aligned} j_{(1)} &\equiv 0 \\ h_{(1)} &\equiv 0 \end{aligned}$$

$$j_{(2)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 1$$

$$h_{(0)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 3$$

$$h_{(2)}^{(p)}(\bar{q}) = 0 \text{ for } p \geq 2$$

we obtain

$$S = h_{(0)} + \frac{1}{4}\left[j_{(2)}, h_{(0)}^{(2)}\right]_+$$

$$T = \left[j_{(2)}, h_{(0)}^{(1)}\right]_-$$

$$U = h_{(2)} + \left[h_{(0)}, j_{(2)}\right]_+ - \frac{1}{2} j_{(2)} h_{(0)}^{(2)} j_{(2)}$$

To simplify these terms further, we assume that the $j_{(i)}^{(p)}$ and $h_{(i)}^{(p)}$ terms are just functions of $\bar{q}$ and therefore that they commute. Then we have $T = 0$. We further neglect $h_{(0)}^{(2)}$ in the $U$ coefficient (but not in the $S$ coefficient), and substitute the following values (taking into account the difference in the definitions of the moment in this work, Eq. (3.179), which contains a power of $i$ factor, compared to Eq. (10.98) in [9])

$$\begin{aligned} j_{(2)} &= \frac{1}{4}\frac{N_2}{N_0} \\ h_{(0)} &= \frac{H_0}{N_0} \\ h_{(2)} &= -\frac{1}{2}\frac{H_2}{N_0} \end{aligned}$$

to obtain

$$\begin{aligned} V(\bar{q}) &\equiv S \\ &= \frac{H_0}{N_0} - \frac{1}{8}\frac{N_2}{N_0}\frac{H_0''}{N_0} \end{aligned}$$

and

$$\begin{aligned} \frac{1}{M(\bar{q})} &\equiv 2U \\ &= \frac{N_2}{N_0}\frac{H_0}{N_0} - \frac{H_2}{N_0} \end{aligned}$$

which just gives Eq. (10.104) in [9].

#### 3.3.3.2 Explicit form of $j_{(i)}^{(p)}$ and $h_{(i)}^{(p)}$

So far, we have used the coefficients $j_{(i)}^{(p)}$ and $h_{(i)}^{(p)}$ without explicitly specifying what they are (other than the very special case at the end of the last section). We go back to Eq. (3.196),

$$\begin{aligned}\mathscr{H}(\bar{q}) &= \left[\hat{J}_{-1/2}(\bar{q})\right]^{\dagger} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \sum_{n=0}^{\infty} \frac{1}{n!} \left[H^{(n)}(\bar{q})\,\hat{P}\right]^{(n)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \hat{J}_{-1/2}(\bar{q}) \\ &\equiv \hat{J}_{-1/2}(\bar{q})\, H(\bar{q})\, \hat{J}_{-1/2}(\bar{q})\end{aligned}$$

where, to second order SOPO's, we have

$$H(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \left[H^{(0)}(\bar{q}) + \left[H^{(1)}(\bar{q})\,\hat{P}\right]^{(1)} + \frac{1}{2}\left[H^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\right] \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \tag{3.207}$$

and we recall from Eq. (3.179) that

$$H^{(n)}(\bar{q}) \equiv i^{n} \int_{-\infty}^{+\infty} ds\, s^{n} H\left(\bar{q}+\frac{s}{2}, \bar{q}-\frac{s}{2}\right)$$

Now we proceed as in section 3.3.2 to absorb the $1/\sqrt{N^{(0)}}$ factors into the Hamiltonian SOPO's. We write

$$\frac{1}{\sqrt{N^{(0)}(\bar{q})}} H^{(0)}(\bar{q}) \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \equiv \bar{H}^{(0)}(\bar{q})$$

Next, using Eq. (.17),

$$\begin{aligned}\frac{1}{\sqrt{N^{(0)}(\bar{q})}} \left[H^{(1)}(\bar{q})\,\hat{P}\right]^{(1)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} &= \left[\bar{H}^{(1)}(\bar{q})\,\hat{P}\right]^{(1)} \\ &\quad + \frac{i}{2} C^{(1)}\left(H^{(1)}(\bar{q}), N^{(0)}(\bar{q})\right)\end{aligned}$$

and using Eq. (.18),

$$\begin{aligned}\frac{1}{\sqrt{N^{(0)}(\bar{q})}} \left[H^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}} &= \left[\bar{H}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} \\ &\quad + \left[iC^{(1)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right)\hat{P}\right]^{(1)} \\ &\quad - C^{(2)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right)\end{aligned}$$

and so we re-write Eq. (3.207) as

$$H(\bar{q}) = \bar{H}^{(0)}(\bar{q}) + \frac{i}{2}C^{(1)}\left(H^{(1)}(\bar{q}), N^{(0)}(\bar{q})\right) - \frac{1}{2}C^{(2)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right)$$
$$+ \left[\left[\bar{H}^{(1)}(\bar{q}) + \frac{i}{2}C^{(1)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right)\right]\hat{P}\right]^{(1)} + \frac{1}{2}\left[\bar{H}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}$$

and if we want to write this as

$$H(\bar{q}) = \sum_{i=0}^{2}\left[h_{(i)}(\bar{q})\,\hat{P}\right]^{(i)}$$

we can then identify

$$h_{(0)} = \bar{H}^{(0)}(\bar{q}) + \frac{i}{2}C^{(1)}\left(H^{(1)}(\bar{q}), N^{(0)}(\bar{q})\right) - \frac{1}{2}C^{(2)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right) \tag{3.208}$$

$$h_{(1)} = \bar{H}^{(1)}(\bar{q}) + \frac{i}{2}C^{(1)}\left(H^{(2)}(\bar{q}), N^{(0)}(\bar{q})\right) \tag{3.209}$$

$$h_{(2)} = \frac{1}{2}\bar{H}^{(2)} \tag{3.210}$$

Next, we do the same thing for $\hat{J}_{-1/2}(\bar{q})$. We return to Eq. (3.188),

$$\hat{J}(\bar{q}) = I + \hat{u}(\bar{q})$$

but this time we keep the odd terms in $\hat{u}(\bar{q})$. Then to second-order SOPO's, Eq. (3.187) gives

$$\hat{u}(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\left\{\left[N^{(1)}(\bar{q})\,\hat{P}\right]^{(1)} + \frac{1}{2}\left[N^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\right\}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}$$

Absorbing the $1/\sqrt{N^{(0)}(\bar{q})}$ factors, we find

$$\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\left[N^{(1)}(\bar{q})\,\hat{P}\right]^{(1)}\frac{1}{\sqrt{N^{(0)}(\bar{q})}} = \left[\bar{N}^{(1)}(\bar{q})\,\hat{P}\right]^{(1)} + \frac{i}{2}C^{(1)}\left(N^{(1)}(\bar{q}), N^{(0)}(\bar{q})\right)$$

and

$$\begin{aligned}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\left[N^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}\frac{1}{\sqrt{N^{(0)}(\bar{q})}} = &\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} \\ &+\left[iC^{(1)}\left(N^{(2)}(\bar{q}),N^{(0)}(\bar{q})\right)\hat{P}\right]^{(1)} \\ &-C^{(2)}\left(N^{(2)}(\bar{q}),N^{(0)}(\bar{q})\right)\end{aligned}$$

and therefore

$$\hat{J}(\bar{q}) = I+\alpha_{(0)}(\bar{q})+\left[W_N(\bar{q})\,\hat{P}\right]^{(1)}+\frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)}$$

with

$$\alpha_{(0)}(\bar{q}) \equiv \frac{i}{2}C^{(1)}\left(N^{(1)}(\bar{q}),N^{(0)}(\bar{q})\right)-\frac{1}{2}C^{(2)}\left(N^{(2)}(\bar{q}),N^{(0)}(\bar{q})\right)$$

and

$$W_N(\bar{q}) \equiv \bar{N}^{(1)}(\bar{q})+\frac{i}{2}C^{(1)}\left(N^{(2)}(\bar{q}),N^{(0)}(\bar{q})\right)$$

Next, we approximate $\hat{J}_{-1/2}(\bar{q})$ by expanding $1/\sqrt{1+\hat{u}(\bar{q})}$, as we did in Eq. (3.201)

$$\hat{J}_{A,-1/2}(\bar{q}) = 1-\frac{1}{2}\hat{u}(\bar{q})+\frac{3}{8}\hat{u}^2(\bar{q})$$

with

$$\hat{u}(\bar{q}) = \alpha_{(0)}(\bar{q})+\left[W_N(\bar{q})\,\hat{P}\right]^{(1)}+\frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\,\hat{P}\right]^{(2)} \tag{3.211}$$

Using Eqs. (.12) and (.14) we can in principle obtain a general expression for $\hat{J}_{A,-1/2}(\bar{q})$, but we first illustrate the case where $N^{(0)}(\bar{q})$, $N^{(1)}(\bar{q})$, and $N^{(2)}(\bar{q})$ are constants independent of $\bar{q}$, then we can write

$$\hat{J}_{A,-1/2}(\bar{q}) = j_{(0)}+\left[j_{(1)}(\bar{q})\,\hat{P}\right]^{(1)}+\left[j_{(2)}(\bar{q})\,\hat{P}\right]^{(2)}$$

where ,

$$j_{(0)} = 1$$

$$j_{(1)} = -\frac{1}{2}\bar{N}^{(1)}(\bar{q})$$

$$j_{(2)} = \frac{3}{8}\left[\bar{N}^{(1)}(\bar{q})\right]^2-\frac{1}{4}\bar{N}^{(2)}(\bar{q})$$

Now we give a more general form of $\hat{J}_{A,-1/2}(\bar{q})$, corresponding to Eq. (36) in [20]. Substituting the value of $\hat{u}(\bar{q})$ in Eq. (3.211),

$$\begin{aligned}\hat{J}_{A,-1/2}(\bar{q}) &= 1 - \frac{1}{2}\hat{u}(\bar{q}) + \frac{3}{8}\hat{u}^2(\bar{q}) \\ &= 1 - \frac{1}{2}\left\{\alpha_{(0)}(\bar{q}) + \left[W_N(\bar{q})\hat{P}\right]^{(1)} + \frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\hat{P}\right]^{(2)}\right\} \\ &\quad + \frac{3}{8}\left\{\alpha_{(0)}(\bar{q}) + \left[W_N(\bar{q})\hat{P}\right]^{(1)} + \frac{1}{2}\left[\bar{N}^{(2)}(\bar{q})\hat{P}\right]^{(2)}\right\}^2\end{aligned}$$

We will assume $\alpha_{(0)}(\bar{q})$ can be neglected (if it cannot, then we can always iterate the procedure described in section 3.3.2 until it does become small). We also ignore derivatives of $W_N(\bar{q})$, and derivatives of order higher than 1 for $\bar{N}^{(2)}(\bar{q})$. Finally, we use Eq. (.12) for the product of two SOPO's to obtain

$$\begin{aligned} j_{(0)} &= 1 \\ j_{(1)} &= -\frac{1}{2}W_N \\ j_{(2)} &= -\frac{1}{4}\bar{N}^{(2)} + \frac{3}{8}(W_N)^2 + \frac{3}{32}i\left[W_N, \left(\bar{N}^{(2)}\right)'\right]_- + \frac{3}{32}\left[\left(\bar{N}^{(2)}\right)'\right]^2 \end{aligned} \tag{3.212}$$

With this, we have in principle all the components needed to calculate $\mathscr{H}(\bar{q})$ in Eq. (3.196) and solve the SCIM equation (3.195).

### *3.3.4 Illustration with the multi-O (4) model*

The SCIM formalism derived in the previous section is rather complicated and its application to more realistic models of nuclei is still in progress. Here, we provide the reader with a concrete illustration of the application of this formalism using the multi-$O(4)$ model (see section 1.6.1). The goal of this section is mainly pedagogical. As we shall see at the end of the section, where we compare the SCIM results to the exact calculation, disagreement between the two should not be taken as a verdict on the limitations of the SCIM in general, but rather as an indicator of improvements needed in the calculations. We outline some of these improvements, but their implementation is beyond the scope of this manuscript.

#### 3.3.4.1 Definitions and notation

For convenience, we introduce the coefficients

$$\begin{aligned} A_\alpha &\equiv (S_{\alpha\alpha}-1)\,u_\alpha^D - T_{\alpha\bar{\alpha}} v_\alpha^D \\ B_\alpha &\equiv S_{\alpha\alpha} v_\alpha^D - Y_{\alpha\bar{\alpha}} u_\alpha^D \\ C_\beta &\equiv S_{\beta\beta} v_{\alpha'}^{D'} + T_{\beta\bar{\beta}} u_{\alpha'}^{D'} \\ D_\beta &\equiv (S_{\beta\beta}-1)\,u_{\alpha'}^{D'} + Y_{\beta\bar{\beta}} v_{\alpha'}^{D'} \end{aligned} \tag{3.213}$$

where the $S$, $T$, and $Y$ coefficients are defined in Eqs. (3.34), (3.35), and (3.36). Note that $Y_{\alpha\bar{\alpha}}$ and $Y_{\beta\bar{\beta}}$ appear in Eq. (3.213), while Eq. (3.36) defines the matrix element $Y_{\bar{\mu}\nu}$, but it is trivial to change the order of the indices and show that $Y_{\nu\bar{\mu}} = -Y_{\bar{\mu}\nu}$. The following identity can be easily proven

$$A_\alpha u_{\alpha'}^{D'} - B_\alpha v_{\alpha'}^{D'} = -\left(C_\alpha v_\alpha^D - D_\alpha u_\alpha^D\right) \tag{3.214}$$

We also define the two-quasiparticle states

$$|\Phi_\alpha(D)\rangle \equiv \eta_{\bar{\alpha}}^\dagger \eta_\alpha^\dagger \,|\Phi_D\rangle$$

Next, we evaluate all the necessary matrix elements. To do this, we express the qp operators in the single-particle basis and use the fact that this basis is the same at all deformations in the multi-$O(4)$ model (i.e., $a_\mu^{D'} = a_\mu^D$). Then the resulting matrix elements can be related to the $S$, $T$, and $Y$ coefficients.

### 3.3.4.2 Norm overlap kernel

We calculate first the overlap between 2-qp states

$$\langle \Phi_\alpha(D)\,|\Phi_{\alpha'}(D')\,\rangle = \left\langle \Phi_D \left| \eta_\alpha^D \eta_{\bar{\alpha}}^D \eta_{\bar{\alpha}'}^{D'\dagger} \eta_{\alpha'}^{D'\dagger} \right| \Phi_{D'} \right\rangle$$

Without dropping any terms from the generalized Wick's theorem, we obtain

$$\begin{aligned} \frac{\langle \Phi_\alpha(D)\,|\Phi_{\alpha'}(D')\,\rangle}{\langle \Phi_D\,|\Phi_{D'}\,\rangle} = \delta_{\alpha\alpha'} &\left[ v_\alpha^D \left( T_{\alpha\bar{\alpha}} u_{\alpha'}^{D'} + S_{\alpha\alpha} v_{\alpha'}^{D'} \right) - u_\alpha^D \left( (S_{\alpha\alpha}-1)\,u_{\alpha'}^{D'} + Y_{\alpha\bar{\alpha}} v_{\alpha'}^{D'} \right) \right]^2 \\ &- \left[ T_{\alpha\bar{\alpha}} \left(v_\alpha^D\right)^2 + Y_{\alpha\bar{\alpha}} \left(u_\alpha^D\right)^2 + (1-2S_{\alpha\alpha})\,u_\alpha^D v_\alpha^D \right] \\ &\times \left[ T_{\alpha'\bar{\alpha}'} \left(u_{\alpha'}^{D'}\right)^2 + Y_{\alpha'\bar{\alpha}'} \left(v_{\alpha'}^{D'}\right)^2 - (1-2S_{\alpha'\alpha'})\,u_{\alpha'}^{D'} v_{\alpha'}^{D'} \right] \end{aligned}$$

In terms of the coefficients defined in Eq. (3.213), we can write this as

$$\begin{aligned} \frac{\langle \Phi_\alpha(D)\,|\Phi_{\alpha'}(D')\,\rangle}{\langle \Phi_D\,|\Phi_{D'}\,\rangle} &= \delta_{\alpha\alpha'} \left( v_\alpha^D C_\alpha - u_\alpha^D D_\alpha \right)^2 \\ &\quad + \left( v_\alpha^D A_\alpha + u_\alpha^D B_\alpha \right) \left( u_{\alpha'}^{D'} C_{\alpha'} + v_{\alpha'}^{D'} D_{\alpha'} \right) \end{aligned}$$

We can also calculate the overlaps between 0 and 2-quasi-particle states,

$$\frac{\langle \Phi_D | \Phi_{\alpha'}(D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \frac{\left\langle \Phi_D \left| \eta_{\bar{\alpha}'}^{D'\dagger} \eta_{\alpha'}^{D'\dagger} \right| \Phi_{D'} \right\rangle}{\langle \Phi_D | \Phi_{D'} \rangle}$$
$$= -\left( u_{\alpha'}^{D'} C_{\alpha'} + v_{\alpha'}^{D'} D_{\alpha'} \right)$$

and

$$\frac{\langle \Phi_\alpha(D) | \Phi_{D'} \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \frac{\langle \Phi_D | \eta_\alpha^D \eta_{\bar{\alpha}}^D | \Phi_{D'} \rangle}{\langle \Phi_D | \Phi_{D'} \rangle}$$
$$= -\left( v_\alpha^D A_\alpha + u_\alpha^D B_\alpha \right)$$

#### 3.3.4.3 Spherical component of the Hamiltonian overlap

Next, we need to do the same for the Hamiltonian overlap. We start with the spherical component,

$$\langle \Phi_\alpha(D) | H_0 | \Phi_{\alpha'}(D') \rangle = \sum_\mu e_\mu^0 \left\langle \Phi_D \left| \eta_\alpha^D \eta_{\bar{\alpha}}^D a_\mu^{D'\dagger} a_\mu^{D'} \eta_{\bar{\alpha}'}^{D'\dagger} \eta_{\alpha'}^{D'\dagger} \right| \Phi_{D'} \right\rangle$$

we can then calculate

$$\frac{\langle \Phi_\alpha(D) | H_0 | \Phi_{\alpha'}(D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \sum_{\mu>0} e_\mu^0 \frac{\left\langle \Phi_D \left| \eta_\alpha^D \eta_{\bar{\alpha}}^D \left( a_\mu^{D'\dagger} a_\mu^{D'} + a_{\bar{\mu}}^{D'\dagger} a_{\bar{\mu}}^{D'} \right) \eta_{\bar{\alpha}'}^{D'\dagger} \eta_{\alpha'}^{D'\dagger} \right| \Phi_{D'} \right\rangle}{\langle \Phi_D | \Phi_{D'} \rangle}$$
$$\begin{aligned} &= 2 \Big\{ \left[ v_\alpha^D A_\alpha + u_\alpha^D B_\alpha \right] \left[ u_{\alpha'}^{D'} C_{\alpha'} + v_{\alpha'}^{D'} D_{\alpha'} \right] \\ &\quad + \delta_{\alpha\alpha'} \left[ v_\alpha^D C_\alpha - u_\alpha^D D_\alpha \right]^2 \Big\} \sum_{\mu>0} e_\mu^0 S_{\mu\mu} \\ &\quad - 2 A_\alpha B_\alpha \left[ u_{\alpha'}^{D'} C_{\alpha'} + v_{\alpha'}^{D'} D_{\alpha'} \right] e_\alpha^0 \\ &\quad - 2 C_{\alpha'} D_{\alpha'} \left[ v_\alpha^D A_\alpha + u_\alpha^D B_\alpha \right] e_{\alpha'}^0 \\ &\quad + 2 \delta_{\alpha\alpha'} \left[ v_\alpha^D C_\alpha - u_\alpha^D D_\alpha \right] \left[ A_\alpha D_\alpha - B_\alpha C_\alpha \right] e_\alpha^0 \end{aligned}$$

For the overlaps between 0- and 2-quasi-particle states we find

$$\frac{\langle \Phi_D | H_0 | \Phi_{\alpha'}(D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = 2 C_{\alpha'} D_{\alpha'} e_{\alpha'}^0 - 2 \left( u_{\alpha'}^{D'} C_{\alpha'} + v_{\alpha'}^{D'} D_{\alpha'} \right) \sum_{\mu>0} e_\mu^0 S_{\mu\mu}$$

and

$$\frac{\langle \Phi_\alpha(D) | H_0 | \Phi_{D'} \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = 2 A_\alpha B_\alpha e_\alpha^0 - 2 \left( v_\alpha^D A_\alpha + u_\alpha^D B_\alpha \right) \sum_{\mu>0} e_\mu^0 S_{\mu\mu}$$

#### 3.3.4.4 Quadrupole component of the Hamiltonian overlap

Next, we consider

$$
\begin{aligned}
H_Q &= -\frac{1}{2}\chi\left(\sum_{\mu} d_\mu \sigma_\mu a_\mu^{D'\dagger} a_\mu^{D'}\right)^2 \\
&= -\frac{1}{2}\chi \sum_{\mu\nu} d_\mu \sigma_\mu d_\nu \sigma_\nu a_\mu^{D'\dagger} a_\mu^{D'} a_\nu^{D'\dagger} a_\nu^{D'}
\end{aligned}
$$

After some simplifications, we find

$$
\begin{aligned}
&\frac{\left\langle \Phi_\alpha (D) \left| H_Q \right| \Phi_{\alpha'} (D') \right\rangle}{\left\langle \Phi_D \right| \left. \Phi_{D'} \right\rangle} \\
&= -\frac{1}{2}\chi \sum_{\mu,\nu>0} d_\mu \sigma_\mu d_\nu \sigma_\nu \frac{1}{\left\langle \Phi_D \right| \left. \Phi_{D'} \right\rangle} \\
&\quad \times \left\langle \Phi_D \left| \eta_\alpha^D \eta_{\bar{\alpha}}^D \left(a_\mu^{D'\dagger} a_\mu^{D'} + a_{\bar{\mu}}^{D'\dagger} a_{\bar{\mu}}^{D'}\right) \left(a_\nu^{D'\dagger} a_\nu^{D'} + a_{\bar{\nu}}^{D'\dagger} a_{\bar{\nu}}^{D'}\right) \eta_{\bar{\alpha}'}^{D'\dagger} \eta_{\alpha'}^{D'\dagger} \right| \Phi_{D'} \right\rangle \\
&= -2\chi \left\{ \left[ \left(A_\alpha v_\alpha^D + B_\alpha u_\alpha^D\right) \left(C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'}\right) + \delta_{\alpha\alpha'} \left(A_\alpha u_{\alpha'}^{D'} - B_\alpha v_{\alpha'}^{D'}\right)^2 \right] \right. \\
&\quad \times \left(\sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu}\right)^2 \\
&\quad - \left(d_\alpha \sigma_\alpha + d_{\alpha'} \sigma_{\alpha'}\right) \left[ A_\alpha B_\alpha \left(C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'}\right) + C_{\alpha'} D_{\alpha'} \left(A_\alpha v_\alpha^D + B_\alpha u_\alpha^D\right) \right. \\
&\quad \left. \left. + \delta_{\alpha\alpha'} \left(B_\alpha C_{\alpha'} - A_\alpha D_{\alpha'}\right) \right] \left(\sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu}\right) + 2 A_\alpha B_\alpha C_{\alpha'} D_{\alpha'} d_\alpha \sigma_\alpha d_{\alpha'} \sigma_{\alpha'} \right\}
\end{aligned}
$$

For the overlaps between 0- and 2-quasi-particle states we find

$$
\begin{aligned}
&\frac{\left\langle \Phi_D \left| H_Q \right| \Phi_{\alpha'} (D') \right\rangle}{\left\langle \Phi_D \right| \left. \Phi_{D'} \right\rangle} \\
&= -\frac{1}{2}\chi \sum_{\mu,\nu>0} d_\mu \sigma_\mu d_\nu \sigma_\nu \left[ 4 C_{\alpha'} D_{\alpha'} \left(\delta_{\nu\alpha'} S_{\mu\mu} + \delta_{\mu\alpha'} S_{\nu\nu}\right) - 4 \left(C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'}\right) S_{\mu\mu} S_{\nu\nu} \right] \\
&= -\frac{1}{2}\chi \left\{ 8 C_{\alpha'} D_{\alpha'} d_{\alpha'} \sigma_{\alpha'} \sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu} - 4 \left(C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'}\right) \left(\sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu}\right)^2 \right\} \\
&= -2\chi \left[ 2 C_{\alpha'} D_{\alpha'} d_{\alpha'} \sigma_{\alpha'} \left(\sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu}\right) - \left(C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'}\right) \left(\sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu}\right)^2 \right]
\end{aligned}
$$

and

$$\begin{aligned}
&\frac{\langle \Phi_\alpha (D) | H_Q | \Phi_{D'} \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} \\
&= -\frac{1}{2}\chi \sum_{\mu,\nu>0} d_\mu \sigma_\mu d_\nu \sigma_\nu \left[ 4 A_\alpha B_\alpha \left( \delta_{\nu\alpha} S_{\mu\mu} + \delta_{\mu\alpha} S_{\nu\nu} \right) - 4 \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) S_{\mu\mu} S_{\nu\nu} \right] \\
&= -\frac{1}{2}\chi \left\{ 8 A_\alpha B_\alpha d_\alpha \sigma_\alpha \left( \sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu} \right) - 4 \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \left( \sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu} \right)^2 \right\} \\
&= -2\chi \left[ 2 A_\alpha B_\alpha d_\alpha \sigma_\alpha \left( \sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu} \right) - \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \left( \sum_{\mu>0} d_\mu \sigma_\mu S_{\mu\mu} \right)^2 \right]
\end{aligned}$$

#### 3.3.4.5 Pairing component of the Hamiltonian overlap

Finally, we consider the pairing Hamiltonian

$$H_P = -\frac{1}{2} G \sum_{\mu,\nu>0} \left[ a_\mu^{D'\dagger} a_{\bar\mu}^{D'\dagger} a_{\bar\nu}^{D'} a_\nu^{D'} + a_{\bar\mu}^{D'} a_\mu^{D'} a_\nu^{D'\dagger} a_{\bar\nu}^{D'\dagger} \right]$$

from which

$$\begin{aligned}
&\frac{\langle \Phi_\alpha (D) | H_P | \Phi_{\alpha'} (D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} \\
&= G \left[ \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \left( C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'} \right) + \delta_{\alpha\alpha'} \left( A_\alpha u_{\alpha'}^{D'} - B_\alpha v_{\alpha'}^{D'} \right)^2 \right] \\
&\quad \times \left( \sum_{\mu>0} T_{\mu\bar\mu} \right) \left( \sum_{\mu>0} Y_{\mu\bar\mu} \right) - G \left[ D_{\alpha'}^2 \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) - B_\alpha^2 \left( C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'} \right) \right. \\
&\quad \left. - 2 \delta_{\alpha\alpha'} B_\alpha D_{\alpha'} \left( A_\alpha u_{\alpha'}^{D'} - B_\alpha v_{\alpha'}^{D'} \right) \right] \left( \sum_{\mu>0} T_{\mu\bar\mu} \right) - G \left[ C_{\alpha'}^2 \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \right. \\
&\quad \left. + 2 \delta_{\alpha\alpha'} A_\alpha C_{\alpha'} \left( A_\alpha u_{\alpha'}^{D'} - B_\alpha v_{\alpha'}^{D'} \right) \right] \left( \sum_{\mu>0} Y_{\mu\bar\mu} \right) - G \left( A_\alpha^2 D_{\alpha'}^2 + B_\alpha^2 C_{\alpha'}^2 \right)
\end{aligned}$$

For the overlaps between 0- and 2-quasi-particle states we find

$$\begin{aligned}
\frac{\langle \Phi_D \left| H_P \right| \Phi_{\alpha'} \left( D' \right) \rangle}{\langle \Phi_D \right| \Phi_{D'} \rangle} &= -\frac{1}{2} G \sum_{\mu,\nu>0} \Big[ \Big( C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'} \Big) \left( T_{\mu\bar{\mu}} Y_{\nu\bar{\nu}} + Y_{\mu\bar{\mu}} T_{\nu\bar{\nu}} \right) \\
&\quad - D_{\alpha'}^2 \left( \delta_{\nu\alpha'} T_{\mu\bar{\mu}} + \delta_{\mu\alpha'} T_{\nu\bar{\nu}} \right) - C_{\alpha'}^2 \left( \delta_{\nu\alpha'} Y_{\mu\bar{\mu}} + \delta_{\mu\alpha'} Y_{\nu\bar{\nu}} \right) \Big] \\
&= -G \left( C_{\alpha'} u_{\alpha'}^{D'} + D_{\alpha'} v_{\alpha'}^{D'} \right) \left( \sum_{\mu>0} T_{\mu\bar{\mu}} \right) \left( \sum_{\mu>0} Y_{\mu\bar{\mu}} \right) \\
&\quad + G D_{\alpha'}^2 \left( \sum_{\mu>0} T_{\mu\bar{\mu}} \right) + G C_{\alpha'}^2 \left( \sum_{\mu>0} Y_{\mu\bar{\mu}} \right)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\langle \Phi_\alpha \left( D \right) \left| H_P \right| \Phi_{D'} \rangle}{\langle \Phi_D \right| \Phi_{D'} \rangle} &= -\frac{1}{2} G \sum_{\mu,\nu>0} \left[ \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \left( T_{\mu\bar{\mu}} Y_{\nu\bar{\nu}} + Y_{\mu\bar{\mu}} T_{\nu\bar{\nu}} \right) \right. \\
&\quad \left. + B_\alpha^2 \left( \delta_{\nu\alpha} T_{\mu\bar{\mu}} + \delta_{\mu\alpha} T_{\nu\bar{\nu}} \right) + A_\alpha^2 \left( \delta_{\nu\alpha} Y_{\mu\bar{\mu}} + \delta_{\mu\alpha} Y_{\nu\bar{\nu}} \right) \right] \\
&= -G \left( A_\alpha v_\alpha^D + B_\alpha u_\alpha^D \right) \left( \sum_{\mu>0} T_{\mu\bar{\mu}} \right) \left( \sum_{\mu>0} Y_{\mu\bar{\mu}} \right) \\
&\quad - G B_\alpha^2 \left( \sum_{\mu>0} T_{\mu\bar{\mu}} \right) - G A_\alpha^2 \left( \sum_{\mu>0} Y_{\mu\bar{\mu}} \right)
\end{aligned}$$

#### 3.3.4.6 Schrodinger-like equation

Using the results above, we have now defined norm and Hamiltonian overlap matrices for the multi-$O(4)$ model,

$$N_{\alpha\beta} \left( D, D' \right) \equiv \begin{cases} \langle \Phi_D \left| \Phi_{D'} \right\rangle & \alpha = \beta = 0 \\ \langle \Phi_D \left| \Phi_\beta \left( D' \right) \right\rangle & \alpha = 0, \beta \geq 1 \\ \langle \Phi_\alpha \left( D \right) \left| \Phi_{D'} \right\rangle & \alpha \geq 1, \beta = 0 \\ \langle \Phi_\alpha \left( D \right) \left| \Phi_\beta \left( D' \right) \right\rangle & \alpha, \beta \geq 1 \end{cases}$$

and similarly,

$$H_{\alpha\beta} \left( D, D' \right) \equiv \begin{cases} \langle \Phi_D \left| H \right| \Phi_{D'} \rangle & \alpha = \beta = 0 \\ \langle \Phi_D \left| H \right| \Phi_{\alpha'} \left( D' \right) \rangle & \alpha = 0, \beta \geq 1 \\ \langle \Phi_\alpha \left( D \right) \left| H \right| \Phi_{D'} \rangle & \alpha \geq 1, \beta = 0 \\ \langle \Phi_\alpha \left( D \right) \left| H \right| \Phi_{\alpha'} \left( D' \right) \rangle & \alpha, \beta \geq 1 \end{cases}$$

For example, we can write the overlap kernels obtained in section 3.3.4.2 explicitly as

$$\frac{\langle \Phi_D | \Phi_{\alpha'}(D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \frac{u_{\alpha'}^D v_{\alpha'}^{D'} - v_{\alpha'}^D u_{\alpha'}^{D'}}{u_{\alpha'}^D u_{\alpha'}^{D'} + v_{\alpha'}^D v_{\alpha'}^{D'}}$$

and

$$\frac{\langle \Phi_\alpha(D) | \Phi_{D'} \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \frac{v_\alpha^D u_\alpha^{D'} - u_\alpha^D v_\alpha^{D'}}{u_\alpha^D u_\alpha^{D'} + v_\alpha^D v_\alpha^{D'}}$$

and

$$\frac{\langle \Phi_\alpha(D) | \Phi_{\alpha'}(D') \rangle}{\langle \Phi_D | \Phi_{D'} \rangle} = \frac{\delta_{\alpha\alpha'}}{\left(u_\alpha^D u_\alpha^{D'} + v_\alpha^D v_\alpha^{D'}\right)^2} + \frac{v_\alpha^D u_\alpha^{D'} - u_\alpha^D v_\alpha^{D'}}{u_\alpha^D u_\alpha^{D'} + v_\alpha^D v_\alpha^{D'}} \times \frac{u_{\alpha'}^D v_{\alpha'}^{D'} - v_{\alpha'}^D u_{\alpha'}^{D'}}{u_{\alpha'}^D u_{\alpha'}^{D'} + v_{\alpha'}^D v_{\alpha'}^{D'}}$$

With this, we are able to calculate the moments for each matrix element,

$$\begin{aligned} N_{\alpha\beta}^{(n)}\left(\bar{D}\right) &\equiv i^n \int_{-\infty}^{+\infty} ds\, s^n N_{\alpha\beta}\left(\bar{D} + \frac{s}{2}, \bar{D} - \frac{s}{2}\right) \\ H_{\alpha\beta}^{(n)}\left(\bar{D}\right) &\equiv i^n \int_{-\infty}^{+\infty} ds\, s^n H_{\alpha\beta}\left(\bar{D} + \frac{s}{2}, \bar{D} - \frac{s}{2}\right) \end{aligned} \tag{3.215}$$

where

$$\begin{aligned} \bar{D} + \frac{s}{2} &= D \\ \bar{D} - \frac{s}{2} &= D' \end{aligned}$$

In practice, we have a set of overlap values $N_{\alpha\beta}(D_i, D_j)$ and $H_{\alpha\beta}(D_i, D_j)$ calculated at discrete deformation values with $i, j = 1, \ldots, N_D$. Therefore, if we have a mesh of regularly spaced deformation values with

$$\delta D \equiv D_{i+1} - D_i$$

the moment integrals are then approximated by discrete sums,

$$\begin{aligned} N_{\alpha\beta}^{(n)}\left(\bar{D} = D_j\right) &\approx i^n \delta D \sum_{k=0}^{\min(j-1, N_D - j)} \left(D_{j+k} - D_{j-k}\right)^n N_{\alpha\beta}\left(D_{j+k}, D_{j-k}\right) \\ H_{\alpha\beta}^{(n)}\left(\bar{D} = D_j\right) &\approx i^n \delta D \sum_{k=0}^{\min(j-1, N_D - j)} \left(D_{j+k} - D_{j-k}\right)^n H_{\alpha\beta}\left(D_{j+k}, D_{j-k}\right) \end{aligned}$$

#### 3.3.4.7 Numerical example

Now, we apply the formalism derived above to the numerical example of section B.5. A major technical challenge in evaluating Eqs. (3.204), (3.205), and (3.206) in this case is the fact that the multi-$O(4)$ model has a maximum value of the deformation $|D|$ for a given set of single-particle states. For the numerical example of section B.5, this maximum value is $|D| = 42$. By contrast, the SME integrals (e.g., Eq. (3.215)) extend from $-\infty$ to $+\infty$. The artificial "walls" introduced by the maximum value of $|D|$ can create points where the $S_{ij}\left(\bar{D}\right)$, $T_{ij}\left(\bar{D}\right)$, and $U_{ij}\left(\bar{D}\right)$ curves are not differentiable. To illustrate this problem, we perform a set of four calculations:

1. Calculation using the standard multi-$O(4)$ model with maximum value of $|D| = 42$.
2. Calculation where the $u$ and $v$ coefficients do not reach 1 or 0 abruptly when $|D| = 42$, but rather are extended by an exponential function to approach their limiting values as $|D| \to \infty$ (in practice the exponential function is matched to the $u$ and $v$ coefficients at $|D| = 40$)
3. Calculation with exponentially extended $u$ and $v$ coefficients, as in 2 above, but in addition, the overlap $\langle \Phi_D | \Phi_{D'} \rangle$ has been replaced by a fit with a Gaussian function of the form
$$\left\langle \Phi_{\bar{D}+\frac{s}{2}} \middle| \Phi_{\bar{D}-\frac{s}{2}} \right\rangle = \exp\left[-\left(\gamma_0 + \gamma_2 \bar{D}^2 + \gamma_4 \bar{D}^4\right) s^2\right]$$
4. Calculation with extended $u$ and $v$ coefficients and fitted overlap, as in 3 above, but in addition with the second derivative of $\left[N^{(0)}\right]^{-1/2}$ set to zero:
$$\left(\frac{1}{\sqrt{N^{(0)}}}\right)'' = 0$$

The results of the SCIM calculations using the Hamiltonian in Eq. (3.203) are shown in Fig. 3.7. All the components of the $S$, $T$, and $U$ matrices that form this Hamiltonian are included in the calculations, but only the "$(0,0)$" components are plotted in Fig. 3.7. The $T_{00}\left(\bar{D}\right)$ values are negligible for all 4 calculations and are therefore not plotted. The calculation with the standard multi-$O(4)$ model (calculation 1) displays "kinks" for both $S_{00}\left(\bar{D}\right)$ and $U_{00}\left(\bar{D}\right)$ curves around $\left|\bar{D}\right| \approx 11.7$. This problem is already alleviated in calculation 2, by extending the $D$ dependence of the $u$ and $v$ coefficients, and therefore allowing the SME integrals to span their full range from $-\infty$ to $+\infty$. Another problem associated with the maximum $|D|$ value can be seen in Fig. 3.8 which shows the overlap $\left\langle \Phi_{\bar{D}+\frac{s}{2}} \middle| \Phi_{\bar{D}-\frac{s}{2}} \right\rangle$ as a function of $s$ for different values of $\bar{D}$. As $\bar{D}$ approaches the maximum value of 42, the overlap curves are defined in a smaller and smaller range of $s$ values. Eventually, when $\bar{D} = 42$, only the $s = 0$ value is allowed (and in that case, $D_1 = D_2 = 42$). The exponential extension of the $u$ and $v$ coefficients alone cannot produce a smooth curve for $\left\langle \Phi_{\bar{D}+\frac{s}{2}} \middle| \Phi_{\bar{D}-\frac{s}{2}} \right\rangle$ as $\bar{D} \to \pm 42$ unless these coefficients are allowed to approach their asymptotic values much more gradually, which would constitute a significant departure from the original multi-$O(4)$ model. An alternative approach is to replace the overlaps $\left\langle \Phi_{\bar{D}+\frac{s}{2}} \middle| \Phi_{\bar{D}-\frac{s}{2}} \right\rangle$ with a fit to a Gaussian form, which is done in calculation 3. The $S_{00}\left(\bar{D}\right)$ curve for this solution in Fig. 3.7 is very similar to the original multi-$O\,(4)$ model result (calculation 1), except that the "kink" near $\left|\bar{D}\right| \approx 11.7$ is not present, and the energy approaches a constant value for $\left|\bar{D}\right| \gtrsim 42$. The difference between calculations 1 and 3 in the $U_{00}\left(\bar{D}\right)$ curves is more pronounced: the values of $U_{00}\left(\bar{D}\right)$ are larger in calculation 3 for $39 \lesssim \bar{D} \lesssim 39$, and $U_{00}\left(\bar{D}\right) \to 0$ as $\bar{D} \to \pm\infty$. Finally in calculation 4, which is essentially the same as calculation 3 but with the second derivatives of the $\left[N^{(0)}\right]^{-1/2}$ matrix set to zero, the $S_{00}\left(\bar{D}\right)$ and $U_{00}\left(\bar{D}\right)$ curves have generally the same shape as for calculation 3 but with larger absolute values (except as $\bar{D} \to \pm\infty$, where the curves for calculations 3 and 4 begin to overlap).

In practice, Eq. (3.196) is solved by discretizing $\bar{D}$ into $\bar{D}_j$ values in steps of $\delta\bar{D} = 0.25$. The wave function solutions are of the form $g_i\left(\bar{D}_j\right)$. Replacing the derivatives in the Hamiltonian of Eq. (3.203) with finite differences, we therefore have to solve the discrete eigenvalue equation

$$\sum_{b,j} K_{(a,i),(b,j)}\, g_b\left(\bar{D}_j\right) = E g_a\left(\bar{D}_i\right) \tag{3.216}$$

We could substitute discretized forms of the derivatives of the wave functions $g_i\left(\bar{D}_j\right)$ into the SCIM equation,

$$\left\{H\left(\bar{q}\right) - E\right\} g\left(\bar{q}\right) = 0$$

to obtain the discretized form of $K_{(a,i),(b,j)}$, however this does not yield a manifestly Hermitian form of the Hamiltonian matrix. Instead, we use Eq. (.1) and write first for first-order SOPO term

$$\left\{\left[T\left(\bar{q}_i\right)\hat{P}\right]^{(1)} g\left(\bar{q}_i\right)\right\}_\alpha = -\frac{1}{2}\sum_\beta \left\{\left[\frac{\partial}{\partial\bar{q}}\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)\right] g_\beta\left(\bar{q}_i\right) + 2\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)\left[\frac{\partial}{\partial\bar{q}} g_\beta\left(\bar{q}_i\right)\right]\right\}$$

and re-arrange the terms as

$$\left\{\left[T\left(\bar{q}_i\right)\hat{P}\right]^{(1)} g\left(\bar{q}_i\right)\right\}_\alpha = -\frac{1}{2}\sum_\beta \left\{\left[\frac{\partial}{\partial\bar{q}}\left(\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right) g_\beta\left(\bar{q}_i\right)\right)\right] + \tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)\left[\frac{\partial}{\partial\bar{q}} g_\beta\left(\bar{q}_i\right)\right]\right\}$$

Discretizing the derivatives leads to

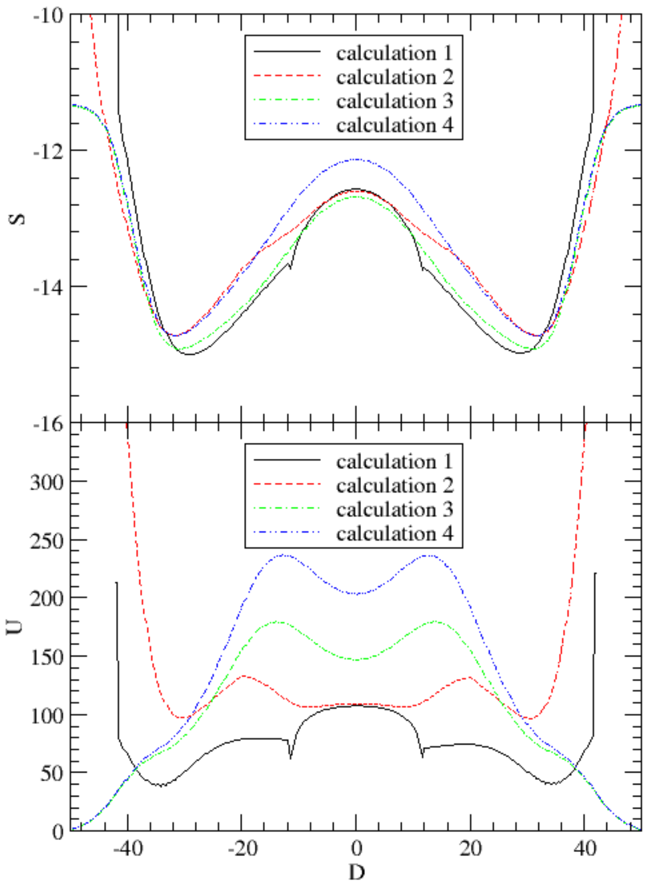


**Fig. 3.7** Coefficients $S$ and $U$ in the SCIM Hamiltonian of Eq. (3.203) compared for the 4 variations of the multi-$O\,(4)$ model (see text).

$$
\begin{aligned}
\left\{ \left[ T\left(\bar{q}_i\right) \hat{P} \right]^{(1)} g\left(\bar{q}_i\right) \right\}_{\alpha} &= -\frac{1}{2} \sum_{\beta} \left\{ \frac{\tilde{T}_{\alpha\beta}\left(\bar{q}_{i+1}\right) g_{\beta}\left(\bar{q}_{i+1}\right) - \tilde{T}_{\alpha\beta}\left(\bar{q}_{i-1}\right) g_{\beta}\left(\bar{q}_{i-1}\right)}{2\Delta\bar{q}} \right. \\
&\qquad \left. + \tilde{T}_{\alpha\beta}\left(\bar{q}_i\right) \frac{g_{\beta}\left(\bar{q}_{i+1}\right) - g_{\beta}\left(\bar{q}_{i-1}\right)}{2\Delta\bar{q}} \right\} \\
&= -\frac{1}{4\Delta\bar{q}} \sum_{\beta} \left\{ \left[ \tilde{T}_{\alpha\beta}\left(\bar{q}_{i+1}\right) + \tilde{T}_{\alpha\beta}\left(\bar{q}_i\right) \right] g_{\beta}\left(\bar{q}_{i+1}\right) \right. \\
&\qquad \left. - \left[ \tilde{T}_{\alpha\beta}\left(\bar{q}_{i-1}\right) + \tilde{T}_{\alpha\beta}\left(\bar{q}_i\right) \right] g_{\beta}\left(\bar{q}_{i-1}\right) \right\}
\end{aligned}
$$

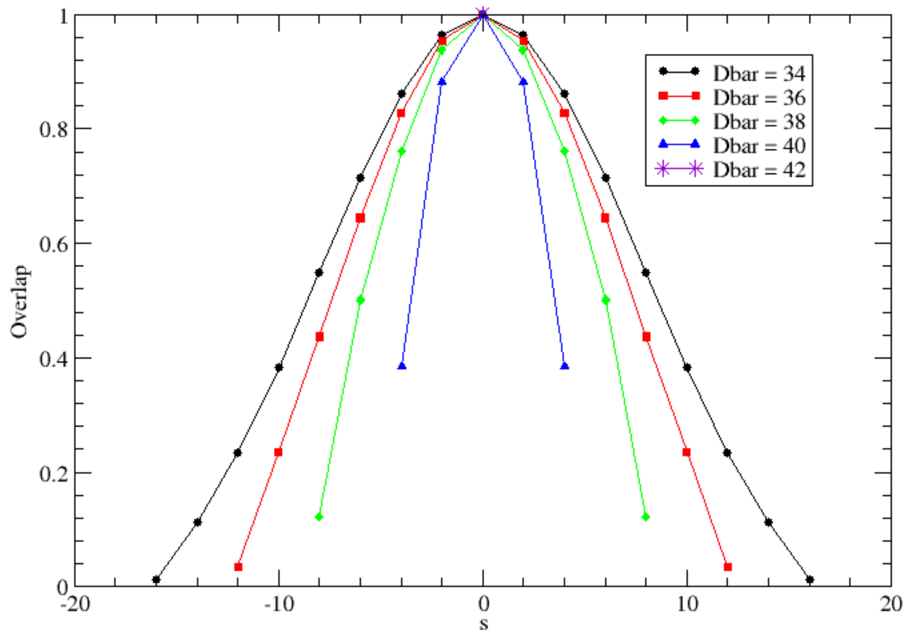


**Fig. 3.8** Kernel overlaps in the multi-$O\,(4)$ model as a function of $s$ for different $\bar{D}$ values showing the effect of the sharp cutoff in deformation of the model.

Let us now define

$$\bar{T}_{(\alpha,i),(\beta,j)} \equiv \frac{1}{4}\delta_{|i-j|,1}\frac{\tilde{T}_{\alpha\beta}\,(\bar{q}_i)+\tilde{T}_{\alpha\beta}\,(\bar{q}_j)}{\bar{q}_i-\bar{q}_j}$$

where

$$\Delta\bar{q} = \bar{q}_{i+1}-\bar{q}_i = \bar{q}_i-\bar{q}_{i-1}$$

so that

$$\begin{aligned}\left\{\left[T\left(\bar{q}_i\right)\hat{P}\right]^{(1)}g\left(\bar{q}_i\right)\right\}_\alpha &= \frac{1}{4}\sum_{\beta j}\left\{\frac{\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)+\tilde{T}_{\alpha\beta}\left(\bar{q}_{i+1}\right)}{\bar{q}_i-\bar{q}_{i+1}}g_\beta\left(\bar{q}_{i+1}\right)\right.\\ &\qquad\left.+\frac{\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)+\tilde{T}_{\alpha\beta}\left(\bar{q}_{i-1}\right)}{\bar{q}_i-\bar{q}_{i-1}}g_\beta\left(\bar{q}_{i-1}\right)\right\}\\ &= \sum_{\beta j}\bar{T}_{(\alpha,i),(\beta,j)}g_\beta\left(\bar{q}_j\right)\end{aligned}$$

and note that we have

$$\begin{aligned}\bar{T}_{(\beta,j),(\alpha,i)} &= \frac{1}{4}\delta_{|j-i|,1}\frac{\tilde{T}_{\beta\alpha}\left(\bar{q}_j\right)+\tilde{T}_{\beta\alpha}\left(\bar{q}_i\right)}{\bar{q}_j-\bar{q}_i}\\ &= \frac{1}{4}\delta_{|i-j|,1}\frac{-\tilde{T}_{\alpha\beta}\left(\bar{q}_j\right)-\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)}{\bar{q}_j-\bar{q}_i}\\ &= \bar{T}_{(\alpha,i),(\beta,j)}\end{aligned}$$

so that the matrix $\bar{T}$ is symmetric. For the second-order term we have

$$\begin{aligned}\left\{\left[U\left(\bar{q}_i\right)\hat{P}\right]^{(2)}g\left(\bar{q}_i\right)\right\}_\alpha &= \sum_\beta\left\{-\frac{1}{4}\left[\frac{\partial^2}{\partial\bar{q}^2}U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_i\right)-\left[\frac{\partial}{\partial\bar{q}}U_{\alpha\beta}\left(\bar{q}_i\right)\right]\left[\frac{\partial}{\partial\bar{q}}g_\beta\left(\bar{q}_i\right)\right]\right.\\ &\qquad\left.-U_{\alpha\beta}\left(\bar{q}_i\right)\left[\frac{\partial^2}{\partial\bar{q}^2}g_\beta\left(\bar{q}_i\right)\right]\right\}\\ &= -\frac{1}{4}\sum_\beta\left\{\left[\frac{\partial^2}{\partial\bar{q}^2}U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_i\right)+4\left[\frac{\partial}{\partial\bar{q}}U_{\alpha\beta}\left(\bar{q}_i\right)\right]\left[\frac{\partial}{\partial\bar{q}}g_\beta\left(\bar{q}_i\right)\right]\right.\\ &\qquad\left.+4U_{\alpha\beta}\left(\bar{q}_i\right)\left[\frac{\partial^2}{\partial\bar{q}^2}g_\beta\left(\bar{q}_i\right)\right]\right\}\end{aligned}$$

We can rearrange the terms as

$$\begin{aligned}\left\{\left[U\left(\bar{q}_i\right)\hat{P}\right]^{(2)}g\left(\bar{q}_i\right)\right\}_\alpha &= -\frac{1}{4}\sum_\beta\left\{2\left[\frac{\partial^2}{\partial\bar{q}^2}\left(U_{\alpha\beta}\left(\bar{q}_i\right)g_\beta\left(\bar{q}_i\right)\right)\right]-\left[\frac{\partial^2}{\partial\bar{q}^2}U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_i\right)\right.\\ &\qquad\left.+2U_{\alpha\beta}\left(\bar{q}_i\right)\left[\frac{\partial^2}{\partial\bar{q}^2}g_\beta\left(\bar{q}_i\right)\right]\right\}\end{aligned}$$

Discretizing the derivatives leads to

$$\begin{aligned}&\left\{\left[U\left(\bar{q}_i\right)\hat{P}\right]^{(2)} g\left(\bar{q}_i\right)\right\}_\alpha\\ &= -\frac{1}{4}\sum_\beta\left\{2\frac{U_{\alpha\beta}\left(\bar{q}_{i+1}\right)g_\beta\left(\bar{q}_{i+1}\right)-2U_{\alpha\beta}\left(\bar{q}_i\right)g_\beta\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_{i-1}\right)g_\beta\left(\bar{q}_{i-1}\right)}{\Delta\bar{q}^2}\right.\\ &\quad-\frac{U_{\alpha\beta}\left(\bar{q}_{i+1}\right)-2U_{\alpha\beta}\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_{i-1}\right)}{\Delta\bar{q}^2}g_\beta\left(\bar{q}_i\right)\\ &\quad\left.+2U_{\alpha\beta}\left(\bar{q}_i\right)\frac{g_\beta\left(\bar{q}_{i+1}\right)-2g_\beta\left(\bar{q}_i\right)+g_\beta\left(\bar{q}_{i-1}\right)}{\Delta\bar{q}^2}\right\}\end{aligned}$$

regrouping terms

$$\begin{aligned}\left\{\left[U\left(\bar{q}_i\right)\hat{P}\right]^{(2)} g\left(\bar{q}_i\right)\right\}_\alpha = -\frac{1}{4\Delta\bar{q}^2}\sum_\beta&\left\{\left[2U_{\alpha\beta}\left(\bar{q}_{i+1}\right)+2U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_{i+1}\right)\right.\\ &+\left[-4U_{\alpha\beta}\left(\bar{q}_i\right)-U_{\alpha\beta}\left(\bar{q}_{i+1}\right)+2U_{\alpha\beta}\left(\bar{q}_i\right)\right.\\ &\left.-U_{\alpha\beta}\left(\bar{q}_{i-1}\right)-4U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_i\right)\\ &\left.+\left[2U_{\alpha\beta}\left(\bar{q}_{i-1}\right)+2U_{\alpha\beta}\left(\bar{q}_i\right)\right]g_\beta\left(\bar{q}_{i-1}\right)\right\}\end{aligned}$$

Next we define

$$\begin{aligned}\bar{U}_{(\alpha,i),(\beta,j)} \equiv -\frac{1}{4\Delta\bar{q}^2}&\left\{2\left[U_{\alpha\beta}\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_j\right)\right]\delta_{|j-i|,1}\right.\\ &\left.-\left[U_{\alpha\beta}\left(\bar{q}_{i+1}\right)+6U_{\alpha\beta}\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_{i-1}\right)\right]\delta_{i,j}\right\}\end{aligned}$$

so that

$$\left\{\left[U\left(\bar{q}_i\right)\hat{P}\right]^{(2)} g\left(\bar{q}_i\right)\right\}_\alpha = \sum_{\beta j}\bar{U}_{(\alpha,i),(\beta,j)}g_\beta\left(\bar{q}_j\right)$$

and note that $\bar{U}$ is symmetric. For completeness, we also define

$$\bar{S}_{(\alpha,i),(\beta,j)} \equiv S_{\alpha\beta}\left(\bar{q}_i\right)\delta_{i,j}$$

Thus we have

$$\begin{aligned}\bar{K}_{(\alpha,i),(\beta,j)} &\equiv \bar{S}_{(\alpha,i),(\beta,j)}+\bar{T}_{(\alpha,i),(\beta,j)}+\bar{U}_{(\alpha,i),(\beta,j)}\\ &= \left\{S_{\alpha\beta}\left(\bar{q}_i\right)+\frac{1}{4\Delta\bar{q}^2}\left[U_{\alpha\beta}\left(\bar{q}_{i+1}\right)+6U_{\alpha\beta}\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_{i-1}\right)\right]\right\}\delta_{i,j}\\ &\quad+\left\{\frac{1}{4}\frac{\tilde{T}_{\alpha\beta}\left(\bar{q}_i\right)+\tilde{T}_{\alpha\beta}\left(\bar{q}_j\right)}{\bar{q}_i-\bar{q}_j}-\frac{1}{2\Delta\bar{q}^2}\left[U_{\alpha\beta}\left(\bar{q}_i\right)+U_{\alpha\beta}\left(\bar{q}_j\right)\right]\right\}\delta_{|i-j|,1}\end{aligned}$$

and we must solve the eigenvalue equation

$$\sum_{\beta j}\bar{K}_{(\alpha,i),(\beta,j)}g_\beta\left(\bar{q}_j\right) = E_{(\alpha,i)}g_\alpha\left(\bar{q}_i\right) \tag{3.217}$$

We have obtained the eigenvalues of $\bar{K}_{(\alpha,i),(\beta,j)}$ for the four calculations defined above. This process presents some technical challenges due to the appearance of many spurious eigenvalues because of the discretization of the problem. In order to more easily identify the physical solutions, we have started with the diagonalization of the submatrix $\bar{K}_{(0,i),(0,j)}$, which does not include any coupling to the quasiparticle states, and introduced a parameter $\kappa$ to introduce this coupling gradually as $\kappa$ is increased in small steps from 0 to 1 and where

$$\bar{K}_{(\alpha,i),(\beta,j)}(\kappa) \equiv \begin{cases} \bar{K}_{(\alpha,i),(\beta,j)} & \alpha = \beta = 0 \\ \kappa \bar{K}_{(\alpha,i),(\beta,j)} & \text{otherwise} \end{cases} \tag{3.218}$$

The eigenvalues as a function of $\kappa$ are plotted for calculation 1 in the top panel of Fig. 3.9. The first few eigenvalues of $\bar{K}_{(0,i),(0,j)}$ can be tracked until $\kappa \approx 0.6$. Beyond $\kappa \approx 0.6$ the eigenvalue spectrum becomes very noisy and it is impossible to track it all the way to $\kappa = 1$. By contrast calculation 2, which replaces the sharp cutoffs at $\bar{D} = \pm 42$ with a more gradual drop-off, is shown in the bottom panel of Fig. 3.9 and appears to be much "cleaner". Calculation 3, which uses the Gaussian overlap approximation, is shown in the too panel of Fig. 3.10. Here again, level repulsions complicate the behavior of the eigenvalues as a function of $\kappa$, especially in the $\kappa = 0.8 - 1$ range. In calculation 4, shown in the bottom panel of Fig. 3.10, the second-order derivative of $\left[N^{(0)}\right]^{-1/2}$ is set to zero and individual states can be discerned in the low-lying spectrum at $\kappa = 1$.

At $\kappa = 0$, a large number of solutions with zero energy are produced by the diagonalization of the discretized SCIM Hamiltonian. A closer examination of the eigenvectors for these solutions shows that they have a zero component in the HFB ground states at all deformations, and that they therefore consist entirely of 2-qp excitations built on those ground states. Since the $\kappa = 0$ limit explicitly excludes these pure 2-qp solutions (see Eq. (3.218)), we will consider them as spurious states. As $\kappa$ is gradually increased from 0 to 1, and the couplings between 0- and 2-qp states and among 2-qp states are introduced, the spurious solutions with only 2-qp components fan out from zero energy at $\kappa = 0$ to "pollute" the entire energy range of the spectrum for the higher $\kappa$ values. For our purposes, we will simply ignore these solutions in our analysis.

The energies of the first few excited states from calculations 2, 3, and 4, where individual levels can be identified in the low-lying spectrum, are compared in table 3.1 to the exact solution from section B.5. The results from calculation 3 in particular should be taken with some caution, given the level of noise in the spectrum at $\kappa = 1$. In general, the SCIM calculations seem to predict a first excited state very close to the ground state, just like the exact solution. The next excited state, at energy 1.606 in the exact calculation, has a closer match in calculations 3 and 4 than calculation 2. The last two excited states in 3.1 are somewhat best reproduced by calculation 4.

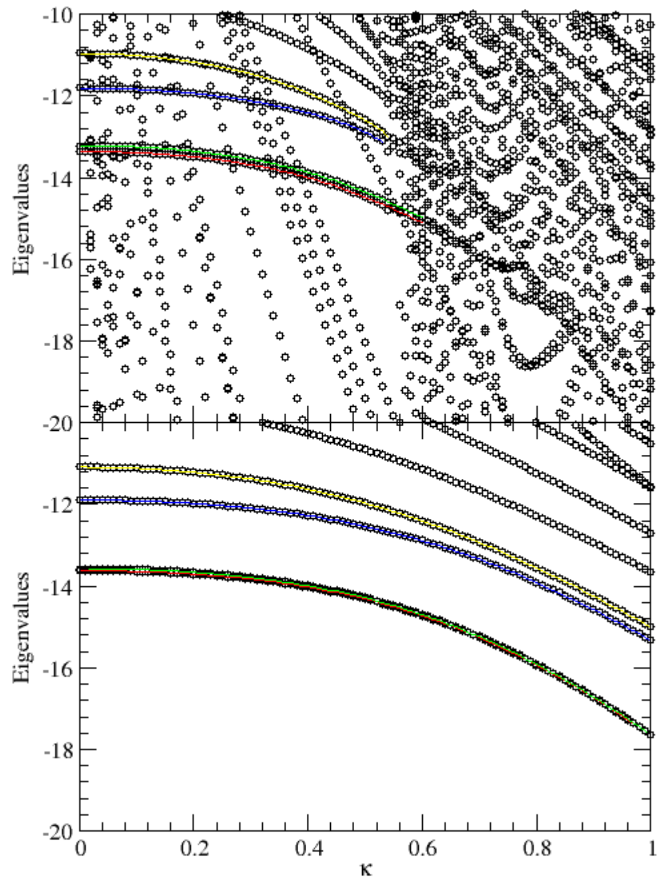


**Fig. 3.9** Eigenvalues for Eq. (3.217) as a function of damping parameter $\kappa$ in Eq. (3.218) for variations 1 (top panel) and 2 (bottom panel) of the multi-$O\,(4)$ model.

| Calc 2 | Calc 3 | Calc 4 | exact |
|---|---|---|---|
| 0.017 | 0.026 | 0.131 | 0.091 |
| 2.321 | 1.012 | 1.148 | 1.606 |
| 2.645 | 2.000 | 2.453 | 2.177 |
| 3.985 | 2.064 | 2.800 | 2.580 |

**Table 3.1** Energies of the first few excited states from variations 2, 3, and 4 of the SCIM calculations compared to the exact result for the multi-$O\,(4)$ model.

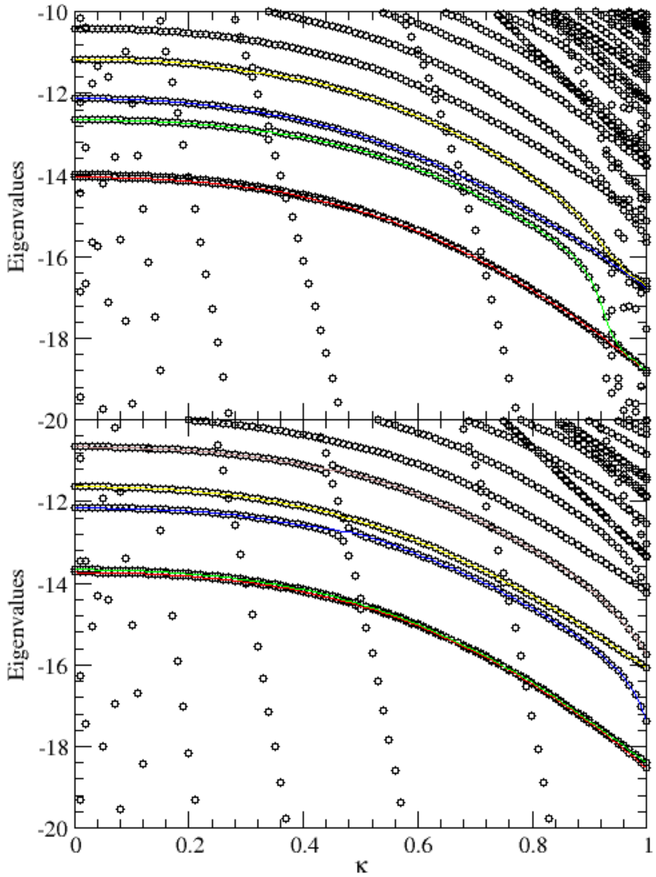


**Fig. 3.10** Same as Fig. 3.9, but for variations 3 (top panel) and 4 (bottom panel) of the multi-$O\,(4)$ model.

These four calculations show the numerical sensitivities of the spectrum, and some of the difficulties inherent in the solution of the SCIM. These difficulties are further complicated by the sharp cutoff at $\bar{D} = \pm 42$ built into the example we are studying. However, these results should only be taken as a pedagogical illustration of the SCIM equation due to some inherent limitations in the present analysis. In particular, we have not enforced good particle number in the calculations, which could be done using the techniques discussed in C. As we saw in section 3.1.4, this could easily affect the level energies by noticeable amounts.

The advantage of the multi-$O(4)$ is that it provides a versatile test bed to explore the SCIM. For example, in addition to comparing the energies of levels, as we did above, the SCIM wave functions themselves could be analyzed on the set of exact multi-$O(4)$ solutions in order to gain a better understanding of the SCIM states. The model can also serve as a check of further extensions to the SCIM such as the inclusion of 4-qp excitations, or of coherent 2-qp excitations (e.g., obtained from local QRPA calculations at each deformation point) which could provide a better set of collective and non-collective qp excitations that will be orthogonal by construction to vibrations in the deformation parameter.

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# Part II
# Application to low-energy fission

In the second part of the book we apply the microscopic method presented in part I to the fission problem. The starting point for microscopic calculation of fission is a set of constrained HFB states calculated with respect to a few collective parameters relevant to fission in the Hartree-Fock-Bogoliubov (HFB) approximation. These collective parameters serve as constraints in the HFB calculation. Once the HFB solutions have been calculated, the Time-Dependent Generator Coordinate Method (TDGCM) is invoked to construct a wave packet from the HFB solutions that describe the fissioning nucleus in a fully quantum-mechanical way. In practice, we do not solve the full Hill-Wheeler equations , but, as explained in section 3.2, an approximation that yields a collective, time-dependent Schrödinger equation (TDSE) . The potential- and kinetic-energy terms of this Schrödinger equation are calculated from the microscopic HFB solutions, and produce a collective Hamiltonian for the system constructed from the underlying microscopic degrees of freedom. The time-independent form of this equation is used first to generate a spectrum of initial collective states expressed as linear superpositions of static HFB solutions. These collective solutions are then evolved in time toward a set of scission configurations by solving the TDSE. The set of scission configurations form a line in calculations with two collective constraints (or a hypersurface of $D-1$ dimensions in $D$ dimensions) that defines a boundary between a pre-scission and a post-scission region. Within the pre-scission region the collective Hamiltonian describes a single (parent) nucleus, and in the post-scission region it describes two fragments moving apart and interacting eventually through their mutual Coulomb repulsion. We will describe this approach in greater detail in this chapter with the goal of computing fission-fragment mass, kinetic-energy and excitation-energy distributions that can be compared with experimental data, and illustrate the results in the case of neutron induced fission on a $^{239}$Pu target (i.e., fission from an excited state of $^{240}$Pu).

# Chapter 4
# General concepts

In this chapter we apply the formalism developed in the first part of the book to fission. We discuss the choice of collective coordinate adapted to the fission problem. We then present a quantum localization technique to progressively identify the wave function of the nascent pre-fragments within the wave function of the parent nucleus, and provide a quantum-mechanical definition of scission. We conclude with a discussion of the calculation of fission-fragment properties, in particular their mass distributions and total kinetic and excitation energies.

## 4.1 The choice of collective constraints

### 4.1.1 Multipole-moment constraints

Multipole moments (e.g. quadrupole $Q_{20}$ and $Q_{22}$, octupole $Q_{30}$, etc.) of the nucleus have been used as constraints in HFB calculations in a variety of applications with great success. The use of these collective parameters can be justified by the experimental observation of low-energy vibrational states of quadrupole, octupole, etc. character. In the case of fission, multipole constraints have already been routinely used with great success [4, 5, 6, 7, 8, 9].

The quadrupole moment of a nucleus described by an axially symmetric one-body density $\rho\,(r,z)$ can be expressed in cylindrical coordinates as

$$Q_{20} = 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\,(r,z) \left[2\,(z-\bar{z})^2 - r^2\right]$$

where

$$\bar{z} = \frac{1}{A} \times 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\,(r,z)\, z$$

is the abscissa of the center of mass of the nucleus on the $z$-axis, and the octupole moment is given by

$$Q_{30} = 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\,(r,z) \left[(z-\bar{z})^3 - \frac{3}{2}\,(z-\bar{z})\, r^2\right]$$

It is customary to impose the condition $Q_{10} = 0$ which forces the global center of mass of the system to lie at the origin of the coordinate system, i.e. we may set $\bar{z} = 0$ in the expression above.

The hexadecapole moment is given by

$$Q_{40} = 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\,(r,z) \left[(z-\bar{z})^4 - 3r^2\,(z-\bar{z})^2 + \frac{3}{8} r^4\right]$$

### *4.1.2 Constraints on the pre-fragments*

As the nucleus nears scission, constraints on the pre-fragments can give a more appropriate description of the fissioning system than global (e.g., multipole) constraints [12, 13]. If we partition the $z$ axis into two regions separated by a point $z = z_0$, then it is straightforward to show that

$$Q_{20} = Q_{20}^{(<)} + Q_{20}^{(>)} + 2\left[A_< \left(\bar{z}_< - \bar{z}\right)^2 + A_> \left(\bar{z}_> - \bar{z}\right)^2\right]$$

where

$$\begin{aligned} A_< &\equiv 2\pi \int_0^\infty dr\, r \int_{-\infty}^{z_0} dz\, \rho\,(r,z)\, z \\ A_> &\equiv 2\pi \int_0^\infty dr\, r \int_{z_0}^{+\infty} dz\, \rho\,(r,z)\, z \end{aligned} \tag{4.1}$$

and

$$\begin{aligned} \bar{z}_< &\equiv \frac{1}{A_<} \times 2\pi \int_0^\infty dr\, r \int_{-\infty}^{z_0} dz\, \rho\,(r,z)\, z \\ \bar{z}_> &\equiv \frac{1}{A_>} \times 2\pi \int_0^\infty dr\, r \int_{z_0}^{+\infty} dz\, \rho\,(r,z)\, z \end{aligned}$$

and

$$\begin{aligned} Q_{20}^{(<)} &\equiv 2\pi \int_0^\infty dr\, r \int_{-\infty}^{z_0} dz\, \rho\,(r,z) \left[2\left(z - \bar{z}_<\right)^2 - r^2\right] \\ Q_{20}^{(>)} &\equiv 2\pi \int_0^\infty dr\, r \int_{z_0}^{+\infty} dz\, \rho\,(r,z) \left[2\left(z - \bar{z}_>\right)^2 - r^2\right] \end{aligned}$$

and using the relations

$$\begin{aligned} A &= A_< + A_> \\ A\bar{z} &= A_<\bar{z}_< + A_>\bar{z}_> \end{aligned}$$

we can re-write the partitioned quadrupole moment in the more compact form

$$\boxed{Q_{20} = Q_{20}^{(<)} + Q_{20}^{(>)} + 2\mu d^2} \tag{4.2}$$

where the reduced mass $\mu$ and separation distance $d$ are given by

$$\begin{aligned} \mu &= \frac{A_< A_>}{A} \\ d &= \bar{z}_> - \bar{z}_< \end{aligned}$$

Similarly, we can show that octupole moment can be written in the partitioned form

$$\boxed{Q_{30} = Q_{30}^{(<)} + Q_{30}^{(>)} + \frac{3}{2}\left[A_{<}Q_{20}^{(>)} - A_{>}Q_{20}^{(<)}\right]\frac{d}{A} + \left(A_{<} - A_{>}\right)\mu\frac{d^3}{A}} \tag{4.3}$$

Eqs. (4.2) and (4.3) hint at the connection between the quadrupole and octupole moment constraints on the one hand, and the separation distance and mass asymmetry constraints we will introduce below.

#### 4.1.2.1 Neck constraint

Another useful constraint defines the number of particles in a "neck" region connecting the pre-fragments [4, 6],

$$Q_N = 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\left(r, z\right) \exp\left[-\frac{\left(z - z_N\right)^2}{a_N^2}\right] \tag{4.4}$$

where $a_N = 1$ fm and $z_N$ is found at each HFB iteration by minimizing the value of $Q_N$ given by Eq. (4.4). As the nucleus deforms and pre-fragments become discernible within its total density function $\rho\left(r, z\right)$, the neck position $z_N$ becomes better defined. Conversely, in the early stages of the fission process where the parent nucleus is only slightly deformed and has not yet developed a pronounced neck, the definition of $z_N$ is less clear. Possible ways of treating this ambiguity are discussed in section 4.1.2.3.

#### 4.1.2.2 Separation distance and mass asymmetry

The separation distance between fragments, $d$, was introduced in Eqs. (4.2) and (4.3):

$$d = \bar{z}_{>} - \bar{z}_{<} \tag{4.5}$$

As the nucleus approaches scission, this parameter provides a more appropriate description of the dynamical evolution of the pre-fragments than the global quadrupole moment $Q_{20}$.

We can also define a mass asymmetry parameter, which already appears in Eq. (4.3),

$$\xi \equiv \frac{A_{<} - A_{>}}{A_{<} + A_{>}} = \frac{A_{<} - A_{>}}{A} \tag{4.6}$$

to replace the octupole moment constraint $Q_{30}$. With the further constraint that the overall center of mass of the fissioning system be fixed at zero,

$$Q_{10} = 2\pi \int_0^{\infty} dr\, r \int_{-\infty}^{+\infty} dz\, \rho\left(r, z\right) z = 0$$

or, separating the integral over $z$ into regions $z \leq z_N$ and $z > z_N$,

$$A_< \bar{z}_< + A_> \bar{z}_> = 0 \tag{4.7}$$

Combining Eqs. (4.5), (4.6), and (4.7) it is easy to show that

$$\bar{z}_< = \frac{1}{2}(\xi - 1)\, d$$
$$\bar{z}_> = \frac{1}{2}(\xi + 1)\, d$$

and

$$A_< = \frac{A}{2}(1 + \xi)$$
$$A > = \frac{A}{2}(1 - \xi)$$

With these results, we can now re-write Eqs. (4.2) and (4.3) as

$$Q_{20} = Q_{20}^{(<)} + Q_{20}^{(>)} + \frac{A}{2}\left(1 - \xi^2\right) d^2$$

and

$$Q_{30} = Q_{30}^{(<)} + Q_{30}^{(>)} + \frac{3}{4}\left[Q_{20}^{(>)} - Q_{20}^{(<)} + \left(Q_{20}^{(>)} + Q_{20}^{(<)}\right)\xi\right] d + \frac{A}{4}\left(1 - \xi^2\right)\xi d^3$$

Thus, even though two points may be close together in the $(Q_{20}, Q_{30})$ plane, large variations in the pre-fragment moments can cause correspondingly large variations in $d$ and/or $\xi$. For example Table 4.1 shows the breakdown of the quadrupole and octupole moments in terms of the individual pre-fragment contributions for two nearby points in the $(Q_{20}, Q_{30})$ plane for $^{240}$Pu. Although the points are close together in $(Q_{20}, Q_{30})$ values, sudden changes in the pre-fragment moments cause a large variation in the asymmetry parameter (from 0.1154 to 0.1880), which corresponds to a variation in the heavy pre-fragment's average mass from 133.9 to 142.6. As a result, 9 mass units are missing in the calculation, and cannot be recovered even by taking finer step sizes in $Q_{20}$ and $Q_{30}$ [1]. The problem of missing masses can also be seen in Fig. 4.1 which shows the heavy pre-fragment mass calculated using Eq. (4.1) as a function of $Q_{30}$ for values of $Q_{20}$ just before and after scission. The case outlined in Table 4.1 can be seen along the pre-scission line, while an even more significant discontinuity can be seen along the post-scission line in going from $Q_{30} = 80\,\mathrm{b}^{3/2}$ to $Q_{30} = 84\,\mathrm{b}^{3/2}$. These types of discontinuities have been studied by Dubray and Regnier in [11].

---

[1] It may be possible to recover the missing masses by introducing many additional multipole constraints, thereby emulating the constraints on the pre-fragments.

| | $(Q_{20} = 36800\ \mathrm{fm}^2, Q_{30} = 60000\ \mathrm{fm}^3)$ | $(Q_{20} = 36400\ \mathrm{fm}^2, Q_{30} = 64000\ \mathrm{fm}^3)$ |
|---|---|---|
| $Q_{20}^{(<)}$ | $201.657\ \mathrm{fm}^2$ | $1116.55\ \mathrm{fm}^2$ |
| $Q_{20}^{(>)}$ | $1841.99\ \mathrm{fm}^2$ | $1295.44\ \mathrm{fm}^2$ |
| $Q_{30}^{(<)}$ | $567.014\ \mathrm{fm}^3$ | $2839.36\ \mathrm{fm}^3$ |
| $Q_{30}^{(>)}$ | $-906.088\ \mathrm{fm}^3$ | $-1054.52\ \mathrm{fm}^3$ |
| $d$ | $17.1056\ fm$ | $17.1359\ fm$ |
| $\xi$ | 0.1154 | 0.1880 |

**Table 4.1** Pre-fragment moments and $(d, \xi)$ values for two neighboring points near scission for $^{240}$Pu.

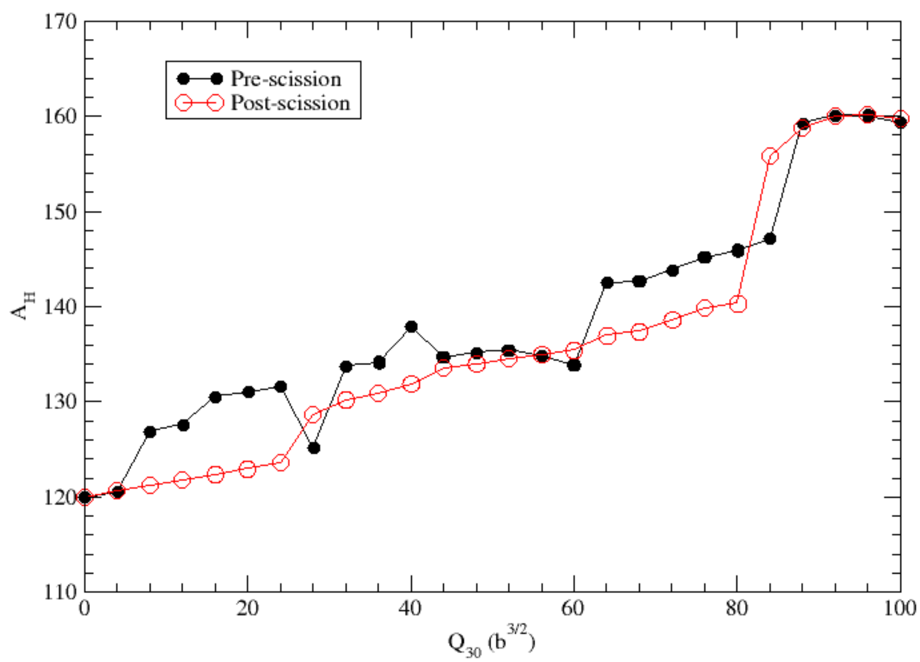


**Fig. 4.1** Fragment mass numbers obtained immediately before and after scission using Eq. (4.1) in $(Q_{20}, Q_{30})$ constrained HFB calculations.

#### 4.1.2.3 A consistent prescription for the neck position

The main challenge in performing the constrained HFB calculation is to define the $(d, \xi)$ coordinates in a consistent manner at all deformations of the fissioning nucleus. The definition of both $d$ and $\xi$, as outlined in section 4.1.2.2 depends on the identification of a neck position $z_N$. In the case of $^{240}$Pu, we find that for $d \geq 11\,\mathrm{fm}$ a neck region can be clearly identified in the total density $\rho\,(r, \varphi, z)$. For $d < 11\,\mathrm{fm}$, it becomes increasingly difficult to recognize a neck region in the total density as the deformation of the nucleus decreases. One possibility would be to treat $z_N$ as a variational parameter at low deformation, and choose the value that minimizes the HFB energy for each given $(d, \xi)$ constraint. However, as Fig. 4.2 shows for a calculation at $d = 6.5\,\mathrm{fm}$ (which corresponds to the first well) and exploring the $z_N$ parameter in discrete steps to minimize the HFB energy, this leads to a linear dependence of $z_N$ on $A_H$, and an energy surface that is nearly flat in $A_H$. Using $(d, \xi)$ to calculate the initial collective states would in turn lead to a much lower density of initial collective states compared to calculations with the $(Q_{20}, Q_{30})$ constraints (see section 5.0.4). Our goal is for the dynamical calculations with the $(d, \xi)$ parameters to reproduce as closely as possible those with $(Q_{20}, Q_{30})$ at low deformation, and therefore we reject the approach where $z_N$ is treated as a variational parameter. Instead, we use the calculations at $d = 11\,\mathrm{fm}$, where the neck position is more easily discerned, and fix those $z_N\,(A_H)$ values for all $d < 11\,\mathrm{fm}$ (as shown in Fig. 4.3 for a few masses $A_H$). We will show in section 5.0.4 that this prescription leads to a density of initial states calculated in the $(d, \xi)$ variables that is very similar to the one obtained with $(Q_{20}, Q_{30})$ variables.

## 4.2 A quantum mechanical picture of scission

We have so far referred to scission configurations of the nucleus without giving a concrete definition for this term. In the microscopic approach to fission that we outlined at the beginning of the section, the concept of scission played a central role in defining a boundary between two regions in the dynamic calculations. In [12] we introduced a quantum-mechanical definition of scission, which has been adopted in subsequent work [9]. This definition of scission was motivated by the need to recognize the wave functions of the pre-fragments within the wave function of the parent nucleus progressively, as the system deforms on the way to its breaking point. We now describe this approach in greater detail, as it relates to the present work.

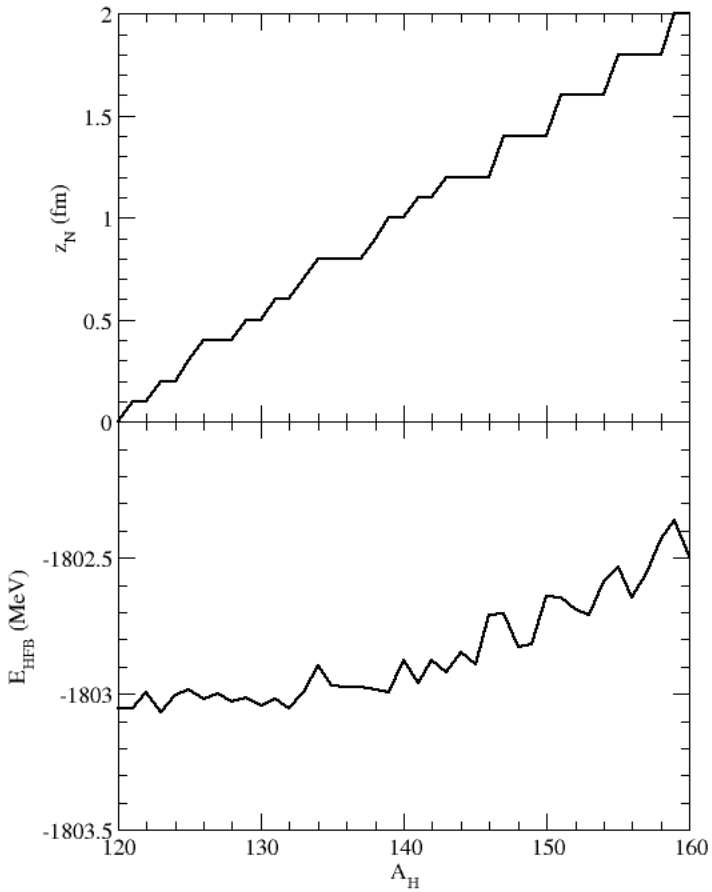


**Fig. 4.2** Top panel: neck position ($z_N$) obtained by minimizing the HFB energy at fixed $d = 6.5$ fm as a function of mass number $A_H$. The bottom panel shows the corresponding (minimized) HFB energy. The stagger in the curves is due to the finite step sized used to vary $z_N$.

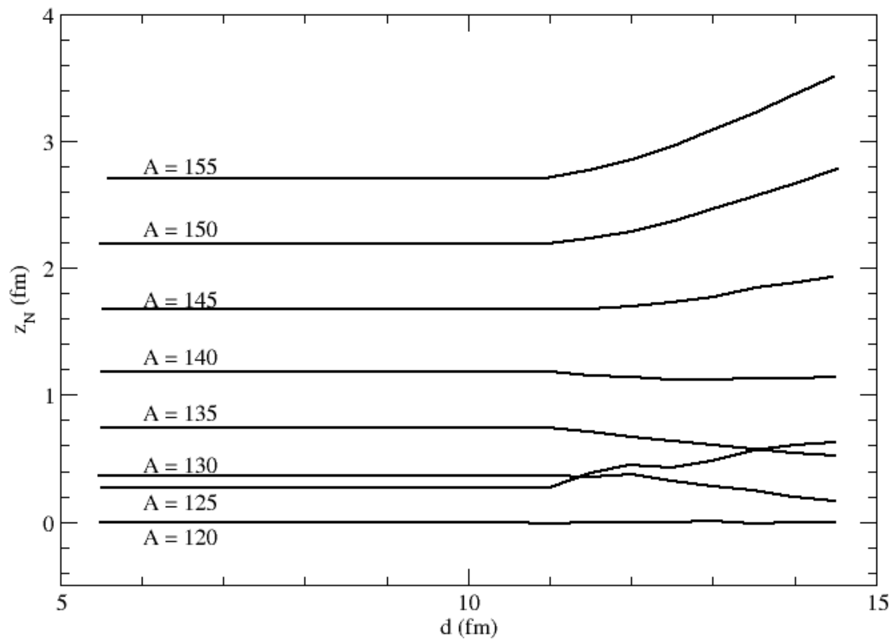


**Fig. 4.3** Neck position $z_N$ obtained using the prescription described in section 4.1.2.3, and plotted as a function of separation distance $d$ between pre-fragments for several mass divisions from $A_H = 120$ to $A_H = 155$.

### *4.2.1 Quantum localization*

For each quasiparticle state $\mu$, we calculate its contribution $\rho_\mu(\mathbf{r})$ to the total density as

$$\rho_\mu(\mathbf{r}) = \sum_{k,k'} V^*_{k'\mu} V_{k\mu} \Phi^*_{k'}(\mathbf{r}) \Phi_k(\mathbf{r})$$

where the $\Phi_k(\mathbf{r})$ are basis states, and the $V_{k\mu}$ are matrix elements of the HFB solution in that basis. Next, we introduce the left and right occupations

$$\left(v_\mu^{(\mathrm{L})}\right)^2 \equiv \int_{-\infty}^{z_N} dz \int_0^{2\pi} d\varphi \int_0^{\infty} r dr \rho_\mu (\mathbf{r})$$
$$\left(v_\mu^{(\mathrm{R})}\right)^2 \equiv \int_{z_N}^{\infty} dz \int_0^{2\pi} d\varphi \int_0^{\infty} r dr \rho_\mu (\mathbf{r})$$

For example, for a quasiparticle with $\left(v_\mu^{(\mathrm{L})}\right)^2 > \left(v_\mu^{(\mathrm{R})}\right)^2$, we can think of that quasiparticle as predominantly localized in the left fragment. To better quantify the "degree" of localization, we then define a localization parameter

$$\ell_\mu \equiv \frac{\left|\left(v_\mu^L\right)^2 - \left(v_\mu^R\right)^2\right|}{\left(v_\mu^L\right)^2 + \left(v_\mu^R\right)^2} \tag{4.8}$$

for each quasiparticle. Thus, for example, a value $\ell_\mu = 0$ corresponds to a completely delocalized quasiparticle that cannot be preferentially assigned to either fragment. We note that localization measures have other useful applications in nuclear physics beyond fission [10].

As we noted in [12], the HFB solution calculated for the parent does not automatically produce well-localized quasiparticles. As a result, if we assign individual quasiparticles to the fragments based on their $\ell_\mu$ values and plot the resulting densities associated with the fragments we typically observe a "tail" from each fragment extending into its complementary partner. These tails may appear relatively small, but because they extend deeply into the complementary pre-fragment, they can contribute a sizable amount of energy to the interaction between the pre-fragments, making it impossible to formulate a criterion for scission based on the wave functions of those pre-fragments or on their mutual interaction energy. In fact, calculations for the most probable fission configuration in $^{240}$Pu at scission shows that for each particle in the tails, the attractive nuclear interaction between pre-fragments binds them by an additional $\approx 50\,\mathrm{MeV}$. This problem is further exacerbated by level crossings as the pre-fragments move apart, which allow tunneling between the individual pre-fragments' potential wells and causes spikes in their mutual interaction energy.

The solution to the problem lies in the fact that in HFB calculations the **global** properties of the nuclear system are not affected by applying an arbitrary unitary transformation to the HFB destruction operators [14, 12, 13]. We are free to choose this transformation to further localize the individual quasiparticle states on their respective pre-fragments, and reduce the size of the tails, without changing any of the global properties of the HFB solution (total energy, moments, etc.). In practice, pairs $(\mu, \nu)$ of quasiparticles are mixed by an orthogonal transformation with angle $\theta_{\mu\nu}$ according to

$$\begin{pmatrix} V_{k\mu}(\theta_{\mu\nu}) \\ V_{k\nu}(\theta_{\mu\nu}) \end{pmatrix} = \begin{pmatrix} \cos\theta_{\mu\nu} & -\sin\theta_{\mu\nu} \\ \sin\theta_{\mu\nu} & \cos\theta_{\mu\nu} \end{pmatrix} \begin{pmatrix} V_{k\mu} \\ V_{k\nu} \end{pmatrix}$$

and where we choose the angle $\theta_{\mu\nu}$ that maximizes the pairwise localization parameter

$$\ell_{\mu\nu}\left(\theta_{\mu\nu}\right) \equiv \sqrt{\left[v_{\mu}^{2}\left(\theta_{\mu\nu}\right)\ell_{\mu}\left(\theta_{\mu\nu}\right)\right]^{2} + \left[v_{\nu}^{2}\left(\theta_{\mu\nu}\right)\ell_{\nu}\left(\theta_{\mu\nu}\right)\right]^{2}}$$

where $\ell_{\mu}$ and $\ell_{\nu}$ are given by Eq. (4.8), and

$$v_{\mu}^{2}\left(\theta_{\mu\nu}\right) = \sum_{k} V_{k\mu}^{*}\left(\theta_{\mu\nu}\right) V_{k\mu}\left(\theta_{\mu\nu}\right)$$

We have chosen this form of $\ell_{\mu\nu}\left(\theta_{\mu\nu}\right)$ because $\partial\ell_{\mu\nu}^{2}/\partial\theta_{\mu\nu} = 0$ yields a quadratic equation that can be solved analytically for $\cos\theta_{\mu\nu}$ and $\sin\theta_{\mu\nu}$. Through a systematic search algorithm, a set of quasiparticle pairs and their mixing angles is then found that minimizes the summed tail size of the two fragments.

In selecting the pairs of quasiparticle orbitals to mix, we take care that 1) their quasiparticle energies before mixing are no too far apart (in practice, less than 2 MeV apart), and 2) that the quasiparticles are not "mirror states". Two states are mirrors of each other if they have similar quasiparticle energies, but are on opposite sides of the Fermi level. In practice, two states were considered to be mirrors if their quasiparticle energies were each greater than 10 MeV but no more than 2 MeV apart, and if one of the quasiparticles had an occupancy smaller than 0.3, while the occupancy of the other was greater than 0.7.

The task of considering all possible sets of pairs of quasiparticles is not computationally tractable for a typical HFB calculation in a heavy nucleus. Therefore, we have adopted an algorithm to select a manageable but relevant set of quasiparticles to mix in pairs. The quasiparticle states are first sorted by decreasing order of their tail size. Then, for each quasiparticle in that ordered list, a partner is found such that

1. the two states are sufficiently close in energy ($\Delta\varepsilon \leq 2\,\mathrm{MeV}$)
2. the states are not mirrors (according to the criteria given above)
3. the optimal mixing angle $\theta_{\mu\nu}$ produces the largest $\ell_{\mu\nu}\left(\theta_{\mu\nu}\right)$, compared to all other possible partners

When two quasiparticle states are matched in this second approach, they are taken out of the set of available states. Thus, in effect, this second approach only constructs a single set of possible pairings (unlike the first approach which constructs many such sets). Given that the quasiparticles have been ordered by tail size, the expectation is that this single set will nevertheless represent a choice of pairings that is likely to significantly reduce the tail sizes of the fragments (and thereby localize them). This procedure was iterated 3 times to further improve the localization. As a rule of thumb, we found in most cases that the total number of particles in the tails (obtained by integrating the densities of the two tails on either side of $z_N$) can be reduced to $\sim Q_N$.

### 4.2.2 Energy partition

After mixing, we divide the quasiparticle states into two sets those that are predominantly to the left of the neck position, and those that are predominantly to its right. In principle there should also a third set consisting of states in the continuum with negligible occupancy and that cannot be definitely assigned to either fragment. In practice, those states do not significantly contribute to any property of the fragments, and arbitrarily assigning them to one or the other as a matter of convenience does not pose any real problems. Thus, we have creation operators for quasiparticles localized on the left ($L$) fragment and right ($R$) fragments

$$\eta^{\dagger}_{\mu\in \mathrm{L}} = \sum_n \left[ U_{n\mu} a^{\dagger}_n + V_{n\mu} a_n \right]$$
$$\eta^{\dagger}_{\nu\in \mathrm{R}} = \sum_n \left[ U_{n\nu} a^{\dagger}_n + V_{n\nu} a_n \right]$$

and corresponding destruction operators. The corresponding density matrix elements are

$$\rho^{(S)}_{mn} = \sum_{\mu\in S} V^{*}_{m\mu} V_{n\mu}$$

where $S = \mathrm{L}$ or R, and the pairing tensor matrix elements are

$$\kappa^{(S)}_{mn} = \sum_{\mu\in S} U^{*}_{m\mu} V_{n\mu}$$

The standard HFB energy can then be broken down into the energies of the individual fragments

$$\begin{aligned} E^{(\mathrm{L})} &= \sum_{mn} t_{mn}\rho^{(\mathrm{L})}_{nm} + \frac{1}{2}\sum_{mnpq} \rho^{(\mathrm{L})}_{pm}\bar{V}_{mnpq}\rho^{(\mathrm{L})}_{qn} + \frac{1}{4}\sum_{mnpq} \kappa^{(\mathrm{L})*}_{pm}\bar{V}_{mnpq}\kappa^{(\mathrm{L})}_{qn} \\ E^{(\mathrm{R})} &= \sum_{mn} t_{mn}\rho^{(\mathrm{R})}_{nm} + \frac{1}{2}\sum_{mnpq} \rho^{(\mathrm{R})}_{pm}\bar{V}_{mnpq}\rho^{(\mathrm{R})}_{qn} + \frac{1}{4}\sum_{mnpq} \kappa^{(\mathrm{R})*}_{pm}\bar{V}_{mnpq}\kappa^{(\mathrm{R})}_{qn} \end{aligned} \tag{4.9}$$

and an interaction energy between them

$$\begin{aligned} V_{\mathrm{int}} = \frac{1}{2}\sum_{mnpq} \rho^{(\mathrm{L})}_{pm}\bar{V}_{mnpq}\rho^{(\mathrm{R})}_{qn} + \frac{1}{4}\sum_{mnpq} \kappa^{(\mathrm{L})*}_{pm}\bar{V}_{mnpq}\kappa^{(\mathrm{R})}_{qn} \\ + \frac{1}{2}\sum_{mnpq} \rho^{(\mathrm{R})}_{pm}\bar{V}_{mnpq}\rho^{(\mathrm{L})}_{qn} + \frac{1}{4}\sum_{mnpq} \kappa^{(\mathrm{R})*}_{pm}\bar{V}_{mnpq}\kappa^{(\mathrm{L})}_{qn} \end{aligned} \tag{4.10}$$

which can be further broken down into the contributions from the nuclear and Coulomb terms of the effective interaction if needed. Note that, for density-dependent interactions ($V_{DD}$), there is a possible ambiguity in terms of which density should be used. In the present work, that part of the interaction was calculated for each fragment, using its own localized density, i.e.,

$$\begin{aligned} V_{DD}^{(\mathrm{L})} &= V_{DD}\left[\rho^{(\mathrm{L})}\right] \\ V_{DD}^{(\mathrm{R})} &= V_{DD}\left[\rho^{(\mathrm{R})}\right] \end{aligned} \tag{4.11}$$

while for the interaction term between the fragments, the density-dependent contribution was obtained as the remainder

$$V_{DD}^{(\mathrm{int})} = V_{DD}\left[\rho\right] - V_{DD}\left[\rho^{(\mathrm{L})}\right] - V_{DD}\left[\rho^{(\mathrm{R})}\right] \tag{4.12}$$

As the fragments separate after scission, and in principle can be better localized using the procedure described in 4.2.1, the spatial overlap between $\rho^{(\mathrm{L})}$ and $\rho^{(\mathrm{R})}$ vanishes, and the interaction contribution in Eq. (4.12) tends to zero, as expected.

Note that any terms that come from the center-of-mass correction have to be removed from the interaction energy in Eq. (4.10) if we are interested in the potential energy between the pre-fragments. Those center-of-mass terms should instead be included in the zero-point-energy $\epsilon_0$ discussed in section 4.2.4. To clarify this point in anticipation of the discussion in section 4.2.4, we give the partition of the kinetic-energy term in detail. The kinetic-energy operator for the $A$-nucleon parent, including two-body center-of-mass corrections ($\bar{K}_A$), is

$$K - \bar{K}_A = -\frac{\hbar^2}{2m}\left(1 - \frac{1}{A}\right)\sum_{i=1}^{A}\boldsymbol{\nabla}_i^2 + \frac{\hbar^2}{mA}\sum_{i>j}\boldsymbol{\nabla}_i\cdot\boldsymbol{\nabla}_j$$

For the left ($L$) and right ($R$) pre-fragments we have similar forms of the kinetic-energy operator,

$$K_S - \bar{K}_S = -\frac{\hbar^2}{2m}\left(1 - \frac{1}{A_S}\right)\sum_{i\in S}\boldsymbol{\nabla}_i^2 + \frac{\hbar^2}{mA_S}\sum_{\substack{i>j\\ i,j\in S}}\boldsymbol{\nabla}_i\cdot\boldsymbol{\nabla}_j$$

where $S = L$ or $R$. Thus, the kinetic-energy operator of the $A$-nucleon system can be written as

$$K - \bar{K}_A = \left(K_L - \bar{K}_L\right) + \left(K_R - \bar{K}_R\right) + \bar{K}_{\mathrm{rel}} \tag{4.13}$$

bringing out a term $\bar{K}_{\mathrm{rel}}$, that corresponds to the relative kinetic energy of the pre-fragments. This term is exactly the zero-point-energy $\epsilon_0$ discussed in section 4.2.4. Formally, it can be written as the difference between total and pre-fragment center-of-mass terms,

$$\bar{K}_{\text{rel}} = \bar{K}_L + \bar{K}_R - \bar{K}_A$$

### 4.2.3 Scission criteria

We reiterate and expand on the three scission criteria that we proposed in [12]:

1. the Coulomb repulsion must greatly exceed the attractive nuclear interaction between the pre-fragments
2. the exchange part of the interaction between the fragments must be small
3. it is possible to excite two-quasiparticle states on each pre-fragment that remain localized on those pre-fragments

The first criterion guarantees that the pre-fragments will fly apart quickly and that their internal degrees of freedom can be treated as "frozen" in a sudden approximation, insofar as the dynamics of the system beyond scission is concerned. Thus, scission marks the boundary between an inner region where the nuclear state is described by adiabatic HFB calculations, and an outer region where individual fragments are in a very complicated excitation configuration relative to their respective ground states. Thanks to the quantum localization procedure described in section 4.2.1, and the definition of the interaction energy in Eq. (4.10), both the Coulomb and nuclear interaction energies can be calculated in a consistent manner from a unique effective interaction between the nucleons. Figure 4.4 shows the nuclear part (i.e., the interaction energy in Eq. (4.10) minus the direct Coulomb contribution) of the interaction energy between the pre-fragments, calculated after quantum localization and plotted along the scission line as a function of neck size $Q_N$ for the different fragmentations (labeled by the heavy fragment mass number $A_H$). The figure shows the nuclear interaction gradually tending to zero as the neck disappears, thanks to the quantum localization procedure. The second scission criterion ensures that the system behaves as two Bogoliubov vacua as far as expectation values of interest are concerned. This is a purely quantum-mechanical criterion that stems from the non-local nature of the HFB wave function. The third and final criterion anticipates future work based on [15] and described earlier in this manuscript, where the GCM is extended to include quasiparticle excitations, in additional to the collective modes. This extension would provide a more complete description of the fission process, which includes the coupling between collective and internal degrees of freedom. Thus, the third criterion ensures that including these internal excitations, of the form

$$|\mu\bar{\nu}\rangle = \eta_\mu^\dagger \eta_{\bar{\nu}}^\dagger \left|\tilde{0}\right\rangle$$

does not automatically destroy the localization of the wave function. With these three criteria, the pre-fragments can be considered as separate entities, each with its own set of excitations, interacting through a (mainly repulsive) force that acts only on their centers of mass.

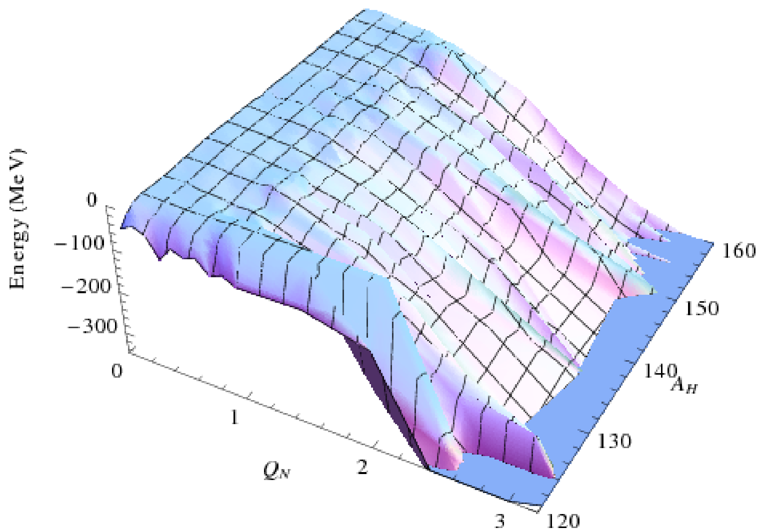


**Fig. 4.4** Nuclear interaction energy between the pre-fragments calculated after quantum localization for $^{240}$Pu near scission.

### 4.2.4 Description of the nucleus beyond scission

Because we wish to extract the excitation and kinetic energies of the fragments, we must halt the variational approach at scission and "freeze" the fragments in their configurations at that point. Beyond scission, we adopt the sudden approximation and assume that the fragments propagate according to a Hamiltonian that depends only on their separation

$$H_{\mathrm{coll}} = -\frac{\mathbf{p}_d^2}{2\mu m} + V\left(d\right) + E_L + E_R + \varepsilon_0 \tag{4.14}$$

where $\mathbf{p}_d$ is the relative momentum of the fragments, $\mu \equiv A_L A_R / A$ is their reduced mass number, and $m$ the nucleon mass, $V(d)$ is the interaction between the fragments (i.e., mainly Coulomb, unless the fragments are still close enough together to feel a small amount of attractive nuclear interaction), $E_L$ and $E_R$ are the internal energies of the fragments (and are constant with respect to $d$ in our sudden approximation) calculated with their center-of-mass correction,

$$E_i = \left\langle \Phi_i \left| H_i - \frac{\mathbf{p}_i^2}{2A_i m} \right| \Phi_i \right\rangle$$

and $\varepsilon_0$ is a zero-point energy that gives the relative center-of-mass-correction [12],

$$\varepsilon_0 \equiv \left\langle \Phi_d \left| \frac{\mathbf{p}_L^2}{2A_L m} + \frac{\mathbf{p}_R^2}{2A_R m} - \frac{\mathbf{p}^2}{2Am} \right| \Phi_d \right\rangle$$

where $\mathbf{p}^2/2Am$ is the center-of-mass energy of the $A$-nucleon system, and which is subtracted throughout the fission process (both before and after scission). At scission (which we denote by $d = d_s$), the energy of the system given by Eq. (4.14) is

$$\langle \Phi_{d_s} \left| H_{\mathrm{coll}} \right| \Phi_{d_s} \rangle = \left\langle \Phi_{d_s} \left| -\frac{\mathbf{p}_d^2}{2\mu m} \right| \Phi_{d_s} \right\rangle + \left\langle \Phi_{d_s} \left| H_L + H_R + V\left(d_s\right) - \frac{\mathbf{p}^2}{2Am} \right| \Phi_{d_s} \right\rangle$$

Note that

$$E_s \equiv \left\langle \Phi_{d_s} \left| H_L + H_R + V\left(d_s\right) - \frac{\mathbf{p}^2}{2Am} \right| \Phi_{d_s} \right\rangle$$

is just the HFB energy of the fissioning parent nucleus at scission, including center-of-mass correction, while

$$E_{\mathrm{pre}} \equiv \left\langle \Phi_{d_s} \left| -\frac{\mathbf{p}_d^2}{2\mu m} \right| \Phi_{d_s} \right\rangle$$

is the so-called pre-scission kinetic energy of the system, acquired dynamically in the evolution from saddle to scission (assuming zero kinetic energy at the saddle). We will return to the calculation of $E_{\mathrm{pre}}$ in section 4.4.2.

## 4.3 Calculation of fragment mass distributions

### *4.3.1 The collective Hamiltonian*

In the microscopic approach developed in [3], we begin with a Bohr-type Hamiltonian written in quantized form according to the expression (3.106) given in Section 3.2.1 (implicit summation over repeated indices is implied here)

$$H_{\mathrm{coll}} = -\frac{\hbar^2}{2} \frac{\partial}{\partial x^k} B_{k,l}(x) \frac{\partial}{\partial x^l} + V(x) + V_K(x) \tag{4.15}$$

Here $x \equiv (d, \xi)$ represent the two collective coordinates adopted for describing the fission mode, $B_{k,l}(x)$ is the collective inertia tensor, the inverse of the collective mass tensor $\mathcal{M}$,

$$B_{k,l}(x) = \left[\mathcal{M}^{-1}(x)\right]_{k,l} \tag{4.16}$$

The potential $V(x)$ is given by (see Eqs. (3.79)-(3.80))

$$\begin{aligned} V(x) &= E_{HFB}(x) - \varepsilon_0(x) \\ \varepsilon_0(x) &= \frac{\hbar^2}{2} g_{k,l} B_{k,l}(x) + \frac{1}{8} g^{k,l} \frac{\partial^2 E_{HFB}(x)}{\partial x^k \partial x^l} + \frac{\hbar^2}{8} \frac{\partial^2 B_{k,l}(q)}{\partial x_k \partial x^l} \end{aligned} \tag{4.17}$$

where $E_{HFB}(x)$ is the HFB potential energy surface in the $(d, \xi)$ variables, $\varepsilon_0(x)$ the so-called "zero-point energy (ZPE) correction", $g_{k,l}$ the elements of the matrix that enters the Gaussian form of the overlap kernel (see Eq. (3.56)) and $g^{k,l}(x)$ the elements of its inverse.
The additional potential $V_K(x)$ is given by Eq. (3.105)

$$V_K(x) = \frac{\hbar^2}{8g^{1/4}} \frac{\partial}{\partial x^k} \left[ B_{k,l}\ g^{-3/4} \frac{\partial g}{\partial x^l} \right]$$

where $g$ is the determinant of the matrix $g_{k,l}$. As explained in Section 4.2.1, this potential arises from the elimination of the $g^{1/2}$ terms that appear as a metric in the kinetic component of the collective Hamiltonian and in the normalization of the collective wave functions.
Let us mention that, in our applications to fission, the last term in $\varepsilon_0(x)$ which is proportional to the second derivative of the inertia is neglected since it is of higher order than the quantities that are kept in the reduction of the Hill-Wheeler equation to a Schrödinger-like equation. On the other hand, a so-called "rotational ZPE" contribution, $\varepsilon_{0_{\text{Rot}}}(x)$ is added to $\varepsilon_0(x)$ whose purpose is to remove from the collective potential the spurious contributions coming from the fluctuations in the orientation in space of the whole nucleus that exist within the constrained HFB states $|\Phi_x\rangle$. This contribution is calculated as in Ref. [19], by summing the ZPE contributions associated with the three quadrupole modes $Q_1 = -2iyz$, $Q_{-1} = -2xz$ and $Q_{-2} = 2ixy$ where $(x, y, z)$ are coordinates in the nucleus intrinsic frame.

The time-dependent Schrödinger equation we have to solve is [5]

$$H_{\text{coll}} \chi(x,t) = i\hbar \frac{\partial}{\partial t} \chi(x,t) \tag{4.18}$$

with the collective wave function $\chi(x,t)$ normalized according to

$$\int |\chi(x,t)|^2 \prod_k dx^k = 1 \tag{4.19}$$

The calculation of the inertia tensor $B_{k,l}(d, \xi)$ from the HFB solutions, is performed using the formalism given in Section 4.2.2 (see also [?]). The elements $\mathcal{M}_{k,l}$ of the inverse of the matrix $B$ (see Eq. 4.16) are expressed in terms of moments $\mathcal{M}_{k,l}^{(-k)}$ as

$$\mathcal{M}_{k,l} = \sum_{r,s=d,\xi} \left(\mathcal{M}^{(-1)}\right)^{-1}_{kr} \left(\mathcal{M}^{(-3)}\right)_{rs} \left(\mathcal{M}^{(-1)}\right)^{-1}_{sl}$$

where the moments are defined as

$$\mathcal{M}_{k,l}^{(-m)} \equiv \sum_{\mu\nu} \frac{\left\langle \Phi\left(d,\xi\right) \left|\hat{x}^{k}\right| \mu\nu \right\rangle \left\langle \mu\nu \left|\hat{x}^{l}\right| \Phi\left(d,\xi\right)\right\rangle}{\left(E_{\mu}+E_{\nu}\right)^{m}}$$

These moments are expressed in terms of the HFB solutions $|\Phi\left(d,\xi\right)\rangle$ and of the two quasiparticle excitations $|\mu\nu\rangle$ built on those HFB states, with $E_\mu + E_\nu$ the energy of the two-quasiparticle states. In this formula, the operators $\hat{x}^k$ and $\hat{x}^l$ stand in for the operators corresponding to the $d$ and $\xi$ coordinates.

### 4.3.2 The direction of fission in the dynamical calculations

In this work, we have taken the increasing $d$ coordinate as the direction of fission near scission and beyond. In [3], a seemingly different approach was adopted to define the direction of fission. These two definitions are in fact compatible.

Since the derivation behind the criterion adopted in [3] is not easily found in the literature, we begin by giving the essential steps. In the $(d, \xi)$ coordinates, we write the metric as

$$ds^2 = \sum_{\alpha,\beta=d,\xi} \mathcal{M}\left(d,\xi\right) d\alpha\, d\beta$$

and seek a new coordinate system $(x, y)$ where the metric takes the form

$$ds^2 = M_{xx} dx^2 + M_{yy} dy^2$$

in other words, in the new coordinate system the mass tensor (and its inverse, the inertia tensor) is diagonal. In fact, it is well known that such a diagonalization can always be carried out in a two-dimensional space [20]. From the general transformation of a metric tensor in curvilinear coordinates , and the equivalence between the inertia and metric tensors (Eq. (**??**)), we therefore have the condition

$$B_{xy} = \sum_{\alpha,\beta=d,\xi} B_{\alpha\beta}\left(d,\xi\right) \frac{\partial x}{\partial\alpha} \frac{\partial y}{\partial\beta} \equiv 0 \tag{4.20}$$

This is essentially Eq. (10) in [3]. We will now show the steps in obtaining Eq. (11) in [3] and describe the numerical solution of this equation.

For convenience, we define the quantities

$$\begin{aligned} A(d,\xi) &\equiv \frac{\partial x(d,\xi)}{\partial d} B_{dd}(d,\xi) + \frac{\partial x(d,\xi)}{\partial \xi} B_{\xi d}(d,\xi) \\ B(d,\xi) &\equiv \frac{\partial x(d,\xi)}{\partial d} B_{d\xi}(d,\xi) + \frac{\partial x(d,\xi)}{\partial \xi} B_{\xi\xi}(d,\xi) \end{aligned} \tag{4.21}$$

where we are free to choose the explicit form of the function $x(d,\xi)$. The goal is then to determine a function $y(d,\xi)$ which satisfies Eq. (4.20), for a given function $x(d,\xi)$. Using the definitions in Eq. (4.21), we re-write Eq. (4.20) as

$$A(d,\xi)\frac{\partial y(d,\xi)}{\partial d} + B(d,\xi)\frac{\partial y(d,\xi)}{\partial \xi} = 0 \tag{4.22}$$

under this condition, the total differential of $y(d,\xi)$ is then

$$Dy(d,\xi) = \left[dy - \frac{B(d,\xi)}{A(d,\xi)}dx\right]\frac{\partial y(d,\xi)}{\partial \xi}$$

Note that the only condition we have to determine $y(d,\xi)$ is given by Eq. (4.22), which only constrains one of the two partial derivatives relative to the other. Therefore, we choose for convenience

$$\frac{\partial y(d,\xi)}{\partial \xi} \equiv 1 \tag{4.23}$$

and look for lines of constant $y(d,\xi)$, given by $Dy(d,\xi) = 0$ or

$$d\xi - \frac{B(d,\xi)}{A(d,\xi)}dd = 0 \tag{4.24}$$

which is a more general version of Eq. (11) in [3].

The solution to Eq. (4.24) is a set of curves in the $(d,\xi)$ plane,

$$S(d,\xi) = C_0$$

where $C_0$ is a constant determined at some initial point by $S(d_0,\xi_0) = C_0$ and

$$S(d,\xi) \equiv \xi - \int_{d_0}^{d} dd' \frac{B(d',\xi(d'))}{A(d',\xi(d'))} \tag{4.25}$$

Indeed, it is straightforward to show that $S(d,\xi)$ has the same partial derivatives as $y(d,\xi)$, given by Eqs. (4.22) and (4.23), and therefore the same total derivative $DS(d,\xi) = Dy(d,\xi)$. Thus the curves defined by $y(d,\xi)$ and $S(d,\xi)$ are the same, up to an irrelevant constant.

It is instructive to describe the numerical construction of the curves defined by Eq. (4.25). Starting from a point $(d_0, \xi_0)$ and a step size $\delta d$, we determine a new point on the curve $S(d,\xi) = C_0 \equiv S(d_0, \xi_0)$ by

$$\begin{aligned} d_1 &= d_0 + \delta d \\ \xi_1 &= \xi_0 + \frac{B(d_0,\xi_0)}{A(d_0,\xi_0)}\delta d \end{aligned}$$

or, in general, from a point $(d_{n-1}, \xi_{n-1})$ we find the next point given by

$$\begin{aligned} d_n &= d_{n-1} + \delta d \\ \xi_n &= \xi_{n-1} + \frac{B(d_{n-1},\xi_{n-1})}{A(d_{n-1},\xi_{n-1})}\delta d \end{aligned} \tag{4.26}$$

which amounts to performing the integral in Eq. (4.25) numerically.

We now return to the definition of the direction of fission adopted in this paper. In the language of [3], the present definition is equivalent to a family of curves $S(d_0, \xi_0) = C_0$ parallel to the $d$ axis. In the numerical construction of the curves described above, this means we have $\xi_n = \xi_{n-1}$ for all $n$. In practice, Eq. (4.26) gives curves that are more or less parallel to the $d$ axis when

$$\frac{B(d_{n-1},\xi_{n-1})}{A(d_{n-1},\xi_{n-1})}\delta d \ll 1$$

Using the definitions in Eq. (4.21), this can be written explicitly in terms of the inertia tensor components as

$$\left[\frac{B_{d\xi}(d,\xi)}{B_{dd}(d,\xi)}\delta d\right] \frac{1 + \left(\frac{\partial x/\partial \xi}{\partial x/\partial d}\right)\frac{B_{\xi\xi}}{B_{d\xi}}}{1 + \left(\frac{\partial x/\partial \xi}{\partial x/\partial d}\right)\frac{B_{\xi d}}{B_{dd}}} \ll \quad 1 \tag{4.27}$$

Numerically, even for a relatively large step size (e.g., $\delta d = 1$ fm) we find in the case of our $^{240}$Pu calculations for the $A_H = 134$ exit point

$$\frac{B_{d\xi}(d,\xi)}{B_{dd}(d,\xi)}\delta d = 1.9 \times 10^{-2} \ll 1$$

and

$$\frac{B_{\xi\xi}(d,\xi)}{B_{d\xi}(d,\xi)}\delta d = 1.3 \times 10^{-1} \ll 1$$

Thus, provided that $x(d,\xi)$ does not vary too slowly with $d$ or too quickly with $\xi$ then Eq. (4.27) is easily satisfied, and the curves defined by Eq. (4.26) are parallel to the $d$ axis. Note that the condition in Eq. (4.27) is similar in form to the condition (see Eq. (4.28))

$$\frac{j^\xi}{j^d}\delta d \ll 1$$

with the partial derivatives of $x\,(d,\xi)$ replaced by terms of the form $\chi^*\partial\chi/\partial d - \chi\partial\chi^*/\partial d$ and $\chi^*\partial\chi/\partial\xi - \chi\partial\chi^*/\partial\xi$.

### *4.3.3 From flux to fragment mass distribution*

The time dependent collective Schrödinger equation

$$H_{coll}\chi\,(d,\xi,t) = E\,\chi\,(d,\xi,t)$$

is solved numerically with the initial condition given by the quasi-stationary states obtained in section 5.0.4,

$$\chi\,(d,\xi,t=0) = \chi_0\,(d,\xi)$$

In order to avoid artificial reflections of the wave packet, both the potential energy surface and inertia tensors shown in Figs 5.1 and 5.2 have been modified to be constant beyond scission (thereby avoiding the discontinuities at scission). Thus, no unusual behavior is expected as the wave packet crosses the scission line. Furthermore, at a large separation distance ($d = 22.9$ fm), the wave packet is absorbed by a damping potential as described in [3] in order to avoid reflections.

The continuity equation is derived from the collective Schrödinger equation in the standard way [16, 5, 17] and gives a current with components

$$\begin{aligned} j^d &= \frac{\hbar}{2i}\left[B_{dd}\left(\chi^*\frac{\partial\chi}{\partial d} - \chi\frac{\partial\chi^*}{\partial d}\right) + B_{d\xi}\left(\chi^*\frac{\partial\chi}{\partial\xi} - \chi\frac{\partial\chi^*}{\partial\xi}\right)\right] \\ j^\xi &= \frac{\hbar}{2i}\left[B_{\xi d}\left(\chi^*\frac{\partial\chi}{\partial d} - \chi\frac{\partial\chi^*}{\partial d}\right) + B_{\xi\xi}\left(\chi^*\frac{\partial\chi}{\partial\xi} - \chi\frac{\partial\chi^*}{\partial\xi}\right)\right] \end{aligned} \tag{4.28}$$

As an example, we show plots of this probability current in Fig. 4.5 for a state near the barrier in $^{240}$Pu and at three different times during the evolution of its wave packet. In this work, we associate the increasing $d$ coordinate with the direction of fission since near scission (and beyond) the increase in this coordinate coincides with the picture we have of the final stage of the fission process where the fragments fly apart as independent nuclei interacting only through the repulsive Coulomb force. Therefore, we will focus on the $j^d$ component of the current to extract fission observables. We note that the same numerical arguments used to justify Eq. (4.27) can be used to explain the predominance of the current in the $d$ direction in Fig. 4.5.

We can then calculate a flux in the fission direction $d$ through a segment of length $\Delta\xi$ as

$$\Phi = j^d \Delta\xi \tag{4.29}$$

Along the scission line, the fragment mass distribution before neutron emission is then obtained by integrating this flux over time,

$$Y(A) = \int_0^{\infty} dt\, \Phi(d_s, \xi, t)$$

The yield $Y(A)$ was normalized according to standard convention so that

$$\sum_{A=0}^{A_{tot}} Y(A) = 200$$

Finally, we must account for fluctuations in particle number of the fragments due to both pairing effects, and the finite number of particles $Q_N$ in the neck region for points along the scission line. For $^{240}$Pu, we find typically $2 \lesssim Q_N \lesssim 5$ along the scission line, and have therefore adopted an average value of 3.5 for the fluctuation in the number of particles $A$ in each fragment. This fluctuation leads to a smoothing of the yield which we calculate as

$$\tilde{Y}(A) \equiv \int_{-\infty}^{\infty} dA'\, Y(A') \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(A-A')^2}{2\sigma^2}\right]$$

with $\sigma = 3.5$.

## 4.4 Calculation of fragment energies

### *4.4.1 Static contribution*

#### 4.4.1.1 Static excitation energies

Although Eq. (4.9) can in principle be used to calculate the individual fragment HFB energies at scission, we also require the ground-state energies of the same fragments in order to extract their excitation energies. On the one hand it is more consistent to extract the ground-state energies in the same basis that was used for the excited states, but on the other hand the fragments would have to be moved very far apart to ensure that there are no polarizing influence from the complementary fragment, which is technically challenging as it would require very large harmonic-oscillator bases. We avoid this problem by calculating both the excited and ground-state energy of each fragment using only its own density (i.e., by removing the density of the complementary fragment). For the excited state at scission, this amounts to using the individual localized densities $\rho^{(\mathrm{L})}$ and $\rho^{(\mathrm{R})}$ defined in section 4.2.2

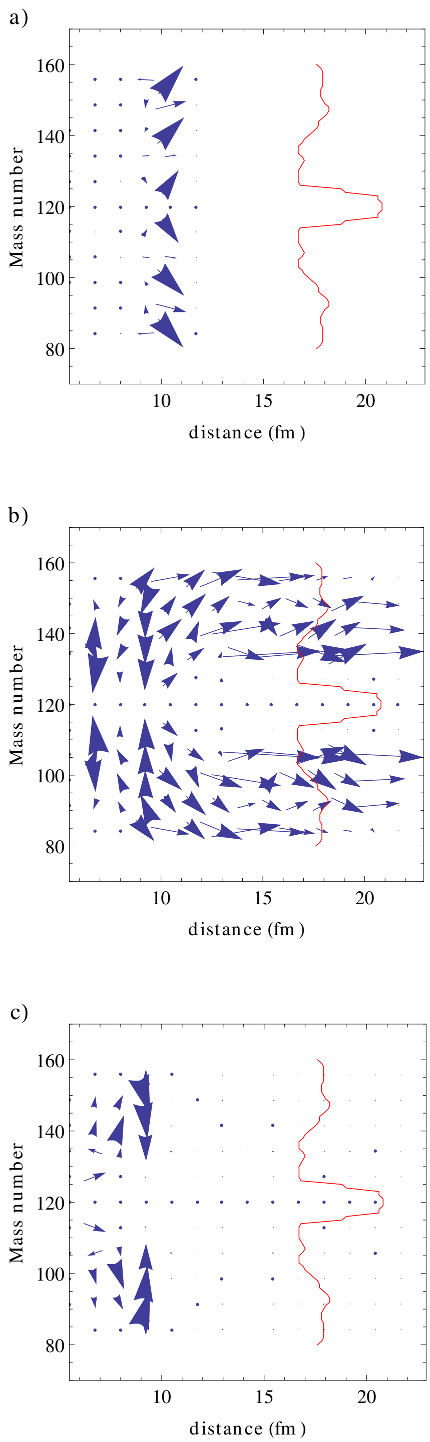


**Fig. 4.5** Probability current calculated using Eq. (4.28) and plotted at three different times: a) before the collective wave function has reached the scission line (red solid line), b) while the wave function is transiting across the scission line, and c) long after the wave function has passed the scission line.

and calculating the corresponding energy directly (i.e., without iterating the HFB code). For the ground state, the average neutron and proton numbers of the individual fragments at scission (which are not necessarily integer values) are imposed as constraints along with the centroid position of the fragment, and the HFB code is iterated and converged separately for each fragment, starting from the density solution at scission, to find the minimum energy-state with those constraints. The excitation energy of the fragments is then obtained as the difference between the excited and ground-state energies for each fragment.

Note that these excitation energies do not include a contribution from the pre-scission dynamics, which will be discussed in section 4.4.2. We also do not explicitly include the impact from the coupling between internal and collective degrees of freedom during the fission process, which is a topic in development [15], but we will try to estimate this contribution to the excitation energies in the discussion in section 5.

#### 4.4.1.2 Static kinetic energies

The total kinetic energy (TKE) acquired by the fragments after scission is calculated from their interaction potential using energy conservation as

$$V\left(d_s\right) - V\left(\infty\right) = V\left(d_s\right)$$

and $V\left(d_s\right)$ is calculated with Eq. (4.10) at a scission configuration. As in the calculation of the excitation energies, this result does not yet include the contribution from the pre-scission dynamics, and the effect of the coupling between internal and collective degrees of freedom during the fission process will only be estimated in section 5.

### *4.4.2 Dynamical contribution*

The calculations in sections 4.4.1.1 and 4.4.1.2 represent only the static contribution to the fragment energies. In addition a dynamic, pre-scission energy contribution must be added to the fragment kinetic and excitation energies. In a semi-classical picture, this energy is gained by the fissioning nucleus in the transition from saddle to scission. The amount of pre-scission energy available in determined by the difference between the total energy of the nucleus, and its potential energy at the scission point. In this section, we present a methodology to estimate the partition of available pre-scission energy between kinetic and excitation energy of the fragments, which will then be added to the static calculations in sections 4.4.1.1 and 4.4.1.2.

The essence of the method relies on comparing, at the scission point, a normalized flux of the wave packet (defined below) in the $(d, \xi)$ coordinates to a normalized flux in a single fission coordinate (which essentially corresponds to the $d$ coordinate describing the separation of the fragments). The loss of flux to the transverse direction deduced from the comparison between these two calculations can then be related to the energy transferred between $d$ and $\xi$ via the WKB approximation, and through an energy-conservation argument to a loss in pre-scission kinetic energy and a commensurate gain in pre-scission excitation energy of the fragments [18, 17].

We define a normalized flux at a scission exit point by dividing the flux in Eq. (4.29) by the squared amplitude of the collective wave function, integrated along the segment length $\Delta\xi$,

$$\begin{aligned} \Phi_N^{(2D)} &\equiv \frac{j^d \Delta\xi}{\int |\chi(d,\xi,t)|^2 \, d\xi} \\ &\simeq \frac{j^d}{|\chi(d,\xi,t)|^2} \end{aligned} \tag{4.30}$$

where we have assumed that the segment length $\Delta\xi$ is sufficiently small that $|\chi(d,\xi,t)|^2$ can be treated as a constant under the integral sign, and where the subscript $(2D)$ serves as a reminder that although we are only using the current in the $d$ direction at scission, the wave packet is free to evolve in both $d$ and $\xi$ coordinates up to that point.

By contrast, we now imagine a wave packet that is constrained to move in the $d$ direction only. Near the scission point, and in the spirit of the WKB approximation, we assume that both the inertia $B_{dd}$ and potential $V$ are slowly varying function of $d$ (remember that we artificially modify both the potential and inertia tensor at scission to insure that there are no discontinuities that might cause reflections in the wave packet). Then the collective Schrödinger equation takes the simple form

$$\left[-\frac{\hbar^2}{2} B_{dd} \frac{\partial^2}{\partial d^2} + V\right] \chi^{(1D)}(d,t) = \hbar i \frac{\partial}{\partial t} \chi^{(1D)}(d,t) \tag{4.31}$$

which has a plane-wave solution

$$\chi^{(1D)}(d,t) = \mathcal{N} \exp\left[i\left(k_d d - \frac{E_{1\mathrm{D}}}{\hbar} t\right)\right] \tag{4.32}$$

where $\mathcal{N}$ is a normalization constant, $k_d$ is the wave number, and $E_{1\mathrm{D}}$ is the energy of the solution. Inserting Eq. (4.32) into Eq. (4.31) leads to the relation

$$k_d = \frac{1}{\hbar} \sqrt{\frac{2}{B_{dd}} (E_{1\mathrm{D}} - V)}$$

From Eq. (4.28) we can calculate the current

$$\begin{aligned} j^d &= \hbar k_d B_{dd} \mathcal{N}^2 \\ &= \mathcal{N}^2 \sqrt{2B_{dd}\left(E_{1\mathrm{D}} - V\right)} \end{aligned}$$

and the normalized flux in Eq. (4.30) takes the form

$$\Phi_N^{(1\mathrm{D})} = \sqrt{2B_{dd}\left(E_{1\mathrm{D}} - V\right)} \tag{4.33}$$

Note that the normalized flux $\Phi_N^{(1\mathrm{D})}$ does not depend on the value of $\mathcal{N}$ and is constant in time. This is a very important property, because it shows that if the WKB approximation is valid, then the normalized flux is insensitive to fluctuations and changes in the wave function. In order to determine the amount of dissipated energy, we interpret the 2D flux $\Phi_N^{(2D)}$ given by Eq. (4.30) using the 1D formula in Eq. (4.33). Unlike the 1D case however, we do not expect the full available energy $E_{1\mathrm{D}} - V$ to be converted to kinetic energy, but rather only a portion $E_{2\mathrm{D}} - V$, with the difference "dissipated" into the transverse degrees of freedom. Then, using Eq. (4.33), the ratio of normalized fluxes is

$$\frac{\Phi_N^{(2D)}}{\Phi_N^{(1\mathrm{D})}} = \sqrt{\frac{E_{2\mathrm{D}} - V}{E_{1\mathrm{D}} - V}} \tag{4.34}$$

from which we deduce the energy in the 2D case

$$E_{2\mathrm{D}} = V + \left(\frac{\Phi_N^{(2D)}}{\Phi_N^{(1\mathrm{D})}}\right)^2 \left(E_{1\mathrm{D}} - V\right)$$

and the dissipated energy is

$$\Delta E_{\mathrm{coll}} \equiv E_{1\mathrm{D}} - E_{2\mathrm{D}} \tag{4.35}$$

Because $d$ is the coordinate describing the separation of the fragments beyond scission, the energy associated with variations in this coordinate is the kinetic energy of the fragments. Therefore $\Delta E_{\mathrm{coll}}$ is energy taken away from the kinetic energy of the fragments, and by conservation of energy we deduce that this energy must appear as excitation of the fragments. In practical calculations, $E_{1\mathrm{D}}$ is given by the energy of the initial state from the time-independent collective Schrödinger equation,

$$H_{coll} \chi_0\left(d, \xi\right) = E_{1D}\, \chi_0\left(d, \xi\right) \tag{4.36}$$

In Fig. 4.6 we show the normalized flux obtained for one such state for $^{240}$Pu using Eq. (4.30), and plotted as a function of time for an exit point corresponding to heavy-fragment mass $A_H = 134$ . We see that, after an initial transient phase, the normalized flux remains remarkably constant in time, in accordance with Eq. (4.33).

Not all states lend themselves to such an analysis. If the collective motion in the $d$ and $\xi$ directions are strongly coupled then the assumptions behind this analysis will not hold, and the normalized flux will not be constant in time as in Fig. 4.6. Starting from the states calculated in section 5.0.4 for $^{240}$Pu, and which span an energy range of $\sim 5$ MeV above the barrier, we plot in Fig. 4.7 the distribution of $\Delta E_{\mathrm{coll}}$ obtained using Eq. (4.35) for the subset of states that have a constant normalized flux and for two different exit points. The exit points correspond to heavy-fragment mass $A_H = 134$ (near the most likely scission configuration for the static calculations) and $A_H = 142$ (near maximum yield in the dynamic calculations). These results will be used in section 5 to calculate the pre-scission energy contribution to the fragment energies.

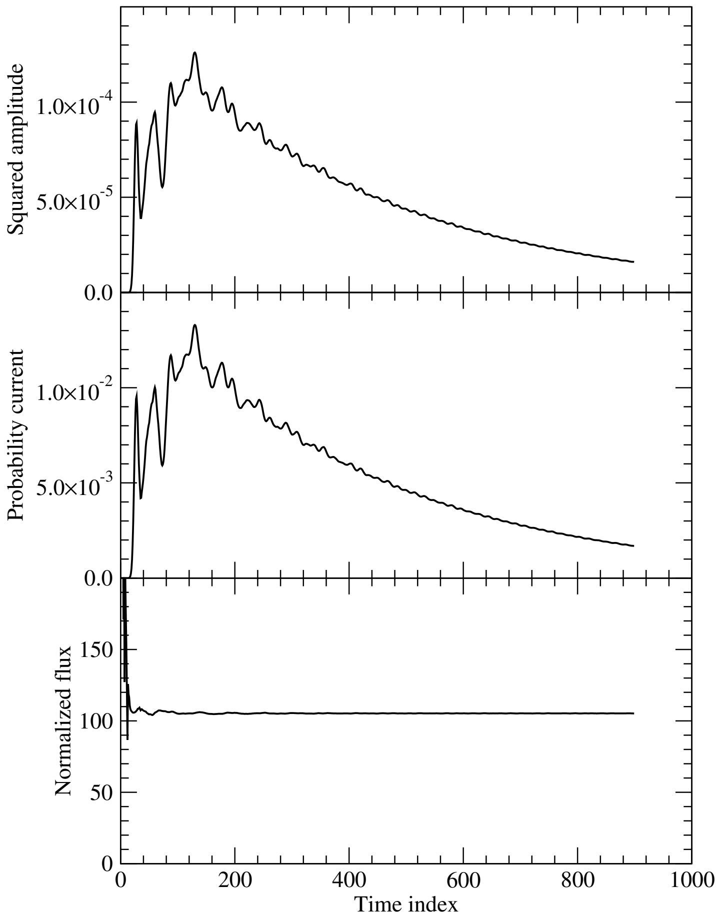


**Fig. 4.6** Calculation of the normalized flux for a state above the first barrier in $^{240}$Pu. The top panel shows $|\chi(d, \xi, t)|^2$, the middle panel shows the current in the $d$ direction, $j^d$, and the bottom panel shows the normalized flux calculated using Eq. (4.30).

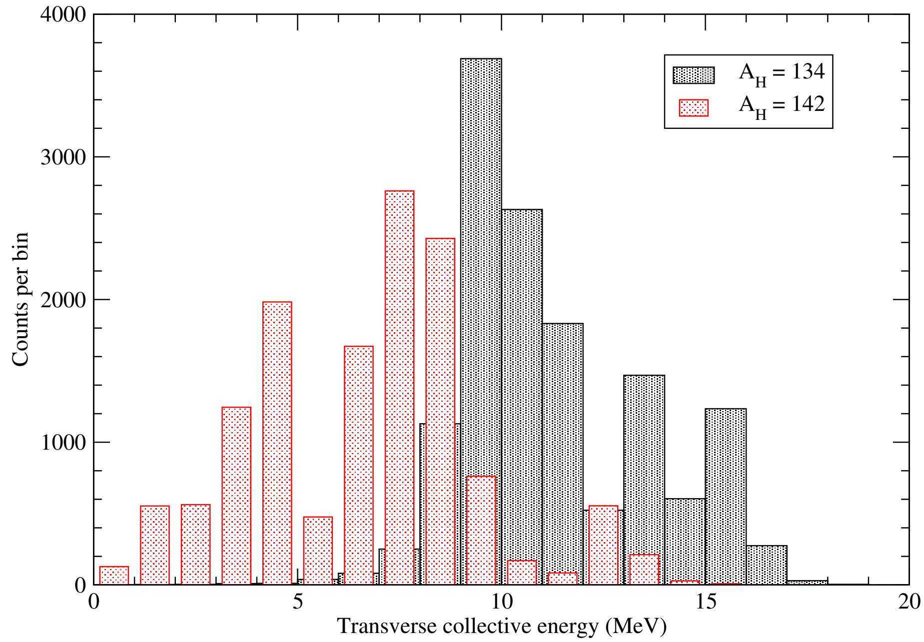


**Fig. 4.7** Distribution in collective energy dissipation given by Eq. (4.35) for calculations at exit point corresponding to $A_H = 134$ and $A_H = 142$.

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Chapter 5

# Numerical application to $^{240}$Pu fission

In this chapter we apply the formalism described in the remainder of the book to the calculation of fission fragment properties following the induced fission of $^{240}$Pu. Fragment mass distributions are obtained for the $^{239}\mathrm{Pu}\,(n,f)$ from thermal up to 5 MeV in incident neutron energy. Total kinetic and excitation energies as a function of mass number are calculated for the fragments for thermal incident neutrons.

### *5.0.3 Potential energy surface and inertia tensor*

Using this prescription for $z_N$ described in section 4.1.2.3, we show in Fig. 5.1 the potential energy surface calculated with the $(d, \xi)$ constraints.

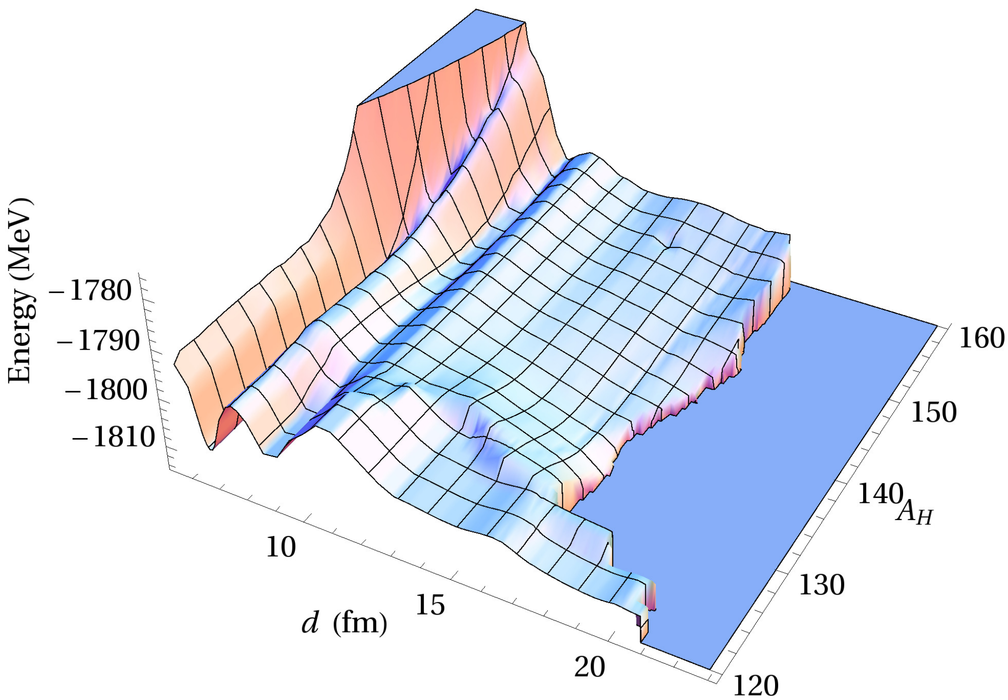


**Fig. 5.1** Potential energy surface calculate in the $(d, \xi)$ coordinates.

The $B_{dd}$, $B_{d\xi}$, and $B_{\xi\xi}$ components of the inertia tensor are plotted in Fig. 5.2 as a function of $(d, \xi)$. As a check of the inertia tensor calculations, we note that for very large separation distance between the fragments, the kinetic energy of the system is governed by the constant reduced mass $\mu$ of the system

$$-\frac{\hbar^2}{2} B_{dd} \frac{\partial^2}{\partial d^2} \longrightarrow \frac{1}{2\mu m} p_d^2$$

with $m$ the nucleon mass and where the momentum in the $d$ coordinate is given by

$$p_d = \frac{\hbar}{i}\frac{\partial}{\partial d}$$

From this we deduce the simple asymptotic formula

$$\hbar^2 B_{dd} \longrightarrow \frac{(\hbar c)^2}{\mu m c^2} \tag{5.1}$$

For example, in the case of $^{240}$Pu fission, typical mass divisions give $\mu \approx 60$ and therefore $\hbar^2 B_{dd} \longrightarrow 0.7\,\mathrm{MeV\,fm}^2$ using Eq. (5.1). Our microscopic calculations for the symmetric and 107/133 (i.e., most likely) mass divisions at $d = 20\,\mathrm{fm}$ also give $\hbar^2 B_{dd} \approx 0.7\,\mathrm{MeV\,fm}^2$.

### *5.0.4 Initial states*

In order to calculate the quasi-stationary states used to construct the initial wave packet, the potential energy surface $V(d,\xi)$ was modified at the second saddle to create a potential well $V_0(d,\xi)$ with high walls [1, 2]. Figure 5.3 shows this modification in the case of $^{240}$Pu for $A_H = 120$. The inertia tensor described above is used to calculate the quasi-stationary states by solving the time-independent collective Schrödinger equation (Eq. (4.36)). The eigenstates $\overline{\chi}_0(d,\xi)$ and corresponding eigenvalues $E$ are obtained by solving the Schrödinger equation numerically (see, e.g., [1]). The cumulative density of levels obtained in this manner for the $(d,\xi)$ parameters is plotted in Fig. 5.4 for $^{240}$Pu, and compared to the same cumulative level density obtained from calculations performed in the $(Q_{20}, Q_{30})$ coordinates. Using the prescription for the $(d,\xi)$ parameters described in section 4.1.2, we find similar level densities between the $(d,\xi)$ and $(Q_{20}, Q_{30})$ formulations. We have used a rather simple prescription for the neck position $z_N$ in the part of the $(d,\xi)$ space relevant to the initial states (see section 4.1.2.3), and in future studies it is possible that the agreement between the curves in Fig. 5.4 could be improved by relaxing the requirement that $z_N$ remain constant as a function of $d$ for $d < 11$ fm.

### *5.0.5 Fragment mass distribution*

As an application of the formalism described in section 4.3, we present calculations of the mass distributions (or yields), total kinetic energy (TKE), and total excitation energy (TXE) of the fragment following the $^{239}$Pu$(n,f)$

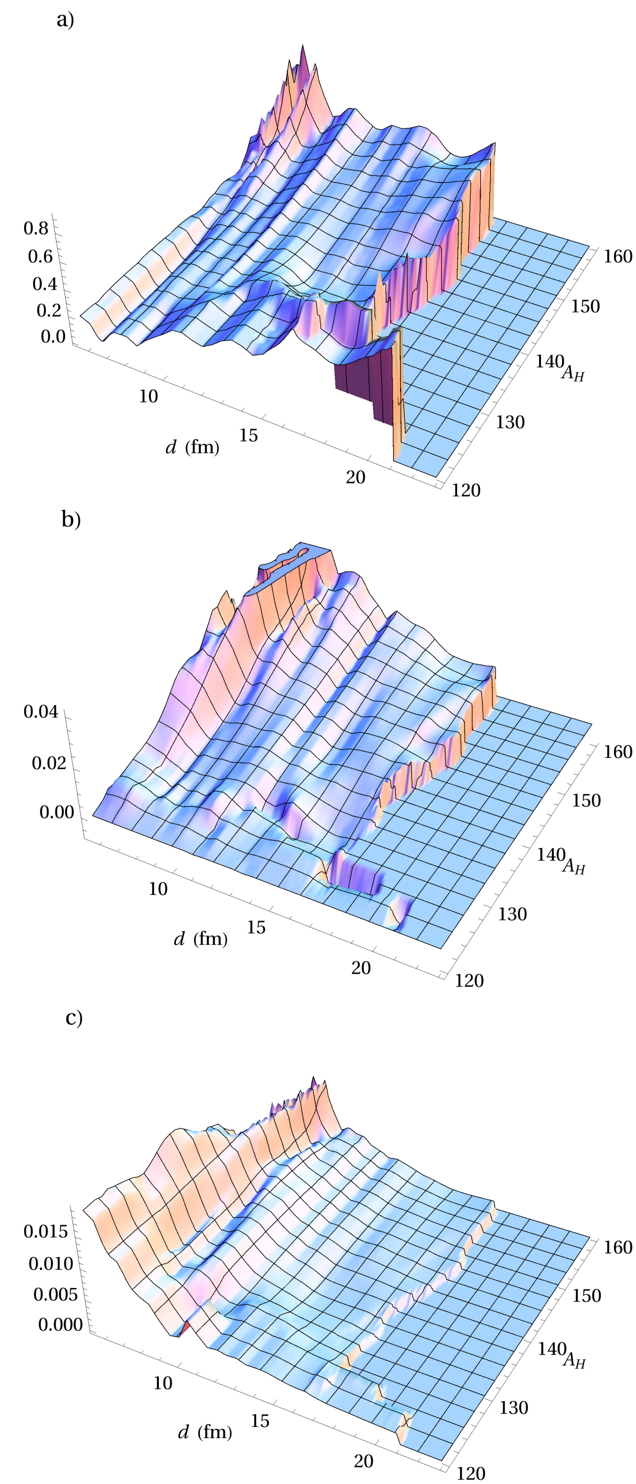


**Fig. 5.2** Plot of the components a) $\hbar^2 B_{dd}\,\mathrm{MeV}\cdot\mathrm{fm}^2$, b) $\hbar^2 B_{d\xi}\,\mathrm{MeV}\cdot\mathrm{fm}$, and c) $\hbar^2 B_{\xi\xi}\,\mathrm{MeV}$ of the inertia tensor.

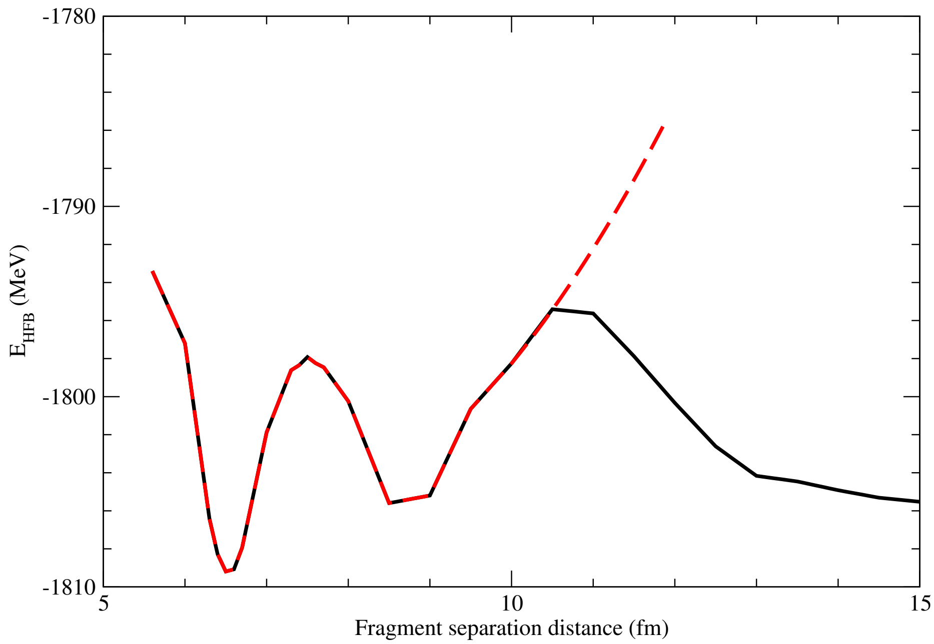


**Fig. 5.3** Extended potential (red dashed line) for symmetric fission, used to calculated the quasi-stationary states for $^{240}$Pu. The black solid line shows the unmodified potential for reference.

reaction. For the fragment energies, we only consider thermal neutron energies, while for the mass distributions we consider incident neutron energies up to $E_n = 5\,\mathrm{MeV}$ , below second-chance fission.

For the yield calculations, we need to simulate the population of states that might follow from a neutron-induced compound-nucleus reaction. For a given incident neutron energy $E_n$ we first need to calculate the excitation energy $E_x$ of the fissioning system. This excitation energy is given by

$$E_x = E_n + E_A - S_n + \Delta\mathrm{ZPE}$$

where $E_A$ is the height of the first saddle, $S_n$ is the separation energy of the neutron in the compound nucleus, and $\Delta$ZPE is the difference in zero-point energy (ZPE) between the first well and the first saddle. In practice, we find that the ZPE is essentially the same in the first well and at the first saddle, and therefore $\Delta\mathrm{ZPE} \approx 0$. Realistic barrier heights $E_A$ can be found in [3], and

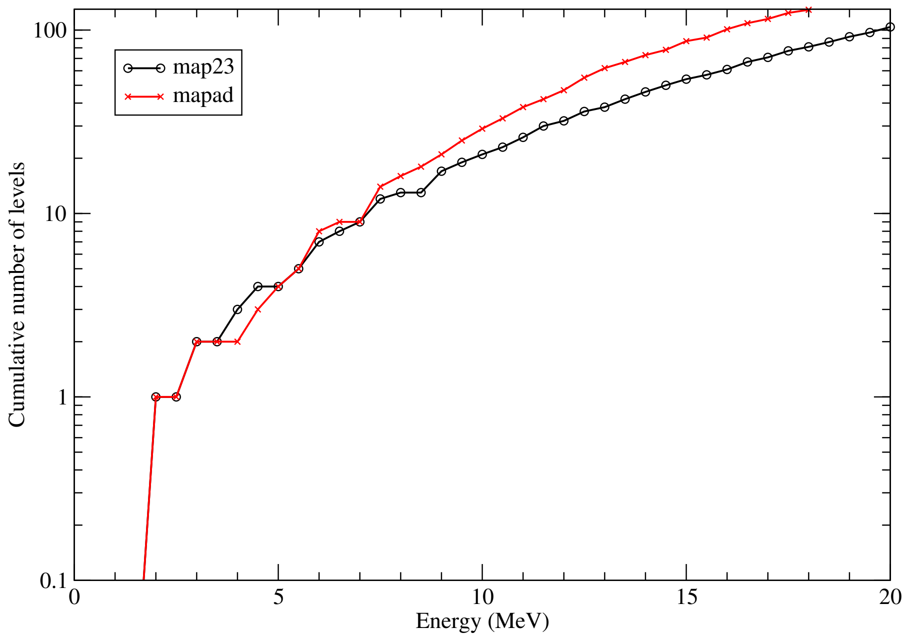


**Fig. 5.4** Cumulative density of collective states as a function of excitation energy obtained by solving Eq. (4.36) in the $(d, \xi)$ variables (labeled "mapad") and compared to the same calculation in the $(Q_{20}, Q_{30})$ coordinates (labeled "map23").

for $^{240}$Pu in particular, $E_A - S_n = 0.53\,\text{MeV}$. For each $E_n$, a collective wave packet was constructed as the superposition of quasi-stationary states within 500 keV of the corresponding $E_x$. Thus, between 8 and 15 equally-weighted states were used for the different energies.

The mass distributions, calculated using the formalism developed in section 4.3.3, are plotted in Fig. 5.5 for different incident energies. In the thermal case we compare with the pre-neutron distributions measured by [4]. At higher energy, where data are not available, we compare to calculations using the phenomenological code GEF [5]. In the thermal case, where data are available, the agreement between microscopic calculation and experiment is quite good. For those masses with reasonable yield ($\geq 1\%$), the agreement between theory and experiment is better than 30% in all cases, and better than 20% in most cases. In this sense, the microscopic approach, starting from neutrons, protons, and an effective interaction performs as well as a more phenomenological calculation that has been specifically adjusted to reproduce the fission data of interest.

### *5.0.6 Fragment energies*

Next, we turn to the calculation of the fission-fragment kinetic and excitation energies as described in section 4.4. Following HFB calculations set up as described in section 4.1.2, we identified for each $\xi$ (or equivalently for each heavy fragment mass $A_H$) a scission distance $d_s$ such that a small increment $\delta d$ would cause a sudden drop in neck size defined in Eq. (4.4) to $Q_N < 0.5$ and a corresponding drop in the HFB energy. For this set of points $(d_s(\xi), \xi)$, we performed another series of calculations with constraints on $\xi$, $d_s(\xi)$, and $Q_N$ (and of course with the dipole moment of the nucleus constrained to zero to prevent spurious center-of-mass shifts during the HFB iterations). The quantum localization algorithm described in section 4.2.1 was applied to the HFB solutions and the nuclear interaction energy ($V_{\text{int}}^N$) and exchange energy ($V_{\text{int}}^{\text{ex}}$) were calculated, and a subset of scission points was selected for which $\left|V_{\text{int}}^N\right| < 15\,\text{MeV}$ and $|V_{\text{int}}^{\text{ex}}| < 2\,\text{MeV}$.

The static contribution to the TKE was extracted as the total interaction energy between the fragments at scission using Eq. (4.10), with the relative kinetic energy ($K_{\text{rel}}$) removed as explained in section 4.2.2. The value of $K_{\text{rel}}$ was found to be relatively constant at $\sim 8\,\text{MeV}$ (give or take $\sim 1\,\text{MeV}$) as a function of both $d$ and $\xi$ near scission. The static excitation energies of the fragments were calculated from their difference in HFB energy at scission and in their respective ground states, using the procedure outlined in section 4.4.

To estimate the dynamic contribution to the fragment energies, we have analyzed the normalized flux in the fission direction, as explained in section 4.4.2. As shown in Fig. 4.7, for $A_H = 134$ this analysis gives an estimate of 5.2 MeV on average transferred from pre-scission kinetic energy to pre-scission excitation energy due to the coupling between the $d$ and $\xi$ collective degrees of freedom. For $A_H = 142$ this average collective "dissipated" energy is 1.9 MeV. The difference in energy between saddle and scission is 15.2 MeV for $A_H = 134$ and 14.8 MeV for $A_H = 142$. In [6] the authors calculated a "dissipated" energy of 2.1 MeV due to orthogonal excitations for calculations in the $(Q_{20}, Q_{40})$ coordinates. In this paper we have only considered two variables for the dynamic calculations ($d$ and $\xi$), but we expect many more to become relevant as the nucleus nears fission (in [7] we postulated that the number of constraints should more or less double near scission to accommodate the degrees of freedom of the nascent fragments). Furthermore, the coupling between collective and quasiparticle degrees of freedom will also contribute to the transfer of energy away from the fission coordinate. Thus, in addition to the values calculated in the present work, we can reasonably expect another 4-5 MeV transferred to transverse modes from the coupling to

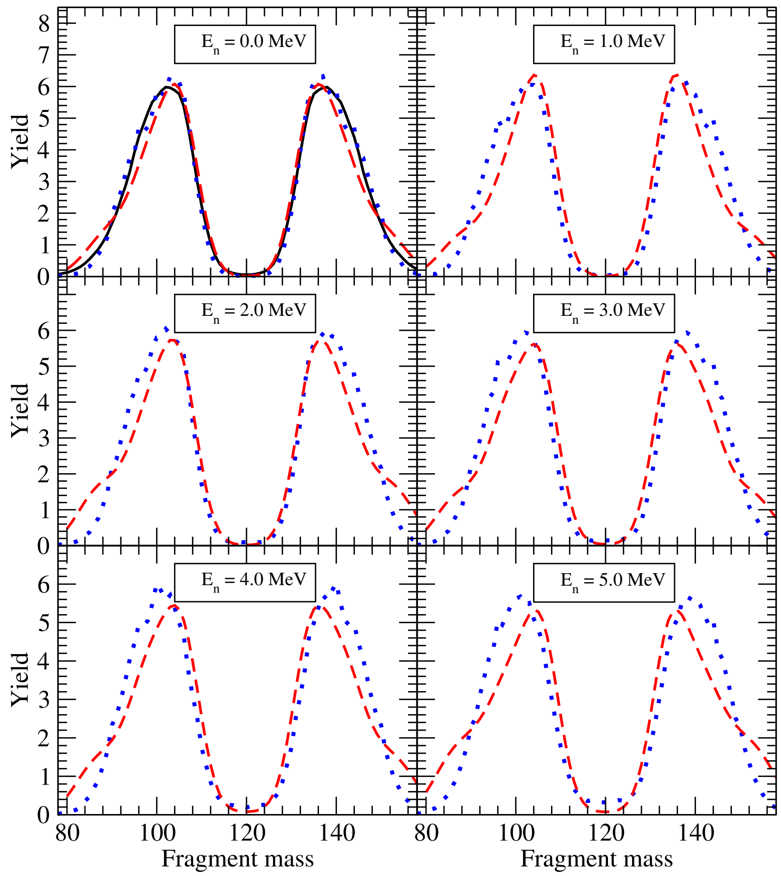


**Fig. 5.5** Theoretical calculations of mass yields, before neutron emission, for the $^{239}\mathrm{Pu}\,(n,f)$ reaction. For thermal neutrons ($E_n = 0.0$ MeV ), microscopic-theory values (dashed lines) are compared to the experimental results of Schillebeeckx et al. (solid black curves) and to calculations using the phenomenological model GEF of Schmidt et al. (dotted line). For $E_n = 1.0$ to 5.0 MeV, the microscopic-theory calculations are compared to the GEF model results only, since no experimental data are available.

other collective and to quasiparticle degrees of freedom near scission. Adding up the contributions, it is then reasonable to expect $\sim 50\%$ of the energy difference between saddle and scission to contribute to the TKE with the rest appearing as additional TXE.

Figure 5.6 shows the calculated TKE and TXE for thermal fission of $^{240}$Pu including both static and dynamic contributions, and assuming a 50/50 split of the available pre-scission energy. The experimental TKE curves are taken from [8, 9, 10], and the one-standard-deviation band around those curves is constructed using the data in [11]. The experimental TXE curve is taken from [12]. We find that the agreement between calculation and experiment is quite good, especially considering the fact that the only phenomenological input is in the parameters of the effective interaction, which were not adjusted to reproduce the data of interest. Even if the assumed 50/50 split of the dynamic contribution to the TKE and TXE is varied within reason (e.g., up to a 25/75 split either way), the results in Fig. 5.6 still remain in good agreement with the data. Interestingly, the calculated TKE slightly overestimate the data, and the TXE correspondingly underestimate the data. It is possible that with additional degrees of freedom, and especially with the inclusion of quasiparticle excitations using an approach such as the SCIM (see section 3.3), these calculations could be brought into even closer agreement with the data.

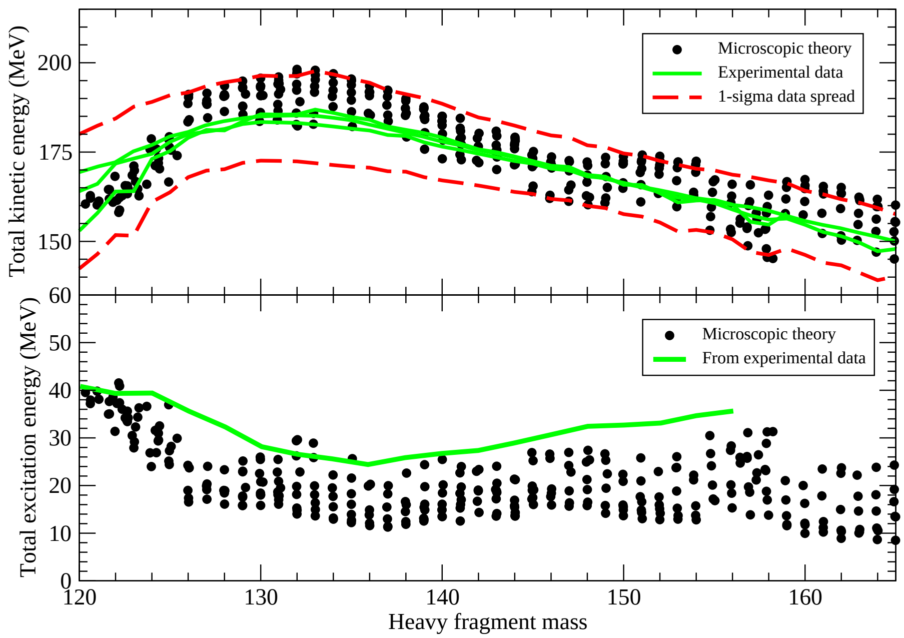


**Fig. 5.6** Comparison of calculated and experimental TKE (top panel) and TXE (bottom panel) for the $^{239}\mathrm{Pu}\,(n, f)$ reaction.

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Chapter 6

# Summary and Outlook for future directions in fission theory

In this final chapter, we summarize the calculations leading up to our estimates of fission-fragment properties following the induced fission of $^{240}$Pu. We conclude with a discussion of possible improvements to the theory, and experimental measurements that can shed light on the fission process and help guide the theory. We also give a brief survey of other theoretical approaches to the description of fission.

## 6.1 Concluding remarks about the methods presented in this work

In the second part of this book we discussed a microscopic approach to the fission problem, starting from protons, neutrons, and an effective interaction between them. Static configurations of the fissioning system were constructed using the constrained Hartree-Fock-Bogoliubov method with a finite-range interaction. We examined the choice of collective coordinates and opted for a set of parameters, the asymmetry and the separation between pre-fragments, to better describe the evolution of the nucleus up to and beyond scission. Next, we discussed in detail a quantum-mechanical definition of scission. The set of scission configurations defines a boundary separating the space in collective coordinates into post- and pre-scission regions. In order to build collectivity from these microscopic solutions, we derived both static and time-dependent collective Schrödinger equations starting from the generator coordinate method with an expansion to second order about the non-locality in the coordinates. The time-independent collective Schrödinger equation was solved with a modified potential energy surface to generate a set of initial states as linear superpositions of HFB solutions. The time-dependent collective Schrödinger equation was then used to evolve these initial wave packets to scission. By integrating the resulting flux across the scission line, the mass distribution was obtained. The difference in HFB energies between fragments at scission and in their relaxed state was used to calculate the static contribution to the fragment excitation energies at scission, while the direct interaction energy between fragments was used to obtain the static part of their total kinetic energy. In addition, an analysis of the flux in the fission direction at scission was used to estimate the dynamic contributions (pre-scission energies) to the kinetic and excitation energies. This entire approach was illustrated for the case of induced fission of $^{240}$Pu.

Moreover, in the first part of the book we gave a broader introduction to some of the tools for a microscopic theory of fission that point the way toward potential future research directions. We discussed an extension of the GCM to include quasiparticle excitations and thereby go beyond the standard adiabatic approximation that is used in many fission calculations. We also covered some projection techniques that could be used to extract fission-fragment properties with exact numbers of protons and neutrons. Projection could and should also be used to calculate these properties as a function of angular momentum [1, 2]. The effective interaction itself could also be improved by eliminating the few remaining dependences on delta functions in favor of finite-range expressions [3, 4], and by moving away from density-dependent interactions [5, 6]. There is also a need for better collective coordinates to describe the fission process from beginning to end. In particular, the parameters that are well-suited to describe the nucleus near its ground state (e.g., quadrupole and octupole moments) are increasingly insufficient as the nucleus nears scission, where one expects at least a "doubling" in the number of parameters required (possibly with the need for even more parameters to describe necking and relative separation), as one nucleus evolves into two (or more) fragments. The question of properly defining those collective coordinates for fission is a fruitful and important one [7], and time-dependent density-functional approaches such as the one presented in [8] could be of great help.

Experimental input would be very helpful in guiding the theoretical research directions proposed above. In particular, we need a more complete understanding of how energy "pumped" into the parent nucleus (i.e., by an incident beam) is partitioned between: 1) the total kinetic and total excitation energies of the fragments and 2) the individual excitation energies of the fragments at scission. This question is directly connected to the coupling among collective and between collective and single-particle degrees of freedom during the dynamical evolution of the nucleus toward scission. Because fission still occurs on time scales too short for direct measurements, multiparameter measurements are needed to reconstruct as completely as possible the state of the nucleus at scission [9]. Alternately, there are probes that can shed some light on the nucleus before and at scission, albeit with model dependences and/or caveats. Among these, we note for example measurements of scission neutrons [10] and their interpretation [11], measurements of fission time scales using a variety of techniques [12, 13, 14][1], as well as experiments involving exotic beams, such as muon-induced fission [15].

## 6.2 Survey of other fission-theory approaches

Finally, we present a brief survey of alternate approaches to the theoretical description of the fission process, focusing on recent developments. First, we review techniques used to extract static properties of the fissioning nucleus. Next, we examine various treatments of fission dynamics. We then conclude this survey with a discussion of the prospects for applying fission theory to nuclear data evaluations.

[1] Some caution is warranted in interpreting fission time measurements because some of these techniques may include the time it takes to form the compound parent nucleus, and not just the saddle-to-scission time.

### 6.2.1 Statics

Static properties of the nucleus (e.g., "shape", potential energy surface, etc.) can be calculated by methods other than the Hartree-Fock-Bogoliubov procedure. We describe a few of these methods below.

#### 6.2.1.1 Macroscopic-microscopic approaches

The macroscopic-microscopic method usually begins with a parametric family of curves that can be used to describe the nuclear shape. Various prescriptions have been used to describe the nuclear shape, for example: expansions in terms of spherical harmonics [16, 17, 18, 19, 20], Cassinian ovaloids [21], Fourier series expansions [22], three-quadratic surface shapes [23, 24], or quasi-molecular shapes [25, 26]. The energy of the nucleus is then obtained as the sum of a macroscopic contribution and microscopic corrections for shell and pairing effects [27]. The macroscopic part of the energy can be calculated by a variety of means: the liquid-drop model [21], the generalized liquid-drop model (GLDM) [25, 26] which includes a proximity energy for configurations near scission, the Lublin-Strasbourg liquid drop model (LSD) [110] which includes curvature- and shape-dependent congruence energy terms [17, 22], the finite-range liquid-drop model (FRLDM) which accounts for the finite range of the nuclear force and the diffuseness of the charge distribution [24, 23], and a Yukawa+exponential folding method [16, 17, 18, 19, 20]. The microscopic shell and pairing corrections can be calculated using a smoothing procedure [28, 29] applied to the single-particle states obtained by solving the Schrödinger equation with, for example, a deformed Woods-Saxon potential [16, 17, 18, 19, 25, 21, 20], or a Yukawa-folded potential [24, 30, 23, 22].

Macroscopic-microscopic methods can be used to calculate a potential energy surface (PES). The PES is an essential ingredient in the description of fission dynamics and can also be used to directly extract fission properties, such as barrier heights and widths, the depth of hyperdeformed minima, spontaneous fission half lives, etc. While they are not direct experimental observables, fission barriers are nevertheless very important to the calculation of fission rates [20]. The identification of features in multi-dimensional PES's , such as barriers and minima, poses a significant challenge and specialized techniques such as the "imaginary water flow" (IWF) method [31, 32, 33, 34] have been used for this task. In this way, extensive tables of fission barriers and other static nuclear properties have been constructed. Möller et al. [23] have calculated fission barriers for 5239 nuclei with $171 \leq A \leq 330$ using a 3-quadratic surface shape parametrization and a FRLDM description. Kowal et al. [16] have calculated barriers for even-even superheavy nuclei in the range $92 \leq Z \leq 126$ and $134 \leq N \leq 192$. More recently, Jachimowicz et al. [20] have obtained barriers for 1305 heavy and superheavy nuclei with $98 \leq Z \leq 126$. These types of calculations have made it possible to identify rare and interesting features in the PES. For example, the existence of a third barrier [19] and third (hyperdeformed) minimum [17, 30] has been investigated using macroscopic-microscopic methods. In the work of Jachimowicz et al. [19], inclusion of a dipole deformation was found to lower the third barrier in $^{232}$Th by more than 4 MeV, and a very shallow third minimum was obtained. The results in [19] are in line with earlier work by Kowal and Skalski [17], who found similar effects due to dipole deformation and very shallow third minima in $^{230,232}$Th. Calculations by Ichikawa et al. [30] predict the strongest candidates for nuclei where the second and third barriers have approximately the same height, namely $^{228-236}$Th and $^{228-236}$U.

Macroscopic-microscopic PES calculations have also been used to estimate spontaneous fission (SF) half lives. These calculations usually require the identification of a 1D fission path on the PES and an inertia tensor along that path. Bao et al. [25] used a semi-empirical macroscopic formula for the inertia tensor and the WKB approximation to obtain SF half lives for heavy and superheavy nuclei with $Z \geq 92$. Their calculations reproduce rather well the experimental data, and relatively long half lives are predicted for many unknown nuclei that could be measured, if they are synthesized in the laboratory. Gao et al. [26] obtained SF half lives from a direct numerical solution of the time-independent Schrödinger equation, without resorting to the WKB approximation. They applied this technique to many heavy and superheavy nuclei between U and Hs, and found more realistic results compared to the WKB approximation. The authors also calculated fission half lives from excited states in $^{238}$Np and $^{239}$U, showing that the numerical solution of the 1D Schrödinger equation is applicable to both SF and excited-state fission. Zhang et al. [35] used a quasi-molecular mechanism within the framework of the generalized liquid drop model [36] to calculate spontaneous fission half lives in good agreement with experiment for many nuclei. These half lives were obtained using the semiclassical expression for barrier penetrability, with a semiempirical model for the inertia.

In another interesting application of static macroscopic-microscopic calculations, the unexpected observation of asymmetric fission in $^{180}$Hg [37] has been studied and contrasted with actinide fission [24]. The calculations have emphasized the importance of the detailed structure of the PES and its impact on fission observables, such as the fragment mass distribution.

#### 6.2.1.2 Two-center shell models

Many surface shape parameterizations used in macroscopic-microscopic approaches, e.g. expansion in spherical harmonics, are not well-suited to describe the nucleus at and beyond scission. One possible solution to this problem, the two-center shell model (TCSM), was developed by Maruhn et al. [38]. This approach is based on the solution of the time-independent Schrödinger equation with two smoothly joined harmonic oscillator potentials. For well-separated potentials, the single-particle states calculated can be sorted into the separate shell structures of the fragments. These single-particle states can then be used in macroscopic-microscopic model to calculate shell and pairing corrections.

Ivanyuk et al. [39] use a TCSM based on two oscillator potentials smoothly joined by a fourth-order polynomial and a parameterized nuclear shape with an asymmetry degree of freedom. They also used a variational prescription devised by Strutinsky [40, 41] to obtain an optimal nuclear shape without imposing a parameterization, which leads to a differential equation for a profile function, solved under constraints on the volume and elongation of the nucleus. The deformation energy calculated using the optimal shapes and the TCSM were found to agree, which was used as a validation of the TCSM. Assuming the fission process is adiabatic, the authors formulated a probability of populating any point on the potential energy surface calculated in a macroscopic-microscopic approach, based on the deformation energy and a collective temperature (similar to the probability used by Wilkins et al. [42]). This probability was used to calculate the fission-fragment mass distributions, their average kinetic and excitation energies, as well as the average number of prompt neutrons emitted by each fragment. The kinetic energies calculated for $^{232}$Th, $^{235}$U, $^{239}$Pu, and $^{245}$Cm were found to be in good agreement with the experimental data.

Mirea et al. [43] used the TCSM to calculate isotopic yields for the cold fission of $^{252}$Cf. The macroscopic energy was obtained using a Yukawa+exponential model, and the pairing and shell corrections were calculated with a Woods-Saxon potential with the TCSM. The penetrabilities were calculated in a semiclassical approximation, with an inertial mass calculated in the cranking approximation along a fission path determined in the multidimensional space of shape coordinates using a least action principle. This work emphasized the impact of magic numbers on the fragment mass distributions. In later work, Mirea [44] used the TCSM to construct time-dependent equations of motion with a dynamically adjusted constraint on the fragment particle numbers. Probabilities of fission into individual mass partitions were calculated using the penetrability of the fission barrier obtained in the WKB approximation. This formalism was then applied to the comparison of probabilities of odd-odd and even-even fragment mass partitions as a function of their excitation energy, in order to study pair-breaking effects in fission.

The TCSM has also been used in spontaneous fission half-life calculations. For example, Poenaru et al. [45] applied the TCSM to estimate the spontaneous fission half life for $^{286}$Fl. They relied on the macroscopic-microscopic model with the macroscopic contribution to the energy obtained from a Yukawa+exponential model, and with the microscopic part based on single-particle states given by the TCSM. The half life was calculated in the WKB approximation, using an inertial mass obtained in the cranking approximation and including BCS pairing correlations based on the TCSM single-particle states.

Malik [46] solved a collective time-independent Schrödinger equation with the TCSM, quantized using the Pauli-Podolski prescription [47, 48]. The mass tensor was calculated in the cranking approximation. Fission-fragment mass distributions following the $^{208}\mathrm{Pb}\left(^{18}\mathrm{O}, f\right)$ reaction were then deduced directly from the wave function solution of the collective time-independent Schrödinger equation.

#### 6.2.1.3 Scission-point models

Scission-point models have a fairly long history dating back at least to the work of Fong [49, 50], and have been used to calculate probability distributions for various fission-fragment properties (e.g., mass, and energy distributions). These models rely on two critical assumptions: 1) fission-fragment properties can be determined entirely from an analysis of the system at scission, and 2) a thermodynamic equilibrium exists between the fission fragments, thereby justifying a statistical treatment. In Fong's approach, the probability of a given mass division is taken as proportional to the number of quantum states available at scission. A variant of the scission-point model approach was later proposed by Wilkins et al. [42], wherein the probability of each division is given by a Boltzmann distribution dependent on the potential energy of the system at scission. The Wilkins approach introduces both an intrinsic temperature common to both fragments, and a separate temperature associated with the collective degrees of freedom of the system.

Andreev et al. [51, 52] have used an improved scission point model to study the fragment properties for the fission of Hg isotopes. In their work, the nucleus at scission is described as two nearly touching coaxial spheroids. The energy of the system is calculated in a macroscopic-microscopic approach, with shell corrections from a TCSM with the Strutinsky smoothing procedure. The shell corrections are damped as a function of excitation energy and angular momentum, and a zero-point contribution is included in the calculation of the individual fragment energies. The interaction energy between the fragments consists of a Coulomb contribution and a nuclear part, calculated using a double-folding integral with a Skyrme-type nucleon-nucleon potential. In this approach, the distance between the fragments is not a free parameter but rather is obtained by minimizing the energy of the system for fixed deformations of the fragments. The mass yield is taken to be proportional to a Boltzmann distribution dependent on the potential energy of the system. Using this formalism, the authors calculated mass distributions and average total kinetic energies for various Hg isotopes, and predicted the evolution of the mass distributions from symmetric for $^{174}\mathrm{Hg}$, to more asymmetric for $^{180}\mathrm{Hg}$, and back to symmetric for $^{192,194,196}\mathrm{Hg}$. They also applied this model to $^{194,196}\mathrm{Po}$, and found a transition from asymmetric to symmetric mass distributions with increasing mass for Ir isotopes, similar to the trend in Hg nuclei. A very similar model was used by Paşca et al. [53] to calculate charge distributions for $^{218-228}$Th and to describe the transition from symmetric to asymmetric distributions as a function of parent nucleus mass. The model was also applied to obtain charge and mass distributions, as well as total kinetic energies of the fragments for the $^{235}\mathrm{U}\,(n,f)$ and $^{239}\mathrm{Pu}\,(n,f)$ reactions, as a function of excitation energy [54].

In a phenomenological variant of the scission point model, Sun et al. [55] used the concept of a dinuclear system to calculate a "driving potential" as the sum of the Q value for a particular division and the Coulomb barrier height in the interaction potential between fragments. A rough mass distribution can be obtained from this driving potential using a Boltzmann exponential factor. A phenomenological potential constructed from 3 harmonic-oscillator functions was also tested and compared to the results with the driving potential. The mass distributions following the $^{238}\mathrm{U}\,(n,f)$, $^{237}\mathrm{Np}\,(n,f)$, $^{235}\mathrm{U}\,(n,f)$, $^{232}\mathrm{Th}\,(n,f)$ and $^{239}\mathrm{Pu}\,(n,f)$ reactions were reproduced reasonably well by this approach.

Panebianco et al. [56] developed an improved version of the Wilkins model that is not restricted to a fixed distance at scission between two coaxial fragments. In the Panebianco et al. approach, the individual fragment energies were obtained from HFB calculations, and the interaction potential between them was calculated as the sum of a Coulomb repulsion between coaxial ellipsoids, and a Blocki proximity potential for the nuclear part [57]. A microcanonical description then gives the fission fragment distributions. In this approach, the distance between fragments was treated as a free parameter. The model gave a qualitative description of the evolution from asymmetric to symmetric division in the Hg isotopes. The same model was used by Goriely et al. [58] to investigate neutron-star mergers as a possible site for the astrophysical r process. They found an $A \approx 165$ rare-earth production peak consistent with abundance patterns in the sun and metal-poor stars. Their results lend support to NS mergers as a leading source of r-process nuclei with $A \gtrsim 140$. Lemaître et al. [59] further developed the model by shifting the HFB energies for individual fission fragments to match experimental masses, and found that they were able to reproduce general trends in mass and charge yields.

#### 6.2.1.4 The sudden approximation

A somewhat different approach has been explored by Carjan and others [60, 61, 62] to account, in particular, for the emission of neutron at scission. The approach uses the sudden approximation to describe the transition from one nucleus just before scission, to two fragments immediately after. Only the neutron eigenstates for the pre- and post-scission configurations are needed in this approach. The scission neutrons suddenly find themselves in a post-scission potential. The nuclear part of the potential is described by a Woods-Saxon form as a function of distance from the nuclear surface, and that surface is represented by Cassini ovals with two parameters, to control the elongation and asymmetry of the nuclear shape. The time-independent Schrödinger equation for this problem is discretized and solved for the neutron eigenstates. The BCS pairing contribution is included for the neutron states at scission. In the sudden approximation, the initial neutron eigenstates in the configuration just before scission become wave packets in the configuration immediately after scission. Overlaps between initial and final eigenstates are then used to calculate the probability that a neutron, initially in a bound state, will be emitted. The sum of these emission probabilities, weighted by the occupation probabilities of the states, give the scission neutron multiplicity. In [60], this model was applied to the thermal neutron-induced fission on $^{235}$U. In addition to the scission neutron multiplicity, the spatial distribution of the neutron emission points was calculated, as well as the total excitation energy which consists of the average energy needed to emit scission neutrons (estimated at $\sim$ 4 MeV), the deformation energy of the fragments at scission, and the excitation energy of the fragments immediately after scission. The scission neutrons were estimated to represent up to 30% of all prompt neutrons for the $^{235}\mathrm{U}\,(n, f)$ reaction at thermal energies. The partition of excitation energy between the light and heavy fragment was investigated in [61] using the sudden-approximation formalism. The probability of each bound neutron to be located in a given fragment was calculated and used to separate the contribution of each fragment to the excitation energy and to the scission neutron multiplicity. The model was also applied to extract scission neutron multiplicities for U, Pu, Cm, and Cf isotopes in [62]. In this work, two different prescriptions to calculate the distance from the nuclear surface were compared: 1) an exact minimization of the point-to-surface distance, and 2) a gradient approximation formula. In this study, scission neutrons were found to account for at most 25% of prompt neutrons, although these estimates were shown to be sensitive to the neck radius before scission. A linear increase of scission neutron multiplicity with mass of the fissioning nucleus was obtained, in agreement with the experimental data for all the isotopes studied, except for Pu which displays a nearly constant behavior for the measured scission neutron multiplicity as a function of mass number.

### *6.2.2 Dynamics*

A variety of techniques have been developed to describe the evolution in time of the fissioning nucleus to scission and beyond. In this section, we survey some of these techniques and highlight their unique features.

#### 6.2.2.1 Time dependent Hartree Fock

The time-dependent Hartree-Fock (TDHF) approach was introduced by P. A. M. Dirac [63] and has been applied to the fission problem since at least the 1970s [64, 65]. The equations of the TDHF method follow from the time derivative of the one-body density in the Hartree-Fock approximation [66]. The TDHF differential equations are solved with a Slater determinant initial solution, and assume the solution remains in the form of a single Slater determinant for all times. There are definite advantages to this approach that have made it an attractive tool for the description of fission dynamics. In TDHF, there is no need to impose coordinate constraints: the system chooses its own path dynamically. There is also no need to derive a coordinate-dependent inertia tensor. Furthermore, "one-body friction" effects which result in the transfer of energy between collective and single-particle degrees of freedom are automatically included, and TDHF is therefore not ipso facto restricted to an adiabatic approximation.

On the other hand, the restriction to a single Slater determinant throughout the evolution of the system can introduce some limitations. The TDHF solution follows a classical-like trajectory by ignoring the superposition principle, and cannot tunnel through potential barriers. Even if the initial Slater determinant is a good approximation to the exact many-body wave function, there is no guarantee that this will remain the case throughout the evolution of the TDHF solution. Finally, spurious final-state interactions can occur because all outgoing channels are subject to the same mean-field potential [66].

Despite these limitations, TDHF theory has proven very useful in the description of fission. In an early application, Koonin et al. [64] used TDHF to study dissipation effects in the fission of $^{236}$U. In a classical system, dissipation represents the irreversible flow of energy from collective to intrinsic modes. Because of the small number of particles in a nucleus, energy can be transferred in both directions between collective and intrinsic degrees of freedom, and in that sense the process differs from classical dissipation. Koonin et al. sought to extract a viscosity coefficient by equating the dissipated energy (i.e., transferred to the intrinsic modes) calculated in a hydrodynamical macroscopic approach on one hand, with the result from TDHF on the other. The authors found a viscosity coefficient considerably larger than the one obtained from a comparison of calculated and experimental fission-fragment energies. They attributed the discrepancy in part to additional degrees of freedom (linked, e.g., to the axial and reflection symmetries of the nucleus) in the descent from saddle to scission.

Later work by Negele et al. [65] expanded on the study in [64] by examining three different dissipation mechanisms within a TDHF framework: two-body viscosity, standard one-body dissipation, and one-body dissipation modified to vanish in the case of uniform translations or rotations. Two-body viscosity is associated with nucleon-nucleon collisions inside the nucleus, but is not expected to play a significant role in nuclei because of the Pauli exclusion principle. The standard one-body dissipation represents collisions on individual nucleons with the moving boundary surface of the nucleus. The standard formulation of this one-body mechanism yields a non-zero dissipation for uniform translational and rotational motion, which is unphysical. Therefore, Negele et al. also studied a version of one-body dissipation modified to give the correct behavior in those cases. The authors found that the TDHF solutions with modified one-body dissipation, along with the two-body viscosity formulation, were most similar to predictions from macroscopic calculations, and that this was not the case for the standard one-body dissipation mechanism.

In more recent work, Simenel et al. [67] used TDHF to study non-adiabatic effects in the symmetric fission of $^{258,264}$Fm. Adiabatic configurations were first calculated using HF+BCS, and the non-adiabatic evolution was obtained using TDHF to account for one-body dissipation. Collective excitations of the fragments were also contained in the TDHF calculations, and it was found that low-lying vibrations were more easily excited than giant resonances, as expected. A non-adiabatic contribution to the the TKE of $\sim$ 19 MeV was obtained, and about 2/3 of the excitation energy of the fragments could be attributed to non-adiabatic effects. Finally, the calculations gave good agreement with the measured TKE for $^{258}$Fm.

Later work by Scamps et al. [68] and Simenel et al. [69] improved on the earlier calculations in [67] by including dynamical BCS pairing. This variant of TDHF, dubbed time-dependent BCS (TDBCS), accounts for changes in occupation numbers when single-particle levels cross the Fermi surface. In this approach, TDBCS equations are solved simultaneously with the TDHF equations, giving the dynamical evolution of the occupation numbers. The TDBCS was used in the descent from saddle to scission in $^{258}$Fm, and the results confirmed that 60-80% of the fission-fragment excitation energy was generated during this descent.

Tanimura et al. [70] proposed a method to calculate conjugate momenta, and the associated collective masses, for a given set of collective variables. This result facilitates the connection between microscopic and macroscopic models of fission. Their method was derived within the framework of a time-dependent energy density functional theory (TD-EDF), which resembles time-dependent Hartree-Fock-Bogoliubov theory (TD-HFB), but allows more flexibility in choosing the effective interaction. From the momentum and collective mass, the authors obtained an expression for the collective kinetic energy. They applied the formalism to the symmetric fission of $^{258}$Fm and, by analyzing the TKE, were able to estimate the energy dissipated into the excitation of the fragments. They also found that the scission point given by the dynamical calculation occurred at a much larger quadrupole moment than the adiabatic path would indicate.

Goddard et al. [71, 72] conducted a series of studies on the impact of the choice of initial state on the subsequent TDHF evolution. In a first paper

[71] they investigated "deformation-induced fission" (DIF) by choosing different initial states from static, quadrupole-moment constrained Hartree-Fock solutions for $^{240}$Pu fission. They found that the different initial conditions produced different fragmentations and they obtained promising results for mass yields. They also calculated the nuclear collective kinetic energy, defined from the current density, and extrapolated to long times using a classical formulation. Their calculated kinetic energy was in reasonable agreement with experimental data. In a follow-up paper [72], they investigated the effect of applying a gauge transformation to the initial-state single-particle wave functions, with the effect of providing an initial velocity boost toward scission, which they called "boost-induced fission" (BIF). They considered two kinds of boosts: instantaneous, and time-dependent. With the time-dependent boost, they found that energy was released gradually into the system and that a lower threshold energy was required to induce fission, compared to an instantaneous boost. Overall, BIF tended to produce more asymmetric fragments compared to DIF.

#### 6.2.2.2 Other microscopic approaches

A variant of the time-dependent GCM put forth by Dietrich et al. [73] formulates the fission process as a microscopic transport theory. The method treats the slow evolution of the nuclear shape explicitly, while using statistical approximations to describe the rapidly varying intrinsic excitations. A local temperature is defined by the requirement that the reference density, describing the slow evolution of the nuclear shape, correctly reproduces the excitation energy for a given shape. The dynamics are described in terms of a statistical density operator, instead of a state vector. The authors then obtain a rigorous equation of motion for the reference density and give a more practical form simplified using the Markov approximation.

Hupin et al. [74] applied a quantum Monte-Carlo technique to the transmission through a fission barrier. They assumed a form for the statistical operator that is separable into system and environment parts, and evolved both parts stochastically. The stochastic evolution of the environment was then projected onto relevant degrees of freedom to make the problem tractable. This method was applied to the case of harmonic potentials coupled to a heat bath, and was shown to be efficient and accurate in reproducing exact solutions.

The spontaneous fission of $^{258}$Fm was investigated by Tanimura et al. [75] using a statistical sampling of initial configurations beyond the outer barrier, evolved to scission using time-dependent density functional theory (TDDFT). The fluctuations in the initial one-body density were formulated using stochastic mean-field theory [76], and were restricted to single-particle states in a narrow energy window. Mass and TKE distributions were obtained and compared to data. The calculations underestimate mass asymmetry after fission, and the results could be improved by a better treatment of the tunneling probability through the barrier, which would impact the quantum weights of the different paths to scission.

The time-dependent superfluid local density approximation (TDSLDA), developed by Bulgac [77, 78, 79, 80] is a fully microscopic extension of density functional theory to include pairing. All degrees of freedom are treated on an equal footing, and all symmetries are correctly implemented in this approach. The equations of motion are derived from an action integral, and are formally equivalent to the time-dependent HFB approximation with local potentials. Extensions of the TDSLDA can be made to calculated two-body observables and dissipation through a stochastic treatment [78]. Recently, this formalism has been applied to the fission dynamics of $^{240}$Pu, by evolving a configuration close to the outer barrier to scission. The calculated TKE is in good agreement with experiment, but the saddle-to-scission time was found to be about an order of magnitude larger than previous estimates [80]. The longer fission time was attributed to collective-shape and pairing-field excitations in the "transverse direction" [80].

Umar et al. [81] have studied fission dynamics using the density-constrained TDHF (DC-TDHF) approach with a collective velocity boost. Applying the technique to $^{240}$Pu, an initial state was generate using TDHF to model the $^{100}\mathrm{Zr} +^{140}\mathrm{Xe}$ fusion into a composite $^{240}$Pu system. By constraining the density along the TDHF trajectory, an ion-ion potential as a function of separation distance was obtained, and a transition state consisting of an isomeric minimum in the potential was identified as an initial configuration for the fission process. From this initial transition state, a very small collective boost was sufficient to initiate fission, resulting in scission into $^{106}$Mo and $^{134}$Te. These types of calculations are a promising start for future investigations of heavy-ion induced fission.

#### 6.2.2.3 Time-dependent semi-phenomenological models

Mirea [82] has investigated the energy partition between fragments using time-dependent pairing equations. In this approach, a fission path is first determined by minimizing the action integral with a macroscopic-microscopic potential. Next, single-particle energy levels are obtained using a Woods-Saxon potential constructed to be consistent with the shape parametrization along the fission path. By assuming a BCS wave function with time-dependent occupations, the variational principle yields the equations of motion as time-dependent pairing equations (TDPE). An approximate measure of dissipated energy can be calculated as the difference between the total energy from the TDPE and the static BCS energy. Applied to the fission of $^{234}$U into $^{102}$Zr and $^{132}$Te, the TDPE approach shows that the excitation energy for the heavy, nearly doubly magic, $^{132}$Te nucleus is smaller than the light one, and the dissipation energy is directly related to the occupation probabilities at scission.

Rizea and Carjan [83] described the dynamics near scission by solving a two-dimensional Schrödinger equation with a time-dependent potential. For the potential, they used a Woods-Saxon function of distance between fragment nuclear shapes described by time-dependent Cassini ovals. In this way, they could calculate probability amplitudes for each eigenstate before scission to be occupied immediately after scission. From these probability amplitudes, they calculated the excitation energies of the fragments after scission and the multiplicity of neutrons released during scission. In addition, they extracted the distribution of emission points and average direction of motion for the emitted neutrons. Applying their methodology to $^{236}$U scission, they found that the emission of scission neutron along the fission axis would make them difficult to distinguish from neutrons evaporated from the accelerated fragments, based on their angular distribution alone.

Scamps and Hagino [84] tackled spontaneous fission by solving a two-dimensional time-dependent Schrödinger equation in a finite box. The two coordinates represent the elongation of the system and an intrinsic degree of freedom. An imaginary potential was used to absorb the outgoing flux at the edge of the box. An initial resonance state was determined using a version of the potential modified to allow for a bound state. From this initial state, the quantum mechanical flow from the solution of the time-dependent Schrödinger equation was obtained and compared to the semiclassical tunneling path. The quantum-mechanical and semiclassical approaches were found to agree.

Randrup et al. [85, 86, 87] calculated fission-fragment mass and charge distributions using a random walk on a five-dimensional potential surface. This approach corresponds to the strong-damping Smoluchowski limit, where the inertia of the system can be ignored. In [85], this approach was used to reproduce the experimental charge distributions for the $^{239}\mathrm{Pu}\,(n,f)$, $^{233,235}\mathrm{U}\,(n,f)$, $^{234}\mathrm{U}\,(\gamma,f)$, and $^{222,224,226,228}\mathrm{Th}\,(\gamma,f)$ reactions. In a follow-up paper [86], the effect of a realistic dissipation tensor as well as the sensitivity to details of the calculation were investigated, confirming the usefulness of a simple random walk to produce the general form of mass distributions for a wide range of nuclei. The technique was then systematically applied to the mass distributions for 987 parent nuclei in the region $74 \leq Z \leq 94$ and $90 \leq N \leq 150$. From these extensive calculations the transition between symmetric and asymmetric fission was found to be at $A \approx 226$ for $84 \leq Z \leq 90$ and, for higher $Z$, a transition line along $N - Z \approx 47$ was identified.

A random walk over a 5D potential surface was also used in [88] to calculate fission-fragment yields for neutron-deficient Hg isotopes, giving approximate agreement with data. In [89], this same technique was used to study excitation energy (as the difference between total and potential) as a function of deformation. The authors found a correlation between the odd-even staggering in fragment charge distributions and the average excitation energy in the deformation region where individual pre-fragments become recognizable.

Ward et al. [90] used a version of the Brownian-motion approach in [91] to study nuclear shape evolution by using a Metropolis walk on a 5D macroscopic-microscopic PES with transition rates determined by microscopic level densities. For consistency, the level densities were calculated by a combinatorial method, using the same single-particle densities as for the pairing and shell corrections, and including the angular momentum dependence. This approach was used to calculate fission-fragment charge distributions for $^{226}$Th, $^{234,236}$U, and $^{240}$Pu, giving good agreement with experimental data.

#### 6.2.2.4 Molecular dynamics

Vonta et al. [92] have described fission using a method adapted from quantum molecular dynamics [93]. Individual nucleons are described by Gaussian wave packets from which phase-space distributions are generated using a Wigner transform. The N-body phase-space distribution is taken simply as the sum of the individual nucleon distributions. The equations of motion follow from the time-dependent Schrödinger equation using a Skyrme-like effective interaction, and the Pauli exclusion principle is enforced in a stochastic way through a phase-space occupation constraint imposed at each time step. The technique was used to study the proton induced fission of $^{232}$Th, $^{235}$U, and $^{238}$U. Satisfactory agreement with cross sections, total fission energies, and neutron multiplicities was obtained, especially at higher incident proton energies (above 60 MeV).

#### 6.2.2.5 The dynamical cluster-decay model

In the dynamical cluster-decay model (DCM), which is based on the quantum-mechanical fragmentation theory of fission, the nucleus is described as preformed clusters or fragments with a nuclear proximity potential between them. The fission cross section in the DCM is written in terms of a preformation probability and a penetrability factor [94]. The preformation probability is obtained from the solution of the stationary Schrödinger equation with respect to an asymmetry coordinate, and the penetrability factor is calculated using a WKB integral [94]. Sawhney et al. [95] recently used the DCM to investigate $^{18}$O and $^{19}$F induced reaction forming many different fissioning Francium isotopes. Effects from nuclear deformation and orientation were included. Measured fission cross sections and anisotropies were reproduced using the DCM. In later work by Kaur et al. [96], the DCM was used to study the $^{239}\mathrm{Np}\,(n,f)$ reaction from 0.62 to 20 MeV, and excellent agreement with the measured cross section was obtained. In [97], Kaur et al. use the DCM to explore fission and quasifission from the $^{286}112^*$, $^{292}114^*$, and $^{296}116^*$ nuclei. Experimental cross sections were well reproduced, and the competition between the compound fission and quasifission processes was investigated, along with the effect of different proximity potentials on the mass and TKE distributions.

#### 6.2.2.6 Langevin dynamics

A different approach to nuclear dynamics consists in describing the evolution of the system as that of a Brownian particle coupled to a heat bath. The Brownian particle represents the collective degrees of freedom of the system, and the heat bath represents the single-particle degrees of freedom. The problem can be formulated quantitatively using the Langevin equation, which gives the classical equation of motion. The Langevin equation is equivalent to the Fokker-Planck equation, but is easier to solve because it reduces the dimensionality of the problem thanks to the use of the Monte-Carlo technique. This approach has been successfully applied to both fusion and fission problems [98]. In the case of fission, the method is typically used to study dissipative effects and their impact on fission probabilities, pre-scission particle emission, and fission-fragment properties (e.g., their mass, charge, and energy distributions). In the Langevin equation, the Brownian motion is dictated by a conservative driving force (in the literature, this force is obtained from the potential, free energy, or from the entropy), a frictional force, and a fluctuating force with a Gaussian probability distribution. The inertia tensor is often calculated in the Werner-Wheeler approximation to the irrotational flow of an incompressible fluid [99]. The Langevin can be coupled at each time step to a statistical calculation of particle emission, using a Monte Carlo procedure, in order to study pre-scission particles [100, 104, 105, 106, 107, 108, 109, 111, 112, 113, 114, 115, 116, 117]. Various dissipation mechanisms have been studied for fission using the Langevin equation. The wall formula [118, 119] couples energy to nucleons colliding with the surface of the nuclear potential. The window formula [119] is based on the assumption that the random exchange of particles through a narrow neck (i.e., the window) between the nascent fragments slows their separations. The wall-and-window model [120, 121, 122, 108, 109] combines the two dissipation mechanisms at the appropriate stages of the fission process. A variant, the chaos-weighted wall-and-window formula [124, 125, 123, 106, 116], uses a shape-dependent wall formula weighted by a chaoticity coefficient between 0 and 1 for shapes without a neck, and adds to it a contribution from the window formula for shapes with a neck. A surface-plus-window model has also been used [119], which includes dissipation due to two-body collisions expected to peak near the nuclear surface.[2]

[2] See also the discussion of dissipation in section 6.2.2.1.

Sadhukhan and Pal [101, 102] revisited the pioneering work of Kramers [103]. Using Langevin calculations with shape-dependent dissipation–one dissipation strength inside the saddle and another outside–they tested the assumption that the fission width depends on the pre-saddle dissipation strength alone, in the case of $^{224}$Th fission [101]. They found that the Kramers fission width, calculated with the pre-saddle dissipation strength, does not represent the true dissipation width. In a subsequent paper [102], they tested the effect of a shape-dependent inertia on the Langevin dynamics for $^{224}$Th fission. They obtained results consistent with the prediction from the Kramers fission width, and extended its domain of validity.

Using a Monte-Carlo treatment of particle evaporation, several groups have studied light-particle and gamma-ray emission before scission. Mazurek et al. [104] compared Langevin calculations with 3 collective degrees of freedom for two different macroscopic potentials: the Finite Range Liquid Drop Model (FRLDM) and the Lublin-Strasbourg Drop (LSD) model. By calculating fission probabilities, pre-scission particle multiplicities, as well fission-fragment mass, charge and TKE distributions, they found a strong dependence of the predictions on details of the PES for the high-energy fission of intermediate-fissility systems, like $^{118}$Ba, but little sensitivity for heavy systems. Ye et al. [112] looked at post-saddle gamma-ray multiplicities in $^{240}$Cf, $^{224}$Th, and $^{200}$Pb high-energy fission to help constrain the friction coefficient. They found that the multiplicity of pre-scission giant dipole resonance gammas was more sensitively dependent on the post-saddle friction coefficient in heavier systems. They also found that their results were not sensitive to using barriers from different macroscopic models. Another study of pre-scission particle emission by Eslamizadeh et al. [116] using a four-coordinate Langevin equation gave very good agreement with neutron multiplicities for $^{210}$Rn fission as a function of excitation energy. Kumar et al. [117] found a dependence of pre-scission neutron multiplicities on deformation from Langevin calculations of the $^{16}\mathrm{O} +^{208} \mathrm{Pb} \rightarrow^{224} \mathrm{Th}$ reaction, as well as three reactions leading to the same $^{251}$Es compound nucleus: $^{19}\mathrm{F} +^{232} \mathrm{Th}$, $^{27}\mathrm{Al} +^{224} \mathrm{Rn}$, and $^{40}\mathrm{Ar} +^{211} \mathrm{Tl}$. Pahlavani et al. [107, 108, 109] used the same statistical treatment of particle emission coupled to the Langevin equation, and including the dynamical evolution of the K quantum number, to study the spectrum of particles evaporated by the fragments. In [107] they found good agreement with data for the initial fragment spin, average energy and multiplicity of emitted neutrons and gammas, following the $^{235}\mathrm{U}(n,f)$ reaction at 20 MeV in excitation. In a study of thermal and fast $^{233,235,238}\mathrm{U}(n,f)$ reactions [108], they obtained good agreement for prompt neutron multiplicities as a function of incident energy, especially at lower energies. Their recent work on the fission of $^{238-242}$Pu [109] also showed good agreement with data for prompt neutron multiplicities, and reproduced the well-known sawtooth behavior.

The excitation energy at scission ($E^*_{\mathrm{sc}}$) has been singled out by Ye et al. [111, 113] as a useful probe of dissipation in highly excited nuclei. Using one-dimensional Langevin calculations coupled to a Monte-Carlo treatment of particle and gamma emission, they studied the sensitivity of $E^*_{\rm sc}$ to the friction coefficient $\beta$ under a variety of conditions [111]. They found that, at high excitation energies of the initial nucleus, $E^*_{\rm sc}$ is not very sensitive to angular momentum, the size of the fissioning nucleus, or to the choice of level-density parameter which enters into the calculation of the driving force in the Langevin equation. In a later paper [113], a different friction coefficient was used before and after the saddle, and the authors found increased dissipation strength with increasing deformation, and increased sensitivity of $E^*_{\rm sc}$ to the post-saddle friction coefficient at higher excitation energies.

Langevin calculations have also shown great success in reproducing measured fission-fragment mass and charge distributions. Sadhukhan et al. [120] compared mass distributions calculated at the saddle and at scission and found a slight increase in variance of the mass peaks from saddle to scission. They also compared dynamical and statistical model predictions and found them to be similar at the saddle, but different at scission. Aritomo et al. [121] obtained good agreement between calculated and measured mass distributions for $^{234,236}$U and $^{240}$Pu fission at 20 MeV in excitation. They also observed [122] that the position of the mass peaks is related to the position of the saddle point, which in turn is determined by the shell corrections to the energy surface, and that the widths of the mass peaks are determined by fluctuations around the scission point. Mazurek et al. [106] used the Langevin method to study the Businaro-Gallone point (the fissility at which mass distributions change from symmetric to asymmetric) in medium mass nuclei from $^{102}$Rh to $^{148}$Pm. Their calculations included K quantum number evolution using an overdamped Langevin equation in order to account for angular momentum effects on fission barriers, which is important in the Businaro-Gallone region. Their analysis revealed a complex interplay between static and dynamic effects in this region. Pahlavani et al. obtained good agreement with experimental mass distributions for neutron-induced fission on $^{233,235,238}$U [108], and later for the fission of $^{238-241}$Pu [109]. The extensive Langevin study carried out by Sierk [119] produced good agreement with data for the energy dependence of fragment yields for the $^{233,235}$U$(n,f)$ reactions, some discrepancies in the details of mass yields for the $^{239}$Pu$(n,f)$ and $^{240}$Pu(SF) reactions, and significant discrepancies for $^{252}$Cf(SF). Usang et al. [118] compared macroscopic (hydrodynamical) and microscopic (Langevin) calculations of mass distributions for the fission of $^{234,236}$U and $^{240}$Pu. They obtained the microscopic transport coefficients (friction and inertia tensors) from linear response theory and local harmonic approximation, adjusted to the local temperature. They found good agreement with measured mass distributions using macroscopic and microscopic transport coefficients, emphasizing the importance of including the temperature dependence in the microscopic transport coefficients. Looking at fission-fragment charge distributions, Mazurek et al. [104] found a strong dependence on the choice of the potential-energy surface (FRLDM vs. LSD) for medium-mass fissioning nuclei (e.g., $^{118}$Ba). In a later study [105], they used a statistical model and experimental data to adjust the width of the charge peak and found good agreement with the measured charge distribution following the fission of $^{250}$Cf at 45 MeV in excitation. Fission-fragment kinetic energies have also been calculated in the Langevin approach. Mazurek et al. [104] studied the TKE following the $^{78}$Kr(429MeV)+$^{40}$Ca $\rightarrow^{118}$ Ba reaction and, as with the charge distributions, found significant differences between the calculations with the FRLDM and LSD energy surfaces. Sierk [119] obtained good agreement for the calculated TKE as a function of incident neutron energy for the $^{235}$U$(n, f)$ reaction.

Fission cross sections and probabilities have been calculated by several groups using the Langevin approach. Pahlavani et al. [108] generated fission probabilities from the Langevin equation, and multiplied them by a formation cross section calculated using an optical model to produce fission cross sections for the $^{233,235}$U$(n, f)$ reactions in good agreement with experimental data. Tian et al. [114, 115] compared cross sections calculated with the Langevin method to statistical model predictions. They found that the sensitivity of the cross section to the pre-saddle friction strength decreases with the size of the fissioning nucleus. Eslamizadeh et al. [116] also compared Langevin and statistical calculations of fission cross sections and observed that the sensitivity of the difference between calculations to the friction coefficient increases for high-isospin low-spin systems.

Vardaci et al. [126] applied Langevin dynamics, coupled to a Hauser-Feshbach model for the evaporation of light particles at each time step, to the fission of $^{132}$Ce at 122 MeV in excitation energy. They performed their calculations using both one- and two-body dissipation mechanisms, and obtained good agreement with data for cross sections as well as mass and energy distributions.

The Langevin approach has also been applied to the calculation of fission-fragment angular distributions. Naderi [123], for example, studied several $^{16}$O induced fission reactions, treating the time evolution of the K quantum number. The resulting fragment angular distributions for the fission of $^{248}$Cf, $^{254}$Fm, and $^{264}$Rf were found to be in good agreement with the data. In [127], Langevin calculations were coupled with a statistical emission model for light particles. An initial K-quantum number distribution was evolved in time by statistical fluctuations sampled at each time step. A comparison with measured pre-scission neutron multiplicities and fragment anisotropies for the fission of Cf isotopes was then used to study viscosity and the dynamics of the K quantum-number evolution.

### 6.2.3 Data evaluations

Finally, the various approaches described above (microscopic and otherwise) can be incorporated into the various tools used for nuclear data evaluations.[3] Some of the developments we discuss in this section already rely on the fission theory tools described thus far, while others could in principle readily incorporate them.

The point-by-point (PbP) model developed by Tudora et al. [131] treats the decay physics for the two isobars per fragment mass that are closest to the most probable charge explicitly. In [132], the model was used to examine the correlation between pre-scission and post-scission observables, brought about by sub-barrier resonances. The fission cross section is the main observable dictated by pre-scission physics, while various fragment properties and the neutron multiplicities are determined by post-scission physics. The PbP model was used to calculate neutron emission and was coupled to a multi-modal fission model, with different fission modes associated with different nuclear shapes at scission [133]. These fission modes contribute to the fission cross section in different amounts, and are populated differently near sub-barrier resonances. This approach was applied to the $^{238}\mathrm{U}\,(n,f)$ reaction, which has sub-barrier resonances for incident neutron energies of $E_n \approx 0.95$ MeV and 1.25 MeV, and the calculations were found to be in good agreement with the measured cross section, as well as with the prompt neutron multiplicities and spectrum. The PbP model was also used to argue for correlations between pre- and post-scission observables near sub-barrier resonances for the $^{232}\mathrm{Th}\,(n,f)$ reaction [134]. In that case, prompt neutron and gamma-ray properties were extracted and found to be in good agreement with experimental data. Pre- and post-scission correlations were also studied in the $^{235}\mathrm{U}\,(n,f)$ reaction [135], with the PbP model used to extract the properties of the fragments and prompt neutrons as a function of incident energy.

More recently [136], the PbP model was applied to the question of the partition of energy between fragments. The prediction for this energy partition given by the PbP model was compared to the one obtained from the energy sorting mechanism of Schmidt and Jurado [137] and implemented in the GEF code [138]. In the PbP model, the excitation energy available at scission is partitioned according to the ratio of level-density parameters of the fragments, while in the energy-sorting approach the available intrinsic energy is transferred entirely to the fragment with lower temperature, the collective energy is shared equally among the fragments, and the deformation and pairing energies are calculated separately for each fragment. The excitation energy of a fragment, according to the energy-sorting mechanism, is then the sum off all these components (intrinsic, collective, deformation, and pairing). Both partition schemes gave good agreement with prompt neu-

[3] For an overview of nuclear data evaluation techniques, see for example [128, 129, 130].

tron multiplicities and average gamma-ray energies as a function of fragment mass.

The Fission Reaction Event Yield Algorithm (FREYA), developed by Randrup and Vogt [139], generates an event-by-event simulation of fission with full kinematic information for all products and emitted neutrons and photons. In its original formulation [139], mass and charge distributions are obtained from fits to data with Gaussian functions, scission energetics are calculated assuming coaxial spheroids with mutual Coulomb repulsion, thermal energy fluctuations are included based on Fermi-gas level density parameters, and neutron and photon emission is treated in a statistical approach. In [140], FREYA was extended to handle spontaneous fission and calculations were performed of mass distributions after neutron emission, TKE and neutron multiplicities as a function of fragment mass, neutron spectrum shape, and neutron-neutron angular correlations for the $^{239}$Pu$(n_{th}, f)$, $^{240}$Pu(SF), $^{252}$Cf(SF), $^{244}$Cm(SF), $^{235}$U$(n_{th}, f)$, and $^{238}$U(SF) reactions. The FREYA code was extended to handle multi-chance fission and pre-equilibrium neutron emission in [141], and was used to study the prompt fission neutron spectrum following the $^{239}$Pu$(n, f)$ reaction up to 20 MeV incident energy. The code was next applied to photon observables in the $^{235}$U$(n_{th}, f)$ and $^{252}$Cf(SF) reactions. Good agreement was obtained with the measured photon multiplicity distribution. In [143] neutron-neutron angular correlations for $^{252}$Cf(SF) and $^{235}$U$(n, f)$ were calculated. Good agreement with data was obtained without the need for scission neutrons, and the results were found to be relatively insensitive to input parameters.

Talou et al. [144] applied a Monte-Carlo approach to the prompt neutron emission from fission fragments. The neutron energies were sampled from an evaporation spectrum, and assumptions were made about the energy partition between fragments at scission by treating the ratio of their temperatures as a free parameter. Gamma-ray emission was not explicitly considered. The approach was applied to fission induced on $^{239}$Pu by thermal and 0.5-MeV neutrons, and the sensitivity to the temperature ratio parameter was investigated for neutron multiplicities and energies.

Moving on to cross sections, the Hauser-Feshbach formalism [147] has long been the prevalent tool used in modern calculations of fission cross sections. Here as well, microscopic ingredients can and have been introduced. Goriely et al. [148] used fission barriers and level densities from mean-field microscopic calculations in the Hauser-Feshbach code TALYS [129]. A one-scale-parameter renormalization was applied to the microscopic barriers, and a scale an shift parameters were used for the level densities. The approach was applied to uranium isotopes and gave good agreement with measured cross sections, while reducing the number of free parameters in the reaction model.

Kawano et al. [149] examined the Hauser-Feshbach model more closely by comparing its prediction for the energy spectra of emitted neutrons to predictions from evaporation theory [150, 151]. In the Hauser-Feshbach model, neutron emission is determined by transmission coefficients and level densities in the residual nucleus. In evaporation theory, the neutron spectrum is formulated directly within a simplified view of the emission process. The approximations introduced by evaporation theory were shown to not always be valid, notably because they ignore the role of the initial spin distribution.

Becker et al. [152] used a Monte-Carlo Hauser-Feshbach approach to model prompt gamma-ray emission from excited fragments. The starting point in the calculations was the excited primary fragment with given spin, parity, and excitation energy. Neutron and gamma emission probabilities were then calculated using level densities and transmission coefficients. This approach gave good agreement with measurements of neutron and gamma-ray properties following the $^{235}$U$(n,f)$, $^{239}$Pu$(n,f)$, and $^{252}$Cf(SF) processes. As in [149], the initial spin distribution of the fragments was found to be one of the most important input quantities.

In Bouland et al. [155], the Hauser-Feshbach formalism was combined with an R-matrix treatment of low-energy fission and applied to $^{236-244}$Pu fission. This model was implemented using Monte-Carlo simulations of class-I and class-II state properties, and of their coupling matrix elements. The calculations also included quasiparticle vibrational transition states and, at higher energies, semi-microscopic combinatorial level densities.

Finally, in a higher-energy regime, Meo et al. [153] studied fission cross sections induced by incident energies from 100 MeV to 1 GeV. The reaction in this case proceeds by an intranuclear cascade mechanism [154] followed by a slow decay stage (particle evaporation, fission, etc.). The calculations were performed using a two-parameter fit by adjusting fission barrier heights and asymptotic level density parameters. Eventually, these parameters could be constrained by microscopic calculations, as in [148]. The calculations gave good agreement with data for a variety of actinide and pre-actinide targets.

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# Appendix A
# Hartree-Fock-Bogoliubov algorithm

The HFB formalism described in chapter 1 is central to the work presented in this manuscript. In this section, we present an algorithm that implements this formalism and that was used to obtain the results discussed throughout the manuscript. This algorithm was discussed in a previous publication [4], and is repeated here for completeness and for the reader's convenience. Other examples of Hartree-Fock and Hartree-Fock-Bogoliubov algorithms and codes can be readily found in the literature [1, 3, 2].

The main steps are shown in Table 1. A list of basis states is generated in step 1 using the formalism described in section 2.2, and grouped according to symmetries required by the user. These groups define the block structure of the various field matrices in the computation. If a starting solution is available, the corresponding densities ($\rho_n$, $\rho_p$) and pairing tensors ($\kappa_n$, $\kappa_p$) are read in along with any Lagrange multipliers for the constraints in step 3. At this point, the main HFB loop begins. Various field matrices are calculated in step 5 for the kinetic energy operator ($T_n$, $T_p$), the mean field ($\mathit{\Gamma}_n$, $\mathit{\Gamma}_p$), and the pairing field ($\mathit{\Delta}_n$, $\mathit{\Delta}_p$) as described in chapter 1. These fields are assembled into the HFB matrix in Eq. (1.13), and diagonalized in step 6 to obtain the $U$ and $V$ matrices. From these new $U$ and $V$ matrices, new densities and pairing tensors for the neutrons and protons in step 7. Next, the change in generalized density from the previous iteration $(i-1)$ is calculated in step 8 to gauge the convergence of the solution: $\varepsilon = \sup|R\,(i) - R\,(i-1)|$. A mixing parameter $\alpha$ between iterations is calculated based on the value of $\varepsilon$ in step 9 according to the formula [4]

$$\alpha = \begin{cases} \alpha_{\max} & \varepsilon \geq \varepsilon_{\max} \\ \alpha_{\max}\frac{\varepsilon-\varepsilon_{\min}}{\varepsilon_{\max}-\varepsilon_{\min}} & \varepsilon_{\min} < \varepsilon \leq \varepsilon_{\max} \\ 0 & \varepsilon < \varepsilon_{\min} \end{cases} \tag{A.1}$$

with typical values $\varepsilon_{\min} = 10^{-4}$, $\varepsilon_{\max} = 10^{-1}$, and $\alpha_{\max} = 0.8$. The solutions are then mixed in step 10,

$$R\,(i) \leftarrow (1-\alpha)R(i) + \alpha R(i-1) \tag{A.2}$$

The Lagrange multipliers and generalized density are adjusted in steps 11 and 12, respectively, as described in section 1.5.2 to satisfy any constraints imposed by the user. The HFB loop terminates if $\varepsilon < \varepsilon_{\min}$ for a set number of consecutive iterations (typically 3) to ensure that the solution is stable.

**Algorithm 1** HFB algorithm pseudocode.

Generate basis state quantum numbers $(n_r, \mathit{\Lambda}, n_z, \sigma)$<br>
Subdivide basis into blocks, according to imposed symmetries<br>
Read initial generalized density $R$ and Lagrange multipliers $\lambda_i$<br>
**repeat**<br>
    Construct Hamiltonian fields<br>
    Diagonalize the HFB Hamiltonian (separately for neutrons and protons)<br>
    Construct the new generalized density<br>
    Calculate maximum change in generalized density<br>
    Adjust mixing parameter<br>
    Mix generalized density from this iteration with the one from the previous iteration<br>
    Adjust Lagrange multipliers<br>
    Adjust generalized density<br>
**until** $\epsilon$ small enough

# References

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# Appendix B
# Exact solution of the multi-$\boldsymbol{O}(4)$ model

The exact solution for this model is obtained by using quasispin methods (see, e.g., chapter 7 in [1]). For this, we first introduce an additional operator

$$\begin{aligned} \hat{B}^{\dagger} &= \sum_j \hat{B}_j^{\dagger} \\ \hat{B}_j^{\dagger} &= \sum_{m>0} \sigma_{jm} a_{jm}^{\dagger} a_{j\bar{m}}^{\dagger} \end{aligned}$$

and then define the quasispin operators [2, 3, 4][1]

$$\begin{aligned} \hat{K}_j^{+} &\equiv \frac{1}{2}\left(\hat{A}_j^{\dagger} + \hat{B}_j^{\dagger}\right) \\ \hat{K}_j^{-} &\equiv \frac{1}{2}\left(\hat{A}_j + \hat{B}_j\right) \\ \hat{K}_j^{0} &\equiv \frac{1}{4}\left(\hat{N}_j + \hat{D}_j - \Omega_j\right) \end{aligned} \tag{B.1}$$

and

$$\begin{aligned} \hat{L}_j^{+} &\equiv \frac{1}{2}\left(\hat{A}_j^{\dagger} - \hat{B}_j^{\dagger}\right) \\ \hat{L}_j^{-} &\equiv \frac{1}{2}\left(\hat{A}_j - \hat{B}_j\right) \\ \hat{L}_j^{0} &\equiv \frac{1}{4}\left(\hat{N}_j - \hat{D}_j - \Omega_j\right) \end{aligned} \tag{B.2}$$

The sets $\left\{\hat{K}_j^{+}, \hat{K}_j^{-}, \hat{K}_j^{0}\right\}$ and $\left\{\hat{L}_{j,}^{+}, \hat{L}_j^{-}, \hat{L}_j^{0}\right\}$ separately form $SU\,(2)$ algebras, and any two elements of different sets commute [3]. In particular, it can be readily verified that

$$\begin{aligned} \left[\hat{K}_j^{+}, \hat{K}_j^{-}\right] &= 2\hat{K}_j^{0} \\ \left[\hat{K}_j^{0}, \hat{K}_j^{\pm}\right] &= \pm\hat{K}_j^{\pm} \\ \left[\hat{K}_j^{-}, \hat{L}_j^{+}\right] &= 0 \\ \left[\hat{L}_j^{+}, \hat{L}_j^{-}\right] &= 2\hat{L}_j^{0} \\ \left[\hat{L}_j^{0}, \hat{L}_j^{\pm}\right] &= \pm\hat{L}_j^{\pm} \end{aligned} \tag{B.3}$$

with all other commutators (e.g., between operators in $j$ and $j'$ where $j \neq j'$) equal to zero. We can then write

[1] Note the factor 1/4 in the definitions of $\hat{K}_j^{0}$ and $\hat{L}_j^{0}$ which is consistent with the definitions in [2], but not [3, 4].

$$\begin{aligned}\hat{A}_j^\dagger &= \hat{K}_j^+ + \hat{L}_j^+ \\ \hat{A}_j &= \hat{K}_j^- + \hat{L}_j^- \\ \hat{D}_j &= 2\left(\hat{K}_j^0 - \hat{L}_j^0\right) \\ \hat{N}_j &= 2\left(\hat{K}_j^0 + \hat{L}_j^0\right) + \Omega_j\end{aligned} \tag{B.4}$$

so that the components in Eq. (1.79) become

$$\hat{H}_0 = \sum_j e_j^0 \left[2\left(\hat{K}_j^0 + \hat{L}_j^0\right) + \Omega_j\right] \tag{B.5}$$

$$\hat{H}_Q = 2\chi \sum_{j,j'} d_j d_{j'} \left(\hat{K}_j^0 - \hat{L}_j^0\right)\left(\hat{K}_{j'}^0 - \hat{L}_{j'}^0\right) \tag{B.6}$$

$$\hat{H}_P = -\frac{1}{2} G \sum_{j,j'} \left[\left(\hat{K}_j^+ + \hat{L}_j^+\right)\left(\hat{K}_{j'}^- + \hat{L}_{j'}^-\right) + \left(\hat{K}_{j'}^- + \hat{L}_{j'}^-\right)\left(\hat{K}_j^+ + \hat{L}_j^+\right)\right] \tag{B.7}$$

## B.1 Useful results for the quasi-spin algebra

### *B.1.1 The action of $\hat{K}_j^0$ on the state $\left(\hat{K}_j^+\right)^n |0\rangle$*

Let us first calculate the effect of $\hat{K}_j^0$ on the particle vacuum $|0\rangle$ where we recall that (see Eq. (B.1))

$$\hat{K}_j^0 \equiv \frac{1}{4}\left(\hat{N}_j + \hat{D}_j - \Omega_j\right)$$

and therefore, using the definitions of the operators $\hat{N}_j$ and $\hat{D}_j$ in Eqs. (1.81) and (1.83), respectively, we find

$$\hat{K}_j^0 |0\rangle = -\frac{\Omega_j}{4} |0\rangle \tag{B.8}$$

Next, we wish to calculate $\hat{K}_j^0 \left(\hat{K}_j^+\right)^n |0\rangle$ for a given integer $n$ with $0 \leq n \leq \Omega_j/2$. Using the $SU(2)$ commutators in Eq. (B.3) we write for example

$$\begin{aligned}\hat{K}_j^0 \hat{K}_j^+ &= \left[\hat{K}_j^0, \hat{K}_j^+\right] + \hat{K}_j^+ \hat{K}_j^0 \\ &= \hat{K}_j^+ \left(1 + \hat{K}_j^0\right)\end{aligned}$$

More generally, if for a given integer $k$ we have

$$\hat{K}_j^0 \left(\hat{K}_j^+\right)^k = \left(\hat{K}_j^+\right)^k \left[k + \hat{K}_j^0\right]$$

then we can show that

$$\begin{aligned}
\hat{K}_j^0 \left(\hat{K}_j^+\right)^{k+1} &= \hat{K}_j^0 \left(\hat{K}_j^+\right)^k \hat{K}_j^+ \\
&= \left(\hat{K}_j^+\right)^k \left[k + \hat{K}_j^0\right] \hat{K}_j^+ \\
&= k \left(\hat{K}_j^+\right)^{k+1} + \left(\hat{K}_j^+\right)^k \left[\hat{K}_j^+ \left(1 + \hat{K}_j^0\right)\right] \\
&= \left(\hat{K}_j^+\right)^{k+1} \left[k + 1 + \hat{K}_j^0\right]
\end{aligned}$$

Therefore, by induction, we conclude that for any integer $n \geq 0$,

$$\hat{K}_j^0 \left(\hat{K}_j^+\right)^n = \left(\hat{K}_j^+\right)^n \left(n + \hat{K}_j^0\right) \tag{B.9}$$

and we can use this with Eq. (B.8) to calculate Eq. (A.8a) in [4]

$$\boxed{\hat{K}_j^0 \left(\hat{K}_j^+\right)^n |0\rangle = \left(n - \frac{\Omega_j}{4}\right) \left(\hat{K}_j^+\right)^n |0\rangle} \tag{B.10}$$

with a similar equation for the $\hat{L}_j^0$ and $\hat{L}_j^+$ operators defined in Eq. (B.2),

$$\boxed{\hat{L}_j^0 \left(\hat{L}_j^+\right)^n |0\rangle = \left(n - \frac{\Omega_j}{4}\right) \left(\hat{L}_j^+\right)^n |0\rangle} \tag{B.11}$$

### B.1.2 The action of $\hat{K}_j^-$ on the state $\left(\hat{K}_j^+\right)^n |0\rangle$

Using the $SU\,(2)$ algebra commutators in Eq. (B.3) we write

$$\begin{aligned}
\hat{K}_j^- \hat{K}_j^+ &= \left[\hat{K}_j^-, \hat{K}_j^+\right] + \hat{K}_j^+ \hat{K}_j^- \\
&= -2\hat{K}_j^0 + \hat{K}_j^+ \hat{K}_j^-
\end{aligned}$$

We use this result to calculate for any integer $n > 0$

$$\hat{K}_j^- \left(\hat{K}_j^+\right)^n = \left(-2\hat{K}_j^0 + \hat{K}_j^+ \hat{K}_j^-\right) \left(\hat{K}_j^+\right)^{n-1}$$

and with the help of Eq. (B.9) this gives a recurrence relation

$$\hat{K}_j^- \left(\hat{K}_j^+\right)^n = -2\left(\hat{K}_j^+\right)^{n-1}\left(n-1+\hat{K}_j^0\right) + \hat{K}_j^+\left[\hat{K}_j^- \left(\hat{K}_j^+\right)^{n-1}\right] \tag{B.12}$$

If we apply this recurrence relation repeatedly to the right-hand side we find

$$\begin{aligned}
\hat{K}_j^- \left(\hat{K}_j^+\right)^n &= -2\left(\hat{K}_j^+\right)^{n-1}\left[(n-1)+(n-2)+\ldots+1+n\hat{K}_j^0\right] \\
&\quad + \left(\hat{K}_j^+\right)^n \hat{K}_j^- \\
&= -2\left(\hat{K}_j^+\right)^{n-1}\left[\frac{1}{2}n\left(n-1\right)+n\hat{K}_j^0\right] + \left(\hat{K}_j^+\right)^n \hat{K}_j^- \\
&= \left(\hat{K}_j^+\right)^{n-1}\left[n\left(1-n\right)-2n\hat{K}_j^0\right] + \left(\hat{K}_j^+\right)^n \hat{K}_j^-
\end{aligned} \tag{B.13}$$

Using Eqs. (B.8) and (B.13), and the (easily verified) fact that $\hat{K}_j^- \left|0\right\rangle = 0$, we now calculate

$$\boxed{\hat{K}_j^- \left(\hat{K}_j^+\right)^n \left|0\right\rangle = n\left(\frac{\Omega_j}{2}-n+1\right)\left(\hat{K}_j^+\right)^{n-1}\left|0\right\rangle} \tag{B.14}$$

We can derive a similar relation for the $\hat{L}_j^-$ and $\hat{L}_j^+$ operators defined in Eq. (B.2),

$$\boxed{\hat{L}_j^- \left(\hat{L}_j^+\right)^n \left|0\right\rangle = n\left(\frac{\Omega_j}{2}-n+1\right)\left(\hat{L}_j^+\right)^{n-1}\left|0\right\rangle} \tag{B.15}$$

### *B.1.3 Normalization of the state* $\left(\hat{K}_j^+\right)^n \left|0\right\rangle$

We define the state

$$\left|n\right\rangle \equiv C_n \left(\hat{K}_j^+\right)^n \left|0\right\rangle$$

where $C_n$ is a normalization constant that we wish to determine such that

$$\left\langle n\right|n\rangle = \left|C_n\right|^2 \left\langle 0\left|\left(\hat{K}_j^-\right)^n \left(\hat{K}_j^+\right)^n\right|0\right\rangle = 1$$

Now we use Eq. (B.14) to write

$$\begin{aligned}
\left\langle 0\left|\left(\hat{K}_j^-\right)^n \left(\hat{K}_j^+\right)^n\right|0\right\rangle &= \left\langle 0\left|\left(\hat{K}_j^-\right)^{n-1} \hat{K}_j^- \left(\hat{K}_j^+\right)^n\right|0\right\rangle \\
&= n\left(\frac{\Omega_j}{2}-n+1\right)\left\langle 0\left|\left(\hat{K}_j^-\right)^{n-1}\left(\hat{K}_j^+\right)^{n-1}\right|0\right\rangle
\end{aligned}$$

and therefore, for any integer $n > 0$

$$\boxed{|C_n|^2 = \frac{|C_{n-1}|^2}{n\left(\frac{\Omega_j}{2} - n + 1\right)}} \tag{B.16}$$

with a similar normalization coefficient for the state $\left(\hat{L}_j^+\right)^n |0\rangle$. Note that Eq. (B.16) only gives a recurrence relation for the normalization coefficients, however that is all we will need in order to calculate the matrix elements of the multi-$O(4)$ Hamiltonian.

## B.2 Many-body basis states

We introduce the basis states for the model [4]

$$|n_K, n_L\rangle = \prod_j |n_{K_j}, n_{L_j}\rangle \tag{B.17}$$

where the integers $n_{K_j}$ and $n_{L_j}$ satisfy the relations

$$0 \le n_{K_j}, n_{L_j} \le \frac{\Omega_j}{2}$$

and

$$\sum_j \left(n_{K_j} + n_{L_j}\right) = \frac{N}{2}$$

In each $j$ shell, we define the states

$$\left|n_{K_j}, n_{L_j}\right\rangle = C_{n_{K_j}} C_{n_{L_j}} \left(\hat{K}_j^+\right)^{n_{K_j}} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle \tag{B.18}$$

where $|0\rangle$ is the particle vacuum, and $C_{n_{K_j}}$ and $C_{n_{L_j}}$ are normalization coefficients given by the recurrence relation in Eq. (B.16). We now calculate the effect of the quasispin operators on the basis states. Using Eqs. (B.10) and (B.11), we readily show that

$$\boxed{\hat{K}_j^0 \left|n_{K_j}, n_{L_j}\right\rangle = \left(n_{K_j} - \frac{\Omega_j}{4}\right) \left|n_{K_j}, n_{L_j}\right\rangle} \tag{B.19}$$

and

$$\boxed{\hat{L}_j^0 \left|n_{K_j}, n_{L_j}\right\rangle = \left(n_{L_j} - \frac{\Omega_j}{4}\right) \left|n_{K_j}, n_{L_j}\right\rangle} \tag{B.20}$$

Next, we calculate

$$\hat{K}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle = \frac{C_{n_{K_j}}}{C_{n_{K_j}+1}} C_{n_{K_j}+1} C_{n_{L_j}} \left(\hat{K}_j^+\right)^{n_{K_j}+1} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle$$
$$= \frac{C_{n_{K_j}}}{C_{n_{K_j}+1}} \left|n_{K_j}+1, n_{L_j}\right\rangle$$

and if we assume, without loss of generality, that the normalization coefficients are real and positive we can use Eq. (B.16) to write

$$\boxed{\hat{K}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{\left(n_{K_j}+1\right)\left(\frac{\Omega_j}{2} - n_{K_j}\right)} \left|n_{K_j}+1, n_{L_j}\right\rangle} \tag{B.21}$$

and similarly,

$$\boxed{\hat{L}_j^+ \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{\left(n_{L_j}+1\right)\left(\frac{\Omega_j}{2} - n_{L_j}\right)} \left|n_{K_j}, n_{L_j}+1\right\rangle} \tag{B.22}$$

Finally, we use Eq. (B.13) to write

$$\hat{K}_j^- \left|n_{K_j}, n_{L_j}\right\rangle = C_{n_{K_j}} C_{n_{L_j}} \left\{ \left(\hat{K}_j^+\right)^{n_{K_j}-1} \left[n_{K_j}\left(1-n_{K_j}\right) - 2n_{K_j}\hat{K}_j^0\right] \right.$$
$$\left. + \left(\hat{K}_j^+\right)^{n_{K_j}} \hat{K}_j^- \right\} \left(\hat{L}_j^+\right)^{n_{L_j}} |0\rangle$$
$$= \left[n_{K_j}\left(1-n_{K_j}\right) - 2n_{K_j}\left(-\frac{\Omega_j}{4}\right)\right] \frac{C_{n_{K_j}}}{C_{n_{K_j}-1}} \left|n_{K_j}-1, n_{L_j}\right\rangle$$

Then we use Eq. (B.16), along with the assumption that the normalization coefficients are real and positive, to write

$$\boxed{\hat{K}_j^- \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{n_{K_j}\left(\frac{\Omega_j}{2} - n_{K_j} + 1\right)} \left|n_{K_j}-1, n_{L_j}\right\rangle} \tag{B.23}$$

with a similar relation for the $\hat{L}_j^-$ operator,

$$\boxed{\hat{L}_j^- \left|n_{K_j}, n_{L_j}\right\rangle = \sqrt{n_{L_j}\left(\frac{\Omega_j}{2} - n_{L_j} + 1\right)} \left|n_{K_j}, n_{L_j}-1\right\rangle} \tag{B.24}$$

These results are in agreement with those found in Appendix A of [4].

## B.3 Matrix elements of the model Hamiltonian

With Eqs. (B.19)-(B.24) we have all the necessary elements to calculate the matrix elements of the Hamiltonian (with components given by Eqs. (B.5), (B.6), and (B.7) in the quasispin representation) between the basis states in Eq. (B.17). Using Eqs. (B.19) and (B.20) we can show that

$$\left[2\left(\hat{K}_j^0+\hat{L}_j^0\right)+\Omega_j\right]\left|n_{K_j},n_{L_j}\right\rangle = 2\left(n_{K_j}+n_{L_j}\right)\left|n_{K_j},n_{L_j}\right\rangle$$

from which we deduce

$$\boxed{\left\langle n_K,n_L\left|\hat{H}_0\right|n'_K,n'_L\right\rangle = 2\left(\prod_j \delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}}\right)\sum_j e_j^0\left(n_{K_j}+n_{L_j}\right)} \tag{B.25}$$

Next, for the quadrupole interaction, Eq. (B.6), we can use Eqs. (B.19) and (B.20) again to show that

$$\begin{aligned}\left(K_i^0-L_i^0\right)\left(K_j^0-L_j^0\right)\left|n_{K_i},n_{L_i}\right\rangle\left|n_{K_j},n_{L_j}\right\rangle &= \left(n_{K_i}-n_{L_j}\right)\left(n_{K_j}-n_{L_j}\right)\\ &\quad\times\left|n_{K_i},n_{L_i}\right\rangle\left|n_{K_j},n_{L_j}\right\rangle\end{aligned}$$

from which we deduce

$$\boxed{\begin{aligned}\left\langle n_K,n_L\left|\hat{H}_Q\right|n'_K,n'_L\right\rangle &= -2\chi\left(\prod_j \delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}}\right)\\ &\quad\times\sum_{i,j} d_i d_j\left(n_{K_i}-n_{L_j}\right)\left(n_{K_j}-n_{L_j}\right)\end{aligned}} \tag{B.26}$$

Finally, we calculate the matrix elements for the pairing term in the Hamiltonian in Eq. (B.7). To simplify the notation, we introduce the quantity

$$p_j(n) \equiv \sqrt{n\left(\frac{\Omega_j}{2}-n+1\right)}$$

for $0 \le n \le \Omega_j/2+1$. Then, with the help of Eqs. (B.21)-(B.24), we can show that

$$\begin{aligned}\left\langle n_{K_j},n_{L_j}\left|\left(\hat{K}_j^+ +\hat{L}_j^+\right)\right|n'_{K_j},n'_{L_j}\right\rangle &= p_j\left(n_{K_j}\right)\delta_{n_{K_j},n'_{K_j}+1}\delta_{n_{L_j},n'_{L_j}}\\ &\quad+p_j\left(n_{L_j}\right)\delta_{n_{K_j},n'_{K_j}}\delta_{n_{L_j},n'_{L_j}+1}\end{aligned}$$

and

$$\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^-\right) \right| n'_{K_j}, n'_{L_j} \right\rangle = p_j \left(n_{K_j} + 1\right) \delta_{n_{K_j}, n'_{K_j}-1} \delta_{n_{L_j}, n'_{L_j}} \\ + p_j \left(n_{L_j} + 1\right) \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}-1}$$

and

$$\begin{aligned} &\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^-\right) \left(\hat{K}_j^+ + \hat{L}_j^+\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \\ &= \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \left[p_j^2 \left(n_{K_j} + 1\right) + p_j^2 \left(n_{L_j} + 1\right)\right] \\ &\quad + \delta_{n_{K_j}, n'_{K_j}+1} \delta_{n_{L_j}, n'_{L_j}-1} p_j \left(n_{K_j}\right) p_j \left(n_{L_j} + 1\right) \\ &\quad + \delta_{n_{K_j}, n'_{K_j}-1} \delta_{n_{L_j}, n'_{L_j}+1} p_j \left(n_{K_j} + 1\right) p_j \left(n_{L_j}\right) \end{aligned}$$

and

$$\begin{aligned} &\left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+\right) \left(\hat{K}_j^- + \hat{L}_j^-\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \\ &= \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \left[p_j^2 \left(n_{K_j}\right) + p_j^2 \left(n_{L_j}\right)\right] \\ &\quad + \delta_{n_{K_j}, n'_{K_j}-1} \delta_{n_{L_j}, n'_{L_j}+1} p_j \left(n_{K_j} + 1\right) p_j \left(n_{L_j}\right) \\ &\quad + \delta_{n_{K_j}, n'_{K_j}+1} \delta_{n_{L_j}, n'_{L_j}-1} p_j \left(n_{K_j}\right) p_j \left(n_{L_j} + 1\right) \end{aligned}$$

We now combine these four results to calculate the full matrix element for the pairing term,

$$\boxed{\begin{aligned} &\left\langle n_K, n_L \left| \hat{H}_P \right| n'_K, n'_L \right\rangle \\ &= -\tfrac{1}{2} G \textstyle\sum_j \left(\prod_{i \neq j} \delta_{n_{K_i}, n'_{K_i}} \delta_{n_{L_i}, n'_{L_i}}\right) \\ &\quad \times \left\{ \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+\right) \left(\hat{K}_j^- + \hat{L}_j^-\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right. \\ &\quad \left. + \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^-\right) \left(\hat{K}_j^+ + \hat{L}_j^+\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right\} \\ &\quad - \tfrac{1}{2} G \textstyle\sum_{i \neq j} \left(\prod_{k \neq i,j} \delta_{n_{K_k}, n'_{K_k}} \delta_{n'_{L_k}, n_{L_k}}\right) \\ &\quad \times \left\{ \left\langle n_{K_i}, n_{L_i} \left| \left(\hat{K}_i^+ + \hat{L}_i^+\right) \right| n'_{K_i}, n'_{L_i} \right\rangle \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^- + \hat{L}_j^-\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right. \\ &\quad \left. + \left\langle n_{K_i}, n_{L_i} \left| \left(\hat{K}_i^- + \hat{L}_i^-\right) \right| n'_{K_i}, n'_{L_i} \right\rangle \left\langle n_{K_j}, n_{L_j} \left| \left(\hat{K}_j^+ + \hat{L}_j^+\right) \right| n'_{K_j}, n'_{L_j} \right\rangle \right\} \end{aligned}} \tag{B.27}$$

Using the matrix elements given by Eqs. (B.25), (B.26) and (B.27), the Hamiltonian matrix can be constructed and diagonalized with a standard numerical algorithm. The result is the spectrum of energies $E_\alpha$ of the many-body states $|\alpha\rangle$ along with their wave functions,

$$|\alpha\rangle = \sum_i C_i^\alpha \left| n_K^i, n_L^i \right\rangle \tag{B.28}$$

## B.4 Transition matrix elements

Using Eqs. (B.4), (B.19) and (B.20) we can calculate the following matrix elements for the operator $\hat{D}_j$,

$$\left\langle n_{K_j}, n_{L_j} \left| \hat{D}_j \right| n'_{K_j}, n'_{L_j} \right\rangle = 2\left(n_{K_j} - n_{L_j}\right) \delta_{n_{K_j}, n'_{K_j}} \delta_{n_{L_j}, n'_{L_j}} \tag{B.29}$$

from which we deduce the transition matrix element for the quadrupole operator $\hat{D}$ between many-body states $|\alpha\rangle$ and $|\beta\rangle$ given by Eq. (B.28) [5, 4],

$$\boxed{\left\langle \alpha \left| \hat{D} \right| \beta \right\rangle = 2 \sum_i \left(C_i^\alpha\right)^* C_i^\beta \sum_j d_j \left(n^i_{K_j} - n^i_{L_j}\right)} \tag{B.30}$$

## B.5 Numerical example and discussion

We illustrate the formulas derived for the multi-$O\,(4)$ with a numerical example taken from [3, 4]. In this example, $N = 28$ particles are distributed among three $j$ shells with the properties given in Table B.1. The interaction strengths are $\chi = 0.04$ and $G = 0.14$. A total of 1894 basis states are generated by looping through all integer values of $n_{K_1}, n_{L_1}, n_{K_2}, n_{L_2}, n_{K_3}, n_{L_3}$ in the ranges $0 \leq n_{K_j}, n_{L_j} \leq \Omega_j/2$ and selecting those that satisfy $\sum_j \left(n_{K_j} + n_{L_j}\right) = N/2{=}14$.

Constructing the Hamiltonian matrix using Eqs. (B.25), (B.26) and (B.27) and diagonalizing it, the energies of the lowest 4 states are

$$\begin{aligned} E_0 &= -16.944 \\ E_1 &= -16.853 \\ E_2 &= -15.338 \\ E_3 &= -14.767 \end{aligned}$$

and the transition matrix elements calculated using Eq. (B.30) are

$$\begin{aligned} \left\langle 0 \left| \hat{D} \right| 3 \right\rangle &= 4.146 \\ \left\langle 2 \left| \hat{D} \right| 3 \right\rangle &= 21.441 \\ \left\langle 1 \left| \hat{D} \right| 2 \right\rangle &= 10.328 \\ \left\langle 0 \left| \hat{D} \right| 1 \right\rangle &= 27.824 \end{aligned}$$

in agreement with the numbers listed in Fig. 5 in [3] and Fig. 7 in [4].

From Eq. (B.29) we see that the basis states in Eq. (B.17) are eigenstates of the quadrupole operator $\hat{D}$,

| shell no. | $j$ | $\Omega_j$ | $e_j^0$ | $d_j$ |
|---|---|---|---|---|
| 1 | $\frac{27}{2}$ | 14 | 0.0 | 2.0 |
| 2 | $\frac{19}{2}$ | 10 | 1.0 | 1.0 |
| 3 | $\frac{7}{2}$ | 4 | 3.5 | 1.0 |

**Table B.1** Properties of the $j$ shells for the numerical example.

$$\begin{aligned}\hat{D}\left|n_K, n_L\right\rangle &= \left[2\sum_j d_j\left(n_{K_j} - n_{L_j}\right)\right]\left|n_K, n_L\right\rangle \\ &\equiv D\left(n_K, n_L\right)\left|n_K, n_L\right\rangle\end{aligned}$$

Thus, for the many-body state in Eq. (B.28) we can calculate a probability weight $P\left(D_0\right)$ for a given value $D\left(n_K, n_L\right) = D_0$,

$$P\left(D_0\right) = \sum_i \left|C_i^\alpha\right|^2 \delta_{D\left(n_K^i, n_L^i\right), D_0} \tag{B.31}$$

These probabilities are plotted in Fig. B.1 for the first few levels in the numerical example. We note for example that ground-state and first excited state have distributions peaked at $D_0 = \pm 32$, even though the overall expectation value for $\hat{D}$ for both levels can be calculated to be zero. In effect, the system in its ground state can be found in both $D_0 = +32$ and $-32$ states with equal probability, hence this is a case of strong shape mixing/coexistence between the two deformations.

These results can also be understood in the context of a microscopic approach starting from a mean-field approximation. The strong mixing between different deformations implies the existence of several local minima in the Hartree-Fock-Bogoliubov energy surface with respect to the deformation $D_0$, and that these minima are connected by a large-amplitude collective motion of the system. The theoretical tools we will apply to describe this behavior in the next sections can also be applied to the problem of fission, which shares some similarities with the phenomenon of shape coexistence.

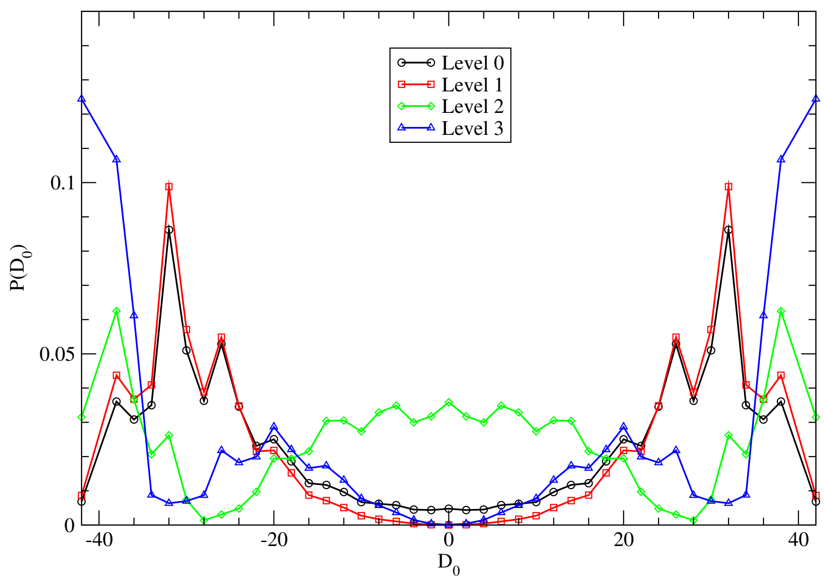


**Fig. B.1** Probability weights $P(D_0)$ as a function of $D_0$ calculated using Eq. (B.31) for the numerical example.

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## Appendix C
# Projection on particle number

For additional discussions of particle-number projection, see for example [1, 6, 5].

## C.1 Different formulations of the Bogoliubov vacuum

We recall the different ways of writing the Bogoliubov vacuum $|\tilde{0}\rangle$ that will be useful in the derivations that follow. First, we write the (unnormalized) vacuum in terms of quasiparticle destruction operators acting on the particle vacuum, $|0\rangle$,

$$|\tilde{0}\rangle = \prod_{\mu} \eta_\mu |0\rangle$$

We may also write the vacuum in the canonical basis (e.g., section 7.2.1 in [1]),

$$\begin{aligned} \alpha_\mu^\dagger &= u_\mu a_\mu^\dagger - v_\mu a_{\bar{\mu}} \\ \alpha_{\bar{\mu}}^\dagger &= u_\mu a_{\bar{\mu}}^\dagger + v_\mu a_\mu \end{aligned}$$

where the canonical particle operators $\left(a_\mu^\dagger, a_{\bar{\mu}}^\dagger\right)$ are related to the "usual" particle operators in Eq. (1.1) by a unitary transformation, and likewise the canonical qp operators $\left(\alpha_\mu^\dagger, \alpha_{\bar{\mu}}^\dagger\right)$ in that same equation by another unitary transformation. Then, it can be shown that [1]

$$\begin{aligned} |\tilde{0}\rangle &= \exp\left[\sum_{\mu>0} \theta_\mu \left(a_\mu^\dagger a_{\bar{\mu}}^\dagger + a_\mu a_{\bar{\mu}}\right)\right] |0\rangle \\ &= \left(\prod_{\mu>0} u_\mu\right) \exp\left[\sum_{\mu>0} \tan\theta_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right] |0\rangle \end{aligned}$$

where we have defined

$$\tan\theta_\mu \equiv \frac{v_\mu}{u_\mu} \tag{C.1}$$

This can also be written as

$$|\tilde{0}\rangle = \left(\prod_{\mu>0} u_\mu\right) \prod_{\mu>0} \left(1 + \tan\theta_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right) |0\rangle \tag{C.2}$$

or

$$|\tilde{0}\rangle = \prod_{\mu>0} \left(u_\mu + v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right) |0\rangle \tag{C.3}$$

In all its forms, the vacuum satisfies

$$\eta_\mu \left|\tilde{0}\right\rangle = \alpha_\mu \left|\tilde{0}\right\rangle = 0$$

## C.2 A "pedestrian" approach

We choose the expression in Eq. (C.2) of the vacuum that we express in the more compact form

$$\left|\tilde{0}\right\rangle = \left(\prod_{\mu>0} u_\mu\right) \prod_{\mu>0} \left(1 + \hat{t}_\mu\right) |0\rangle \tag{C.4}$$

where

$$\hat{t}_\mu \equiv \tan\theta_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}}$$

and where we have

$$\left[\hat{t}_\mu, \hat{t}_\nu\right] = 0 \tag{C.5}$$

The operators $\hat{t}_\mu$ create a pair of nucleons $(\mu, \bar{\mu})$. By expanding the product in Eq. (C.4) it is straightforward to project out the contribution of a number $p$ of pairs to the vacuum defined in Eq. (C.2). If we define the (even) number of particles $N$ as $N = 2p$, then the state with the correct number of particles $N$ is given by the expression

$$|(p)\rangle = \left(\prod_{\mu>0} u_\mu\right) \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_p} |0\rangle \tag{C.6}$$

In what follows, for the sake of simplicity we do not write the normalization factor $\left(\prod_{\mu>0} u_\mu\right)$ explicitly unless it is necessary. Note that Eq. (C.6) does not take into account the dimension $D$ of the particle basis. In practice, the indices $\mu_i$ in Eq. (C.6) should satisfy

$$\mu_1 \leq D - p + 1,\ \mu_2 \leq D - p + 2, \ldots,\ \mu_p \leq D \tag{C.7}$$

For practical reasons, as we will see later, it is convenient to introduce an equivalent form which has the advantage of being symmetric,

$$|(p)\rangle = \frac{1}{p!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_p} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_p} |0\rangle \tag{C.8}$$

with the further restrictions on the indices,

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p \tag{C.9}$$

### C.2.1 Illustration with a simple example

To illustrate these results, we consider a simple system with $N = 6$ particles (i.e., $p = 3$ pairs) in 4 doubly degenerate levels labeled $1, 2, 3, 4$. We write the corresponding state according to Eq. (C.8),

$$\begin{aligned}|(3)\rangle = \frac{1}{3!}\{&\hat{t}_1\hat{t}_2\hat{t}_3 + \hat{t}_1\hat{t}_3\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_3 + \hat{t}_2\hat{t}_3\hat{t}_1 + \hat{t}_3\hat{t}_1\hat{t}_2 + \hat{t}_3\hat{t}_2\hat{t}_1 \\ &+ \hat{t}_1\hat{t}_2\hat{t}_4 + \hat{t}_1\hat{t}_4\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_1 + \hat{t}_4\hat{t}_1\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_1 \\ &+ \hat{t}_1\hat{t}_3\hat{t}_4 + \hat{t}_1\hat{t}_4\hat{t}_3 + \hat{t}_3\hat{t}_1\hat{t}_4 + \hat{t}_3\hat{t}_4\hat{t}_1 + \hat{t}_4\hat{t}_1\hat{t}_3 + \hat{t}_4\hat{t}_3\hat{t}_1 \\ &+ \hat{t}_2\hat{t}_3\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_3 + \hat{t}_3\hat{t}_2\hat{t}_4 + \hat{t}_3\hat{t}_4\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_3 + \hat{t}_4\hat{t}_3\hat{t}_2\}\,|0\rangle\end{aligned} \tag{C.10}$$

We can also use Eq. (C.5) to reorder and combine terms in Eq. (C.10) to recover the form in Eq. (C.6),

$$|(3)\rangle = \left(\hat{t}_1\hat{t}_2\hat{t}_3 + \hat{t}_1\hat{t}_2\hat{t}_4 + \hat{t}_1\hat{t}_3\hat{t}_4 + \hat{t}_2\hat{t}_3\hat{t}_4\right)|0\rangle \tag{C.11}$$

In later calculations in this appendix we will need numerical values for the occupation probabilities, for which we take

$$v_1^2 = 0.9, \quad v_2^2 = 0.6, \quad v_3^2 = 0.4, \quad v_4^2 = 0.1$$

### C.2.2 Normalization

First we can show by Wick's theorem that

$$\begin{aligned}&\sum_{\substack{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_p \\ \mu'_1 \neq \mu'_2 \neq \ldots \neq \mu'_p}} \left\langle 0 \left| \hat{t}^\dagger_{\mu'_1}\hat{t}^\dagger_{\mu'_2}\ldots\hat{t}^\dagger_{\mu'_p}\hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_p} \right| 0 \right\rangle \\ &= p! \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_p} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_p}\right)^2\end{aligned} \tag{C.12}$$

Then, starting from Eq. (C.8) and re-introducing the normalization of the state, the calculation of the norm is straightforward giving

$$\langle (p)|\,(p)\rangle = \frac{\left(\prod_{\mu=1}^{D} u_\mu^2\right)}{p!} \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_p} \left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_p}\right)^2 \tag{C.13}$$

with the restrictions on the indices given in Eq. (C.9). Similarly, Eq. (C.6) or (C.8) yields

$$\langle (p) | (p) \rangle = \left( \prod_{\mu=1}^{D} u_\mu^2 \right) \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \left( \tan\theta_{\mu_1} \tan\theta_{\mu_2} \ldots \tan\theta_{\mu_p} \right)^2 \tag{C.14}$$

with the restrictions on the indices given by Eq. (C.7). Notice that using Eq. (C.1), we could also write these as

$$\langle (p) | (p) \rangle = \sum_{0<\mu_1<\mu_2<\ldots<\mu_p} \left( \prod_{\nu=\mu_{p+1}}^{D} u_\nu^2 \right) \left( v_{\mu_1} v_{\mu_2} \ldots v_{\mu_p} \right)^2 \tag{C.15}$$

or

$$\langle (p) | (p) \rangle = \frac{1}{p!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_p} \left( \prod_{\nu=\mu_{p+1}}^{D} u_\nu^2 \right) \left( v_{\mu_1} v_{\mu_2} \ldots v_{\mu_p} \right)^2 \tag{C.16}$$

In the formalism of [2], this normalization is denoted as

$$\langle (p) | (p) \rangle = R_0^0 \tag{C.17}$$

In the expansion of Eq. (C.15) or (C.16) it is clear that each term is the probability to find a Slater determinant with $N$ particles, and their sum $\langle (p) | (p) \rangle = R_0^0$ can then be interpreted as the overall probability to find $N$ particles in the BCS vacuum.

### C.2.3 One-body density matrix

Next we consider the matrix elements $\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle$. For this calculation, Eq. (C.8) is the most convenient and we get (using $\left[ a_\mu^\dagger a_\mu, a_\nu^\dagger a_{\bar{\nu}}^\dagger \right] = \delta_{\mu\nu} a_\nu^\dagger a_{\bar{\nu}}^\dagger$)

$$a_\mu^\dagger a_\mu \left| (p) \right\rangle = \frac{\hat{t}_\mu}{(p-1)!} \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1}; \mu_i \neq \mu} \hat{t}_{\mu_1} \hat{t}_{\mu_2} \ldots \hat{t}_{\mu_{p-1}} \left| 0 \right\rangle \tag{C.18}$$

where the notation indicates that the state $\mu$ is to be taken out of all the summations, and where we have the further restrictions

$$0 < \mu_i \leq D, \; i = 1, 2, \ldots, p-1$$

We can illustrate this result with the simple example in section C.2.1. Thus starting from Eq. (C.10), we have for example

$$a_2^\dagger a_2 \left|(3)\right\rangle = \frac{1}{3!}\left\{\hat{t}_1\hat{t}_2\hat{t}_3 + \hat{t}_1\hat{t}_3\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_3 + \hat{t}_2\hat{t}_3\hat{t}_1 + \hat{t}_3\hat{t}_1\hat{t}_2 + \hat{t}_3\hat{t}_2\hat{t}_1\right.$$
$$+\hat{t}_1\hat{t}_2\hat{t}_4 + \hat{t}_1\hat{t}_4\hat{t}_2 + \hat{t}_2\hat{t}_1\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_1 + \hat{t}_4\hat{t}_1\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_1$$
$$\left.+\hat{t}_2\hat{t}_3\hat{t}_4 + \hat{t}_2\hat{t}_4\hat{t}_3 + \hat{t}_3\hat{t}_2\hat{t}_4 + \hat{t}_3\hat{t}_4\hat{t}_2 + \hat{t}_4\hat{t}_2\hat{t}_3 + \hat{t}_4\hat{t}_3\hat{t}_2\right\}\left|0\right\rangle$$

where we used $\left[a_\mu^\dagger a_\mu, a_\nu^\dagger a_{\bar{\nu}}^\dagger\right] = \delta_{\mu\nu} a_\nu^\dagger a_{\bar{\nu}}^\dagger$. Then, factoring out $\hat{t}_2$ and combining like terms,

$$\begin{aligned} a_2^\dagger a_2 \left|(3)\right\rangle &= \frac{\hat{t}_2}{3!}\left(3\hat{t}_1\hat{t}_3 + 3\hat{t}_3\hat{t}_1 + 3\hat{t}_1\hat{t}_4 + 3\hat{t}_4\hat{t}_1 + 3\hat{t}_3\hat{t}_4 + 3\hat{t}_4\hat{t}_3\right)\left|0\right\rangle \\ &= \frac{\hat{t}_2}{2!}\left(\hat{t}_1\hat{t}_3 + \hat{t}_3\hat{t}_1 + \hat{t}_1\hat{t}_4 + \hat{t}_4\hat{t}_1 + \hat{t}_3\hat{t}_4 + \hat{t}_4\hat{t}_3\right)\left|0\right\rangle \end{aligned} \tag{C.19}$$

which is just what Eq. (C.18) predicts. We can also show that

$$a_{\bar{\mu}}^\dagger a_{\bar{\mu}} \left|(p)\right\rangle = a_\mu^\dagger a_\mu \left|(p)\right\rangle \tag{C.20}$$

Now taking the scalar product with the projected state $|(p)\rangle$ and using Eq. (C.12) we find

$$\left\langle (p)\left|a_\mu^\dagger a_\mu\right|(p)\right\rangle = \frac{\tan^2\theta_\mu}{(p-1)!}\sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-1};\mu_i\neq\mu}\left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_{p-1}}\right)^2 \tag{C.21}$$

with

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-1$$

We can also write this as

$$\left\langle (p)\left|a_\mu^\dagger a_\mu\right|(p)\right\rangle = \tan^2\theta_\mu \sum_{\mu_1<\mu_2<\ldots<\mu_{p-1};\mu_i\neq\mu}\left(\tan\theta_{\mu_1}\tan\theta_{\mu_2}\ldots\tan\theta_{\mu_{p-1}}\right)^2 \tag{C.22}$$

with the restrictions

$$0 < \mu_1 \leq D-p+1,\ 0 < \mu_2 \leq D-p+2, \ldots,\ 0 < \mu_{p-1} \leq D$$

After inserting the normalization, we obtain

$$\left\langle (p)\left|a_\mu^\dagger a_\mu\right|(p)\right\rangle = \frac{v_\mu^2}{(p-1)!}\sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-1};\mu_i\neq\mu}\left(\prod_{\nu=\mu_p}^{\mu_D} u_\nu^2\right)\left(v_{\mu_1}v_{\mu_2}\ldots v_{\mu_{p-1}}\right)^2$$

or

$$\left\langle (p)\left|a_\mu^\dagger a_\mu\right|(p)\right\rangle = v_\mu^2 \sum_{\mu_1<\mu_2<\ldots<\mu_{p-1};\mu_i\neq\mu}\left(\prod_{\nu=\mu_p}^{\mu_D} u_\nu^2\right)\left(v_{\mu_1}v_{\mu_2}\ldots v_{\mu_{p-1}}\right)^2 \tag{C.23}$$

This is simply related to the quantity $R_1^1(\mu)$ defined in the residue approach of Dietrich et al. [2] through the relation

$$\left\langle (p)\left| a_\mu^\dagger a_\mu \right| (p)\right\rangle = v_\mu^2 R_1^1(\mu) \tag{C.24}$$

We can use the 4-level example in section C.2.1 to illustrate these results by calculating $\left\langle (3)\left| a_2^\dagger a_2 \right| (3)\right\rangle$ either by taking the overlap of the states in Eqs. (C.19) and (C.11) and explicitly evaluating the Wick's contractions, or by applying Eq. (C.22). In either case we find

$$\left\langle (3)\left| a_2^\dagger a_2 \right| (3)\right\rangle = \tan^2\theta_2\left(\tan^2\theta_1\tan^2\theta_3 + \tan^2\theta_1\tan^2\theta_4 + \tan^2\theta_3\tan^2\theta_4\right)$$

Including the normalization, this becomes

$$\left\langle (3)\left| a_2^\dagger a_2 \right| (3)\right\rangle = v_2^2\left(u_4^2 v_1^2 v_3^3 + u_3^2 v_1^2 v_4^3 + u_1^2 v_3^2 v_4^3\right)$$

### *C.2.4 Two-body density matrix*

We will first calculate (for $\mu \neq \nu$)

$$\left\langle (p)\left| a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu \right| (p)\right\rangle = \left\langle (p)\left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p)\right\rangle$$

Starting from Eq. (C.18) we find

$$a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \left|(p)\right\rangle = \frac{\hat{t}_\nu \hat{t}_\mu}{(p-2)!} \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-2};\{\mu_i\neq\mu,\nu\}} \hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_{p-2}}\left|0\right\rangle$$

with

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-2$$

which leads to

$$\left\langle (p)\left| a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu \right| (p)\right\rangle = \frac{(\tan\theta_\mu \tan\theta_\nu)^2}{(p-2)!} \times \sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-2};\{\mu_i\neq\mu,\nu\}} (\tan\theta_1\tan\theta_2\ldots\tan\theta_{p-2})^2$$

with the restrictions stated above,

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-2$$

or, if we order the indices,

$$\left\langle (p)\left|a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu\right|(p)\right\rangle = (\tan\theta_\mu \tan\theta_\nu)^2 \times \sum_{\mu_1<\mu_2<\ldots<\mu_{p-2};\{\mu_i\neq\mu,\nu\}} (\tan\theta_1\tan\theta_2\ldots\tan\theta_{p-2})^2 \tag{C.25}$$

Again, if we multiply by the normalization, the correct form is

$$\left\langle (p)\left|a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu\right|(p)\right\rangle = (v_\mu v_\nu)^2 \sum_{\mu_1<\mu_2<\ldots<\mu_{p-2};\{\mu_i\neq\mu,\nu\}} \left( \prod_{\substack{\alpha=\mu_{p-1}\\ \alpha\neq\mu,\nu}}^{\mu_D} u_\alpha^2 \right) \times (v_1 v_2\ldots v_{p-2})^2$$

which we can relate to the $R_2^2(\mu,\nu)$ of Dietrich et al. [2] by

$$\left\langle (p)\left|a_\nu^\dagger a_\nu a_\mu^\dagger a_\mu\right|(p)\right\rangle = R_2^2(\mu,\nu)\,(v_\mu v_\nu)^2 \tag{C.26}$$

We illustrate this result with the 4-level example of section C.2.1 by first applying $a_3^\dagger a_3$ to Eq. (C.19) to obtain

$$a_3^\dagger a_3 a_2^\dagger a_2 \left|(3)\right\rangle = \frac{\hat{t}_3\hat{t}_2}{1!}\left(\hat{t}_1+\hat{t}_4\right)|0\rangle$$

Then, taking the dot product with Eq. (C.11) we get

$$\begin{aligned}\left\langle (p)\left|a_3^\dagger a_3 a_2^\dagger a_2\right|(p)\right\rangle &= \left\langle (p)\left|\hat{t}_3^\dagger\hat{t}_2^\dagger\hat{t}_1^\dagger\hat{t}_1\hat{t}_2\hat{t}_3+\hat{t}_4^\dagger\hat{t}_3^\dagger\hat{t}_2^\dagger\hat{t}_2\hat{t}_3\hat{t}_4\right|(p)\right\rangle\\ &= \tan^2\theta_2\tan^2\theta_3\left(\tan^2\theta_1+\tan^2\theta_4\right)\end{aligned}$$

which we can also obtain directly from Eq. (C.25).

As we shall see in section C.2.5, we also need to calculate the matrix elements $\left\langle (p)\left|a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu} a_\nu\right|(p)\right\rangle$. For this, we can use Eq. (C.8) and the commutator

$$\left[a_{\bar\nu}a_\nu, a_\mu^\dagger a_{\bar\mu}^\dagger\right] = \delta_{\mu\nu}\left(1-a_\mu^\dagger a_\nu - a_{\bar\mu}^\dagger a_{\bar\nu}\right)$$

to calculate

$$a_{\bar\nu}a_\nu\left|(p)\right\rangle = \frac{\tan\theta_\nu}{(p-1)!}\sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-1};\{\mu_i\neq\nu\}}\hat{t}_{\mu_1}\hat{t}_{\mu_2}\ldots\hat{t}_{\mu_{p-1}}|0\rangle$$

and

$$\left\langle (p)\right| a_\mu^\dagger a_{\bar\mu}^\dagger = \frac{\tan\theta_\mu}{(p-1)!}\langle 0|\sum_{\mu_1\neq\mu_2\neq\ldots\neq\mu_{p-1};\{\mu_i\neq\mu\}}\hat{t}_{\mu_{p-1}}^\dagger\ldots\hat{t}_{\mu_2}^\dagger\hat{t}_{\mu_1}^\dagger$$

with the usual restrictions

$$0 < \mu_i \leq D,\ i = 1, 2, \ldots, p-1$$

The desired matrix element is obtained by taking the scalar product which leads to

$$\left\langle (p) \left| a_\mu^\dagger a_{\bar{\mu}}^\dagger a_{\bar{\nu}} a_\nu \right| (p) \right\rangle = \frac{\tan\theta_\mu \tan\theta_\nu}{(p-1)!} \times \sum_{\mu_1 \neq \mu_2 \neq \ldots \neq \mu_{p-1}; \{\mu_i \neq \mu, \nu\}} \left(\tan\theta_1 \tan\theta_2 \ldots \tan\theta_{p-1}\right)^2 \tag{C.27}$$

After taking care of the normalization, this gives

$$\left\langle (p) \left| a_\mu^\dagger a_{\bar{\mu}}^\dagger a_{\bar{\nu}} a_\nu \right| (p) \right\rangle = u_\mu v_\mu u_\nu v_\nu \sum_{\mu_1 < \mu_2 < \ldots < \mu_{p-1}; \{\mu_i \neq \mu, \nu\}} \left( \prod_{\substack{\alpha = \mu_p \\ \alpha \neq \mu, \nu}}^{\mu_D} u_\alpha^2 \right) \times \left(v_1 v_2 \ldots v_{p-1}\right)^2$$

which is related to the coefficient defined by Dietrich et al. [2] through

$$\left\langle (p) \left| a_\mu^\dagger a_{\bar{\mu}}^\dagger a_{\bar{\nu}} a_\nu \right| (p) \right\rangle = u_\mu v_\mu u_\nu v_\nu R_1^2 (\mu, \nu) \tag{C.28}$$

We illustrate this result with the 4-level example by calculating $\left\langle (p) \left| a_3^\dagger a_{\bar{3}}^\dagger a_{\bar{2}} a_2 \right| (p) \right\rangle$. From Eq. (C.11), we first calculate

$$a_{\bar{2}} a_2 \left|(3)\right\rangle = \tan\theta_2 \left(\hat{t}_1 \hat{t}_3 + \hat{t}_1 \hat{t}_4 + \hat{t}_3 \hat{t}_4\right) \left|0\right\rangle$$

and similarly,

$$a_{\bar{3}} a_3 \left|(3)\right\rangle = \tan\theta_3 \left(\hat{t}_1 \hat{t}_2 + \hat{t}_1 \hat{t}_4 + \hat{t}_2 \hat{t}_4\right) \left|0\right\rangle$$

and taking the scalar product,

$$\left\langle (p) \left| a_3^\dagger a_{\bar{3}}^\dagger a_{\bar{2}} a_2 \right| (p) \right\rangle = \tan\theta_2 \tan\theta_3 \left(\tan^2\theta_1 \tan^2\theta_4\right)$$

which we can also get directly from Eq. (C.27).

### C.2.5 Projected expectation value of the two-body potential

We now wish to calculate

$$V(p) \equiv \frac{1}{4} \sum_{\mu_1,\mu_2,\mu_3,\mu_4} \left\langle \mu_1, \mu_2 \left| V \right| \widetilde{\mu_3, \mu_4} \right\rangle \left\langle (p) \left| a_{\mu_1}^\dagger a_{\mu_2}^\dagger a_{\mu_4} a_{\mu_3} \right| (p) \right\rangle$$

where the notation $\left|\widetilde{\mu_3, \mu_4}\right\rangle \equiv \left|\mu_3, \mu_4\right\rangle - \left|\mu_4, \mu_3\right\rangle$ serves as a reminder that the matrix elements of $V$ are anti-symmetrized. The summation indices $(\mu_1, \mu_2, \mu_3, \mu_4)$ are not independent, but must be chosen such that the four operators conserve the number of pairs when applied to the projected state $|(p)\rangle$. This condition is satisfied only by combinations of the type

$$a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu, \quad a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu} a_\nu$$

Thus we will write

$$\begin{aligned} V(p) &= \frac{1}{4} \sum_{\mu,\nu} \left\langle \mu, \nu \left| V \right| \widetilde{\mu, \nu} \right\rangle \left\langle (p) \left| a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu \right| (p) \right\rangle \\ &+ \frac{1}{4} \sum_{\mu,\nu} \left\langle \mu, \bar\mu \left| V \right| \widetilde{\nu, \bar\nu} \right\rangle \left\langle (p) \left| a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu} a_\nu \right| (p) \right\rangle \end{aligned} \tag{C.29}$$

We take into account the fact that the indices run over positive $(\mu, \nu > 0)$ and negative $(\bar\mu, \bar\nu)$ values and that we have time-reversal invariance. In particular, we have the following properties under action of the time-reversal operator $\hat K$ (and choosing a representation where all the matrix elements are real),

$$\begin{aligned} \left\langle \bar\mu, \bar\nu \left| V \right| \bar\mu, \bar\nu \right\rangle &= \left( \left\langle \bar\mu, \bar\nu \right| \hat K \right) V \left( \hat K \left| \bar\mu, \bar\nu \right\rangle \right) \\ &= \left\langle \mu, \nu \left| \hat K^\dagger V \hat K \right| \mu, \nu \right\rangle^* \\ &= \left\langle \mu, \nu \left| V \right| \mu, \nu \right\rangle^* \\ &= \left\langle \mu, \nu \left| V \right| \mu, \nu \right\rangle \end{aligned}$$

and also,

$$\hat K \left|(p)\right\rangle = \left|(p)\right\rangle$$

As a result,

$$\left\langle (p) \left| a_\mu^\dagger a_\nu^\dagger a_\nu a_\mu \right| (p) \right\rangle = \left\langle (p) \left| a_{\bar\mu}^\dagger a_{\bar\nu}^\dagger a_{\bar\nu} a_{\bar\mu} \right| (p) \right\rangle$$

and

$$\left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p) \right\rangle = \left\langle (p) \left| a^\dagger_{\bar\mu} a^\dagger_\mu a_\nu a_{\bar\nu} \right| (p) \right\rangle$$

Let us now consider the first term in Eq. (C.29). The summation in this term can be expanded as

$$\sum_{\mu,\nu} = \sum_{\mu>0,\nu>0} + \sum_{\mu<0,\nu<0} + \sum_{\mu>0,\nu<0} + \sum_{\mu<0,\nu>0}$$

and according to the properties under time reversal demonstrated above, this term reduces to

$$\begin{aligned}\frac{1}{4}\sum_{\mu,\nu} \langle \mu,\nu\, |V|\, \widetilde{\mu,\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p)\right\rangle = \frac{1}{2}\sum_{\mu,\nu>0} \Big(& \langle \mu,\nu\, |V|\, \widetilde{\mu,\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p)\right\rangle \\ & \langle \mu,\bar\nu\, |V|\, \widetilde{\mu,\bar\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\nu} a_{\bar\nu} a_\mu \right| (p)\right\rangle \Big)\end{aligned}$$

Referring back to Eq. (C.20) it is clear that

$$\left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p)\right\rangle = \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\nu} a_{\bar\nu} a_\mu \right| (p)\right\rangle$$

and therefore we finally obtain

$$\begin{aligned}\frac{1}{4}\sum_{\mu,\nu} \langle \mu,\nu\, |V|\, \widetilde{\mu,\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p)\right\rangle = \frac{1}{2}\sum_{\mu,\nu>0} & \left(\langle \mu,\nu\, |V|\, \widetilde{\mu,\nu}\rangle + \langle \mu,\bar\nu\, |V|\, \widetilde{\mu,\bar\nu}\rangle\right) \\ & \times \left\langle (p) \left| a^\dagger_\mu a^\dagger_\nu a_\nu a_\mu \right| (p)\right\rangle\end{aligned}$$

By proceeding in a similar manner, the second term in Eq. (C.29) takes the form

$$\frac{1}{4}\sum_{\mu,\nu} \langle \mu,\bar\mu\, |V|\, \widetilde{\nu,\bar\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p)\right\rangle = \sum_{\mu,\nu>0} \langle \mu,\bar\mu\, |V|\, \widetilde{\nu,\bar\nu}\rangle \left\langle (p) \left| a^\dagger_\mu a^\dagger_{\bar\mu} a_{\bar\nu} a_\nu \right| (p)\right\rangle$$

Finally, the projected expectation value of the energy takes the form

$$\begin{aligned}\frac{\left\langle (p) \left| \hat H \right| (p)\right\rangle}{\langle (p) |\, (p)\rangle} = \frac{1}{R^0_0} \Bigg\{ & 2\sum_{\mu>0} \left\langle \mu \left| \hat T \right| \mu \right\rangle R^1_1(\mu)\, v^2_\mu \\ & + \frac{1}{2}\sum_{\mu,\nu>0} \left(\langle \mu,\nu\, |V|\, \widetilde{\mu,\nu}\rangle + \langle \mu,\bar\nu\, |V|\, \widetilde{\mu,\bar\nu}\rangle\right) R^2_2(\mu,\nu)\,(v_\mu v_\nu)^2 \\ & + \sum_{\mu,\nu>0} \langle \mu,\bar\mu\, |V|\, \widetilde{\nu,\bar\nu}\rangle\, R^2_1(\mu,\nu)\, u_\mu v_\mu u_\nu v_\nu \Bigg\}\end{aligned} \tag{C.30}$$

where we have used Eqs. (C.17), (C.24), (C.26), and (C.28).

This derivation concludes the pedestrian approach to particle-number projection. In principle, the expression in Eq. (C.30) can always be evaluated numerically, and there are recursion relations for the $R_i^j$ coefficients [2]. In practice, these calculations can be cumbersome and time-consuming. Next, we examine the projector proposed by Dietrich et al. [2] as another way of enforcing particle-number conservation.

## C.3 A projection operator on particle number

### C.3.1 Basic definitions

Let us first introduce the problem of projection with basic and straightforward definitions that will be useful in what follows. Clearly the problem arises when we use a description with an indefinite number of particles, and consequently it is important to define a complete set of states adapted to such a situation. We assume that we have a complete set of vectors to describe any system with a given number of particles. We denote by

$$\{|(i)\,,N\rangle\} \tag{C.31}$$

The basis for a system with $N$ particles. More precisely, any wave function with $N$ particles can be expanded as

$$|\Psi\rangle = \sum_i \langle\,(i)\,,N|\,\Psi\rangle\,|(i)\,,N\rangle$$

The expansion of a wave function with an indefinite number of particles is given by

$$|\Psi\rangle = \sum_{N,i} \langle\,(i)\,,N|\,\Psi\rangle\,|(i)\,,N\rangle$$

The closure relation or the identity operator in the Fock space reads

$$\hat{I} = \sum_{N,i} |(i)\,,N\rangle\,\langle(i)\,,N|$$

Now if $P^{(N)}$ is a projector in the $N$-particle space, it satisfies

$$P^{(N)}\,|(i)\,,N'\rangle = \begin{cases} |(i)\,,N\rangle & N' = N \\ 0 & N' \neq N \end{cases} \tag{C.32}$$

and consequently

$$P^{(N)} = P^{(N)}\hat{I} = \sum_i |(i), N\rangle \langle (i), N|$$

Thus we recover the well-known result that the closure relation in the $N$-space provides a representation of this projector. This expression is useful in the formalism, but not for practical applications. Therefore, we have to resort to other representations, one of them being the projector proposed by Dietrich et al. [2]. Its construction is straightforward thanks to the fact that the eigenvalues of the particle number operator are integers. In effect, to satisfy Eq. (C.32) we seek an operator that behaves like a Kronecker delta symbol when acting on the basis defined in Eq. (C.31). One such possible operator clearly is

$$P^{(N)} \equiv \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{i\varphi\left(\hat{N}-N\right)} \tag{C.33}$$

since

$$P^{(N)}|(i), N'\rangle = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{i\varphi\left(N'-N\right)}|(i), N'\rangle = \begin{cases} |(i), N\rangle & N' = N \\ 0 & N' \neq N \end{cases}$$

It is worth pointing out that the operator in Eq. (C.33) could also be written as

$$P^{(N)} = \frac{1}{2\pi}\int_\alpha^{2\pi+\alpha} d\varphi\, e^{i\varphi\left(\hat{N}-N\right)}$$

for an arbitrary real number $\alpha$. This last remark is useful for certain demonstrations (e.g., that $P^{(N)\dagger} = P^{(N)}$, as expected).

### *C.3.2 Application*

For practical applications, we re-write the operator of Eq. (C.33) in the form

$$P^{(N)} = \frac{1}{2\pi i}\oint dz\, \frac{z^{\hat{N}}}{z^{N+1}}, \quad z = e^{i\varphi}$$

The integration contour is the unit circle. Let us now see the effect of this projector on a BCS state,

$$P^{(N)}|\mathrm{BCS}\rangle = \frac{1}{2\pi i}\oint dz\, \frac{z^{\hat{N}}}{z^{N+1}}|\mathrm{BCS}\rangle$$

To clarify the meaning of the operator $z^{\hat{N}}$ we go over to the exponential form

$$z^{\hat{N}} = e^{\hat{N}\ln z}$$

When applied to a pair state $a^\dagger_\mu a^\dagger_{\bar{\mu}} |0\rangle$ this operator gives

$$\begin{aligned} z^{\hat{N}} a^\dagger_\mu a^\dagger_{\bar{\mu}} |0\rangle &= e^{\hat{N}\ln z} a^\dagger_\mu a^\dagger_{\bar{\mu}} |0\rangle \\ &= e^{2\ln z} a^\dagger_\mu a^\dagger_{\bar{\mu}} |0\rangle \\ &= z^2 a^\dagger_\mu a^\dagger_{\bar{\mu}} |0\rangle \end{aligned}$$

and therefore

$$P^{(N)} |\mathrm{BCS}\rangle = \frac{1}{2\pi i} \oint dz \, \frac{1}{z^{N+1}} \prod_{\mu>0} \left( u_\mu + z^2 v_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}} \right) |0\rangle$$

If we set $N = 2p$ and $\varsigma = z^2$, we recover Eq. (2.3) in [2],

$$P^{(N)} |\mathrm{BCS}\rangle = C \oint d\varsigma \, \frac{1}{\varsigma^{p+1}} \prod_{\mu>0} \left( u_\mu + \varsigma v_\mu a^\dagger_\mu a^\dagger_{\bar{\mu}} \right) |0\rangle$$

with $C$ a normalization constant. With this form of the projector it is clear that the integration picks out the coefficient of $\varsigma^p$ in the expansion of the product, that is, the component with $p$ pairs. This is essentially what the pedestrian approach described above does. The same remark applies to the calculation of the one- and two-body matrices with this residue method.

## C.4 Another point of view

### *C.4.1 Alternate form of the one-body density*

We illustrate another way to use the Dietrich et al. projection operator described above by re-visiting the calculation of the one-body matrix elements. We could have chosen to start with the calculation of the projected norm, $\left\langle \mathrm{BCS} \middle| P^{(N)} \middle| \mathrm{BCS} \right\rangle$, but the one-body operator is a better choice to introduce some general techniques. The matrix elements of the one-body density operator calculated with the projected states can be written as

$$\begin{aligned} \left\langle (p) \middle| a^\dagger_\mu a_\mu \middle| (p) \right\rangle &= \left\langle \mathrm{BCS} \middle| a^\dagger_\mu a_\mu P^{(N=2p)} \middle| \mathrm{BCS} \right\rangle \\ &= \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\varphi N} \left\langle \mathrm{BCS} \middle| a^\dagger_\mu a_\mu e^{i\hat{N}\varphi} \middle| \mathrm{BCS} \right\rangle \end{aligned} \tag{C.34}$$

Now instead of first projecting the BCS state and then calculating the matrix element as we did previously, we take out the integration and examine the quantity

$$\left\langle \mathrm{BCS} \left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \mathrm{BCS} \right\rangle \tag{C.35}$$

Thanks to the simplicity of the particle operator, the calculation is straightforward. In effect, we introduce the quantity

$$\hat{\chi} \equiv e^{i\hat{N}\varphi} \tag{C.36}$$

with the properties

$$\hat{\chi}^\dagger \hat{\chi} = 1, \quad \hat{\chi} \left|0\right\rangle = \left|0\right\rangle \tag{C.37}$$

Furthermore, since we can readily show that $\left[\hat{N}, a^\dagger\right] = a^\dagger$ and $\left[\hat{N}, a\right] = -a$, it follows by the Baker-Campbell-Hausdorff relation that

$$\begin{aligned} \hat{\chi} a^\dagger \hat{\chi}^\dagger &= e^{i\varphi} a^\dagger \\ \hat{\chi} a \hat{\chi}^\dagger &= e^{-i\varphi} a \end{aligned}$$

and therefore,

$$\begin{aligned} \hat{\chi} a_\mu^\dagger a_{\bar{\mu}}^\dagger \hat{\chi}^\dagger &= \hat{\chi} a_\mu^\dagger \hat{\chi}^\dagger \hat{\chi} a_{\bar{\mu}}^\dagger \hat{\chi}^\dagger \\ &= e^{2i\varphi} a_\mu^\dagger a_{\bar{\mu}}^\dagger \end{aligned}$$

By applying the operator $\hat{\chi}$ and using the properties just given we easily obtain the transformed BCS state,

$$\begin{aligned} e^{i\hat{N}\varphi} \left|\mathrm{BCS}\right\rangle &= \hat{X} \left[ \prod_{\mu>0} \left( u_\mu + v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger \right) \right] \hat{\chi}^\dagger \hat{\chi} \left|0\right\rangle \\ &= \prod_{\mu>0} \left[ \hat{\chi} \left( u_\mu + v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger \right) \hat{\chi}^\dagger \right] \left|0\right\rangle \\ &= \prod_{\mu>0} \left( u_\mu + e^{2i\varphi} v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger \right) \left|0\right\rangle \\ &\equiv \left|\mathrm{BCS}\left(\varphi\right)\right\rangle \end{aligned} \tag{C.38}$$

As expected, the BCS state transformed with the $\hat{\chi}$ operator is still a BCS state. More generally, if we transform any Bogoliubov state

$$\left|\tilde{0}\right\rangle \equiv \prod_\mu \eta_\mu \left|0\right\rangle$$

with the operator $\hat{\chi}$, the transformed state is again a Bogoliubov vacuum of the quasiparticle destruction operators as defined below,

$$\begin{aligned} \eta_\mu \left|\tilde{0}\right\rangle &= 0 \\ \Rightarrow \hat{\chi} \eta_\mu \hat{\chi}^\dagger \hat{\chi} \left|\tilde{0}\right\rangle &= 0 \end{aligned}$$

which we can write as

$$\eta_\mu(\varphi)\left|\tilde{0}\right\rangle = 0$$

with

$$\begin{aligned}\eta_\mu(\varphi) &\equiv \hat{\chi}\eta_\mu\hat{\chi}^\dagger \\ &= \sum_{n>0}\left(u_{n\mu}\hat{\chi}a_n\hat{\chi}^\dagger - v_{n\mu}\hat{\chi}a_{\bar{n}}^\dagger\hat{\chi}^\dagger\right) \\ &= \sum_{n>0}\left(u_{n\mu}e^{-i\varphi}a_n - v_{n\mu}e^{i\varphi}a_{\bar{n}}^\dagger\right)\end{aligned}$$

and in the simple case of BCS quasiparticles, this reduces to

$$\eta_\mu(\varphi) = u_\mu e^{-i\varphi}a_\mu - v_\mu e^{i\varphi}a_{\bar{\mu}}^\dagger$$

and similarly,

$$\eta_{\bar{\mu}}(\varphi) = u_\mu e^{-i\varphi}a_{\bar{\mu}} + v_\mu e^{i\varphi}a_\mu^\dagger$$

Then we can calculate

$$\begin{aligned}\left|\tilde{0}(\varphi)\right\rangle &= \prod_{\mu>0}\eta_\mu(\varphi)\,\eta_{\bar{\mu}}(\varphi)\left|0\right\rangle \\ &= \left(\prod_{\mu>0}v_\mu\right)\prod_{\mu>0}\left(u_\mu + e^{2i\varphi}v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger\right)\left|0\right\rangle \\ &= \left(\prod_{\mu>0}v_\mu\right)\left|\mathrm{BCS}(\varphi)\right\rangle\end{aligned}$$

Note that this last expression contains the normalization of the state. We now have all the necessary ingredients to express Eq. (C.35) in the simple form

$$
\begin{aligned}
\left\langle \mathrm{BCS} \left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \mathrm{BCS} \right\rangle &= \left\langle 0 \left| \left[ \prod_{\alpha>0} \left(u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha\right) \right] a_\mu^\dagger a_\mu \right.\right. \\
&\quad \times \left.\left. \left[ \prod_{\beta>0} \left( u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger \right) \right] \right| 0 \right\rangle \\
&= \langle 0| \left[ \prod_{\alpha>0} \left(u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha\right) \right] \left[ \prod_{\substack{\beta > 0 \\ \beta \neq \mu}} \left( u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger \right) \right] \\
&\quad \times \left[ a_\mu^\dagger a_\mu, u_\mu + e^{2i\varphi} v_\mu a_\mu^\dagger a_{\bar{\mu}}^\dagger \right] |0\rangle
\end{aligned}
$$

where we have used the fact that $a_\mu^\dagger a_\mu$ commutes with all the terms $\left( u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger \right)$ except when $\beta = \mu$ to introduce the commutator in the second line. Therefore

$$
\begin{aligned}
\left\langle \mathrm{BCS} \left| a_\mu^\dagger a_\mu e^{i\hat{N}\varphi} \right| \mathrm{BCS} \right\rangle &= e^{2i\varphi} v_\mu^2 \left\langle \left| \left[ \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left(u_\alpha + v_\alpha a_{\bar{\alpha}} a_\alpha\right) \right] \right.\right. \\
&\quad \times \left.\left. \left[ \prod_{\substack{\beta > 0 \\ \beta \neq \mu}} \left( u_\beta + e^{2i\varphi} v_\beta a_\beta^\dagger a_{\bar{\beta}}^\dagger \right) \right] \right| 0 \right\rangle \\
&= e^{2i\varphi} v_\mu^2 \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left( u_\alpha^2 + e^{2i\varphi} v_\alpha^2 \right)
\end{aligned}
$$

where the second line follows follows from a standard calculation of a BCS state norm. Inserting this into Eq. (C.34) we obtain finally

$$
\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\varphi(N-2)} \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left( u_\alpha^2 + e^{2i\varphi} v_\alpha^2 \right)
$$

or, writing $N = 2p$ and making the substitution $2\varphi \to \varphi$, we get

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\varphi(p-1)} \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} \left( u_\alpha^2 + e^{i\varphi} v_\alpha^2 \right)$$

For numerical applications, it is convenient to re-write this integral in a different form. First, we write

$$u_\alpha^2 + e^{i\varphi} v_\alpha^2 = \left( 1 - 2v_\alpha^2 \sin^2 \frac{\varphi}{2} \right) + i v_\alpha^2 \sin\varphi$$

and define the norm

$$\begin{aligned} n_\alpha(\varphi) &\equiv \left| u_\alpha^2 + e^{i\varphi} v_\alpha^2 \right| \\ &= \sqrt{1 - 4v_\alpha^2 \left(1 - v_\alpha^2\right) \sin^2 \frac{\varphi}{2}} \end{aligned}$$

and the argument[1]

$$\Omega_\alpha = \tan^{-1} \left( 1 - 2v_\alpha^2 \sin^2 \frac{\varphi}{2}, v_\alpha^2 \sin\varphi \right)$$

This allows us to write the projected matrix element as

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\left[\varphi(p-1) - \sum_{\alpha\neq\mu} \Omega_\alpha(\varphi)\right]} \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} n_\alpha(\varphi)$$

Taking into account the fact that the matrix element is real, this reduces to

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, \cos\left[ \sum_{\alpha\neq\mu} \Omega_\alpha(\varphi) - \varphi(p-1) \right] \prod_{\substack{\alpha > 0 \\ \alpha \neq \mu}} n_\alpha(\varphi)$$

As a matter of convenience, we define the following quantities which are independent of $\mu$,

$$\begin{aligned} n(\varphi) &\equiv \prod_{\alpha>0} n_\alpha(\varphi) \\ \Omega(\varphi) &\equiv \sum_{\alpha>0} \Omega_\alpha(\varphi) \end{aligned}$$

and re-write the projected matrix element as

---

[1] The notation $\tan^{-1}(x, y)$ refers to the arctangent, taking into account the quadrant that the point $(x, y)$ is in.

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{2\pi} \int_0^{2\pi} d\varphi \, \exp\left[\ln n(\varphi) - \ln n_\mu(\varphi)\right] \\ \times \cos\left[\Omega(\varphi) - \Omega_\mu(\varphi) - \varphi(p-1)\right]$$

Finally by using the symmetry properties

$$n_\alpha(-\varphi) = n_\alpha(\varphi) \\ \Omega_\alpha(-\varphi) = -\Omega_\alpha(\varphi)$$

which follow straight from the definitions of $n_\alpha$ and $\Omega_\alpha$, and which also hold for the summed quantities $n(\varphi)$ and $\Omega(\varphi)$, we can reduce the domain of integration by half and write

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle = \frac{v_\mu^2}{\pi} \int_0^{\pi} d\varphi \, \exp\left[\ln n(\varphi) - \ln n_\mu(\varphi)\right] \\ \times \cos\left[\Omega(\varphi) - \Omega_\mu(\varphi) - \varphi(p-1)\right]$$

Notice that all the quantities occurring in this expression are very simple to calculate. The only remaining problem is to evaluate the integral by an efficient method. Fortunately, these types of integrals have been considered in the literature (see, e.g., [3, 4] and section 11.4.3 in [1]), and it has been shown that they can be calculated by discretizing the angle $\varphi$ as

$$\varphi_k = \frac{\pi k}{L}$$

over a small number of values $k = 0, 1, \ldots, L$. Note that the integrand is 1 when $\varphi = 0$ giving us the first integration point. In other words,

$$\left\langle (p) \left| a_\mu^\dagger a_\mu \right| (p) \right\rangle \approx \frac{v_\mu^2}{L} \sum_{k=0}^{L-1} \exp\left[\ln n(\varphi_k) - \ln n_\mu(\varphi_k)\right] \\ \times \cos\left[\Omega(\varphi_k) - \Omega_\mu(\varphi_k) - \varphi_k(p-1)\right] \tag{C.39}$$

We show in Fig. C.1 the convergence of this quantity for the simple 4-level example described in section C.2.1.

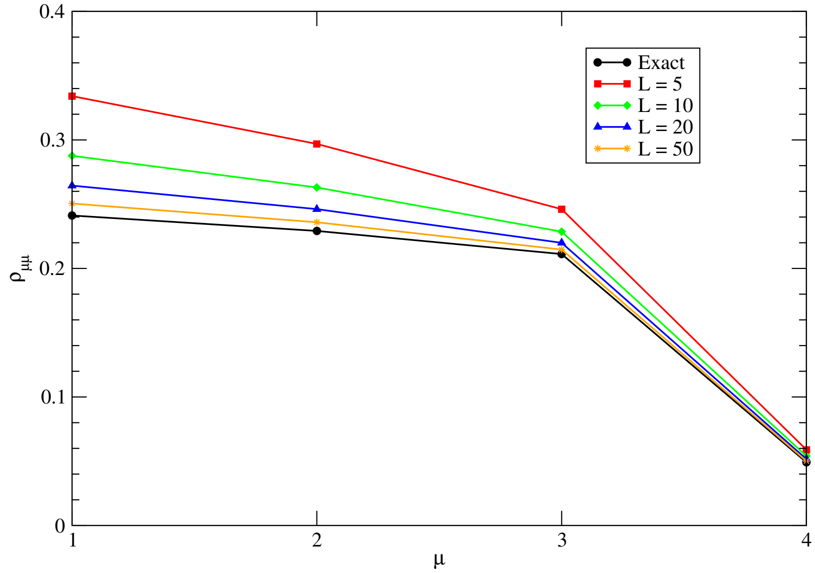


**Fig. C.1** Plot of the density matrix elements $\rho_{\mu\mu} = \left\langle (p) \middle| a_\mu^\dagger a_\mu \middle| (p) \right\rangle$ as a function of state $\mu$ for the 4-level example of section C.2.1. The curve labeled "Exact" corresponds the calculation using Eq. (C.23), the other curves were obtained using Eq. (C.39) for different number $L$ of integration points.

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# Appendix D
# Particle-number projected GCM matrix elements

## D.1 General results

In this appendix we derive expressions for particle-number projected matrix elements between BCS states at different deformation by combining the projection approach described in section C.4 with the procedure developed in [1] to calculate non-diagonal matrix elements. In general, this will involve the calculation of matrix elements of the form

$$\begin{aligned}\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} \hat{O} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle &= \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, e^{-i\left(\varphi'-\varphi\right)N} \\ &\quad \times \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q \varphi} \hat{O} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle\end{aligned} \tag{D.1}$$

for some operator $\hat{O}$ and where we have labeled the number operator and its corresponding projection operator by deformation parameters $q$ and $q'$ as a reminder that the operators are expanded on a basis which may vary as a function of deformation. For example, for the number operator we would write

$$\hat{N}_q = \sum_\mu a_\mu^{q\dagger} a_\mu^q$$

with the commutation relations between single-particle creation and destruction operators described in [1],

$$\left\{ a_\mu^{q'\dagger}, a_\nu^q \right\} = \tau_{\mu\nu}^{qq'} \tag{D.2}$$

$$\left\{ a_\mu^{q'}, a_\nu^q \right\} = \left\{ a_\mu^{q'\dagger}, a_\nu^{q\dagger} \right\} = 0 \tag{D.3}$$

In the special case where $q = q'$, $\tau_{\mu\nu}^{qq'} = \delta_{\mu\nu}$, but in general it is given by the overlap between the single-particle wave functions. In practice, since we consider Hamiltonians that conserve particle number, we will be led to the evaluation of integrals of the form

$$\mathscr{I} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f\left(\varphi' - \varphi\right)$$

where $f(x)$ is a function satisfying the properties

$$f(x + k\pi) = f(x) \tag{D.4}$$

for any integer $k$, and

$$f^*(x) = f(-x) \tag{D.5}$$

Then by changing variables to

$$\bar{\varphi} = \frac{\varphi + \varphi'}{2}$$
$$\xi = \varphi' - \varphi$$

we reduce the problem to a one-dimensional integral,

$$\mathscr{I} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\xi \, (2\pi - \xi) \left[ f(\xi) + f(-\xi) \right]$$

and by using the properties in Eqs. (D.4) and (D.5), we can reduce this to the result

$$\frac{1}{(2\pi)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f(\varphi' - \varphi) = \frac{1}{\pi} \int_0^{\pi} d\xi \, \mathrm{Re} \left[ f(\xi) \right] \tag{D.6}$$

## D.2 Norm overlap

In Eq. (C.38) we wrote a BCS state, adapted for use in particle-number projection integrals, for what follows we will need to write this state with the deformation label $q$ and number of pairs $p$

$$\begin{aligned} \left| \varPhi_q^{(p)}(\varphi) \right\rangle &\equiv \hat{\chi}(\varphi) \left| \varPhi_q^{(p)} \right\rangle \\ &= \prod_{\nu > 0} \left( u_\nu^q + e^{2i\varphi} v_\nu^q a_\nu^{q\dagger} a_{\bar{\nu}}^{q\dagger} \right) |0\rangle \end{aligned}$$

where $\hat{\chi}(\varphi)$ is the operator defined in Eq. (C.36). We introduce an operator $\hat{X}_q(\varphi)$, analogous to the one in [1], defined by

$$\begin{aligned} \hat{X}_q(\varphi) &\equiv \sum_{\mu > 0} e^{2i\varphi} \frac{v_\mu^q}{u_\mu^q} a_\mu^{q\dagger} a_{\bar{\mu}}^{q\dagger} \\ &\equiv \sum_{\mu > 0} e^{2i\varphi} \tan \theta_\mu^q a_\mu^{q\dagger} a_{\bar{\mu}}^{q\dagger} \end{aligned}$$

where we have introduced the quantity

$$\tan \theta_\mu^q \equiv \frac{v_\mu^q}{u_\mu^q} \tag{D.7}$$

defined in Eq. (3.21) in [1]. This operator allows us to relate the state $\left| \varPhi_q^{(p)}(\varphi) \right\rangle$ to the particle vacuum via

$$\left| \varPhi_q^{(p)}(\varphi) \right\rangle = \left\langle 0 \right| \varPhi_q^{(p)}(\varphi) \Big\rangle e^{\hat{X}_q(\varphi)} |0\rangle \tag{D.8}$$

and where the normalization is

$$\begin{aligned}\left\langle 0\middle| \Phi_q^{(p)}(\varphi)\right\rangle &= \left\langle 0\middle|\prod_{\mu>0}\left(u_\mu^q + e^{2i\varphi}v_\mu^q a_\mu^{q\dagger}a_{\bar{\mu}}^{q\dagger}\right)\middle|0\right\rangle \\ &= \prod_{\mu>0}u_\mu^q\end{aligned} \tag{D.9}$$

Then we can generalize Eq. (3.18) in [1] to

$$\begin{aligned}R(x,\varphi,\varphi') &= \left\langle 0\middle|e^{x\hat{X}_q^\dagger(\varphi)}e^{\hat{X}_{q'}(\varphi')}\middle|0\right\rangle \\ &\equiv \frac{\left\langle \Phi_q^{(p)}(x,\varphi)\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle}{\left\langle \Phi_q^{(p)}(\varphi)\middle|0\right\rangle\left\langle 0\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle}\end{aligned} \tag{D.10}$$

and the norm overlap is then given by

$$\left\langle \Phi_q^{(p)}(\varphi)\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle = \left\langle \Phi_q^{(p)}(\varphi)\middle|0\right\rangle\left\langle 0\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle R(1,\varphi,\varphi') \tag{D.11}$$

We can then differentiate Eq. (D.10) to get

$$\frac{\partial}{\partial x}R(x,\varphi,\varphi') = \mathrm{Tr}\left[e^{-2i\varphi}\tan\theta^q A(x,\varphi,\varphi')\right] \tag{D.12}$$

where $\tan\theta^q$ is a diagonal matrix whose elements are given by Eq. (D.7). The matrix $A(x,\varphi,\varphi')$ is defined as

$$A_{\mu\nu}(x,\varphi,\varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(x,\varphi)\middle|a_{\bar{\nu}}^q a_\mu^q\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle}{\left\langle \Phi_q^{(p)}(\varphi)\middle|0\right\rangle\left\langle 0\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle} \tag{D.13}$$

We also define a corresponding matrix

$$B_{\mu\nu}(x,\varphi,\varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(x,\varphi)\middle|a_\nu^{q'\dagger}a_{\bar{\mu}}^{q'\dagger}\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle}{\left\langle \Phi_q^{(p)}(\varphi)\middle|0\right\rangle\left\langle 0\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle} \tag{D.14}$$

Now we can use Eq. (D.8) to write

$$\begin{aligned}\frac{\left\langle \Phi_q^{(p)}(x,\varphi)\middle|a_{\bar{\nu}}^q a_\mu^q\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle}{\left\langle 0\middle|\Phi_{q'}^{(p)}(\varphi')\right\rangle} &= \left\langle \Phi_q^{(p)}(x,\varphi)\middle|a_{\bar{\nu}}^q a_\mu^q e^{\hat{X}_{q'}(\varphi')}\middle|0\right\rangle \\ &= \left\langle \Phi_q^{(p)}(x,\varphi)\middle|e^{\hat{X}_{q'}(\varphi')}e^{-\hat{X}_{q'}(\varphi')}a_{\bar{\nu}}^q a_\mu^q e^{\hat{X}_{q'}(\varphi')}\middle|0\right\rangle\end{aligned}$$

and expand using the Baker-Campbell-Hausdorf relation

$$e^{-\hat{X}_{q'}(\varphi')}a^q_{\bar{\nu}}a^q_{\mu}e^{\hat{X}_{q'}(\varphi')} = a^q_{\bar{\nu}}a^q_{\mu} - \left[\hat{X}_{q'}\left(\varphi'\right), a^q_{\bar{\nu}}a^q_{\mu}\right] + \frac{1}{2}\left[\hat{X}_{q'}\left(\varphi'\right), \left[\hat{X}_{q'}\left(\varphi'\right), a^q_{\bar{\nu}}a^q_{\mu}\right]\right] + \dots$$

We can readily show that

$$\left[\hat{X}_{q'}\left(\varphi'\right), a^q_{\bar{\nu}}a^q_{\mu}\right] = e^{2i\varphi'}\sum_{\alpha>0}\tan\theta^{q'}_{\alpha}\left[\tau^{qq'}_{\bar{\nu}\bar{\alpha}}a^{q'\dagger}_{\alpha}a^q_{\mu} + \tau^{qq'}_{\mu\alpha}a^{q'\dagger}_{\bar{\alpha}}a^q_{\bar{\nu}} - \tau^{qq'}_{\mu\alpha}\tau^{qq'}_{\bar{\nu}\bar{\alpha}}\right]$$

and

$$\left[\hat{X}_{q'}\left(\varphi'\right), \left[\hat{X}_{q'}\left(\varphi'\right), a^q_{\bar{\nu}}a^q_{\mu}\right]\right] = -2e^{4i\varphi'}\sum_{\alpha,\beta>0}\tan\theta^{q'}_{\alpha}\tan\theta^{q'}_{\beta}\tau^{qq'}_{\bar{\nu}\bar{\alpha}}\tau^{qq'}_{\mu\beta}a^{q'\dagger}_{\alpha}a^{q'\dagger}_{\bar{\beta}}$$

and clearly, the expansion ends after the second commutator. Therefore we find

$$A_{\mu\nu}\left(x,\varphi,\varphi'\right) = e^{2i\varphi'}\sum_{\alpha>0}\tan\theta^{q'}_{\alpha}\tau^{qq'}_{\mu\alpha}\tau^{qq'}_{\bar{\nu}\bar{\alpha}}R\left(x,\varphi,\varphi'\right) - e^{4i\varphi'}\sum_{\alpha,\beta>0}\tan\theta^{q'}_{\alpha}\tan\theta^{q'}_{\beta}\tau^{qq'}_{\bar{\nu}\bar{\alpha}}\tau^{qq'}_{\mu\beta}B_{\beta\alpha}\left(x,\varphi,\varphi'\right)$$

or, in matrix form

$$\boxed{\begin{aligned} A\left(x,\varphi,\varphi'\right) &= e^{2i\varphi'}\tau^{qq'}\tan\theta^{q'}\tau^{qq'\dagger}R\left(x,\varphi,\varphi'\right) \\ &- e^{2i\varphi'}\tau^{qq'}\tan\theta^{q'}B\left(x,\varphi,\varphi'\right)\tau^{qq'}\tan\theta^{q'}\tau^{qq'\dagger}\end{aligned}} \tag{D.15}$$

Next, we need the equation for $B\left(x,\varphi,\varphi'\right)$. Proceeding as for $A\left(x,\varphi,\varphi'\right)$, we calculate

$$\frac{\left\langle \Phi^{(p)}_q\left(x,\varphi\right)\left|a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}\right|\Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle}{\left\langle \Phi^{(p)}_q\left(\varphi\right)\middle|0\right\rangle} = \left\langle 0\left|e^{x\hat{X}^{\dagger}_q(\varphi)}a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}e^{-x\hat{X}^{\dagger}_q(\varphi)}e^{x\hat{X}^{\dagger}_q(\varphi)}\right|\Phi^{(p)}_{q'}\left(\varphi'\right)\right\rangle$$

We expand again in terms of commutators,

$$e^{x\hat{X}^{\dagger}_q(\varphi)}a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}e^{-x\hat{X}^{\dagger}_q(\varphi)} = a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}} + x\left[\hat{X}^{\dagger}_q\left(\varphi\right), a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}\right] + \frac{x^2}{2}\left[\hat{X}^{\dagger}_q\left(\varphi\right), \left[\hat{X}^{\dagger}_q\left(\varphi\right), a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}\right]\right] + \dots$$

and find

$$\left[\hat{X}^{\dagger}_q\left(\varphi\right), a^{q'\dagger}_{\nu}a^{q'\dagger}_{\bar{\mu}}\right] = e^{-2i\varphi}\sum_{\alpha>0}\tan\theta^q_{\alpha}\left(\tau^{qq'}_{\alpha\nu}\tau^{qq'}_{\bar{\alpha}\bar{\mu}} - \tau^{qq'}_{\bar{\alpha}\bar{\mu}}a^{q'\dagger}_{\nu}a^q_{\alpha} - \tau^{qq'}_{\alpha\nu}a^{q'\dagger}_{\bar{\mu}}a^q_{\bar{\alpha}}\right)$$

and

$$\left[\hat{X}_q^\dagger(\varphi), \left[\hat{X}_q^\dagger(\varphi), a_\nu^{q'\dagger} a_{\bar{\mu}}^{q'\dagger}\right]\right] = -2e^{-4i\varphi} \sum_{\alpha,\beta>0} \tan\theta_\alpha^q \tan\theta_\beta^q \tau_{\bar{\alpha}\bar{\mu}}^{qq'} \tau_{\beta\nu}^{qq'} a_{\bar{\beta}}^q a_\alpha^q$$

Once again, the expansion ends after the second commutator. Therefore we have

$$\begin{aligned} B_{\mu\nu}(x,\varphi,\varphi') = {} & xe^{-2i\varphi} \sum_{\alpha>0} \tan\theta_\alpha^q \tau_{\alpha\nu}^{qq'} \tau_{\bar{\alpha}\bar{\mu}}^{qq'} R(x,\varphi,\varphi') \\ & -x^2 e^{-4i\varphi} \sum_{\alpha,\beta>0} \tan\theta_\alpha^q \tan\theta_\beta^q \tau_{\bar{\alpha}\bar{\mu}}^{qq'} \tau_{\beta\nu}^{qq'} A_{\alpha\beta}(x,\varphi,\varphi') \end{aligned}$$

which we can write in matrix form

$$\boxed{\begin{aligned} B(x,\varphi,\varphi') = {} & xe^{-2i\varphi} \tau^{qq'\dagger} \tan\theta^q \tau^{qq'} R(x,\varphi,\varphi') \\ & - x^2 e^{-4i\varphi} \tau^{qq'\dagger} \tan\theta^q A(x,\varphi,\varphi') \tan\theta^q \tau^{qq'} \end{aligned}} \tag{D.16}$$

To calculate the norm overlap we need to solve Eqs. (D.15) and (D.16) simultaneously, and for this we proceed as in [1] and define

$$C_1(x,\varphi,\varphi') \equiv e^{-2i\varphi} \tan\theta^q A(x,\varphi,\varphi') \tag{D.17}$$

$$C_2(x,\varphi,\varphi') \equiv e^{2i\varphi'} \left(\tau^{qq'\dagger}\right)^{-1} B(x,\varphi,\varphi') \tan\theta^{q'} \tau^{qq'\dagger} \tag{D.18}$$

$$M^q(\varphi,\varphi') \equiv e^{2i\left(\varphi'-\varphi\right)} \tan\theta^q \tau^{qq'} \tan\theta^{q'} \tau^{qq'\dagger} \tag{D.19}$$

Using Eq. (D.15) we can show

$$C_1(x,\varphi,\varphi') = M^q(\varphi,\varphi') R(x,\varphi,\varphi') - M^q(\varphi,\varphi') C_2(x,\varphi,\varphi') \tag{D.20}$$

and using Eq. (D.16) we get

$$C_2(x,\varphi,\varphi') = xM^q(\varphi,\varphi') R(x,\varphi,\varphi') - x^2 C_1(x,\varphi,\varphi') M^q(\varphi,\varphi') \tag{D.21}$$

Combining Eqs. (D.20) and (D.21) we then find

$$\begin{aligned} C_1(x,\varphi,\varphi') = {} & M^q(\varphi,\varphi') R(x,\varphi,\varphi') - x\left[M^q(\varphi,\varphi')\right]^2 R(x,\varphi,\varphi') \\ & -x^2 M^q(\varphi,\varphi') C_1(x,\varphi,\varphi') M^q(\varphi,\varphi') \end{aligned}$$

which we can iterate to find

$$C_1(x,\varphi,\varphi') = \left[1 + xM^q(\varphi,\varphi')\right]^{-1} M^q(\varphi,\varphi') R(x,\varphi,\varphi') \tag{D.22}$$

Combining Eqs. (D.12), (D.17), and (D.22) we then get

$$\frac{\partial}{\partial x} R\left(x, \varphi, \varphi'\right) = \operatorname{Tr}\left[e^{-2i\varphi} \tan\theta^q A\left(x, \varphi, \varphi'\right)\right]$$
$$= R\left(x, \varphi, \varphi'\right) \operatorname{Tr}\left\{\left[1 + x M^q\left(\varphi, \varphi'\right)\right]^{-1} M^q\left(\varphi, \varphi'\right)\right\}$$

Next, we integrate this result from $x = 0$ to $x = 1$

$$\ln \frac{R\left(1, \varphi, \varphi'\right)}{R\left(0, \varphi, \varphi'\right)} = \int_0^1 dx \, \frac{\partial}{\partial x} \operatorname{Tr}\left\{\ln\left[1 + x M^q\left(\varphi, \varphi'\right)\right]\right\}$$

By inspection of Eq. (D.10) we can see that $R\left(0, \varphi, \varphi'\right) = 1$, and therefore

$$R\left(1, \varphi, \varphi'\right) = \exp\left\{\operatorname{Tr}\left\{\ln\left[1 + M^q\left(\varphi, \varphi'\right)\right]\right\}\right\}$$

By a corollary to Jacobi's formula for the derivative of a matrix determinant, this can be written as

$$R\left(1, \varphi, \varphi'\right) = \det\left[1 + M^q\left(\varphi, \varphi'\right)\right] \tag{D.23}$$

Using this result in Eq. (D.11), and with the normalization given by Eq. (D.9) we get

$$\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle = \left(\prod_{\mu > 0} u_\mu^q u_\mu^{q'}\right) \det\left[1 + e^{2i\left(\varphi' - \varphi\right)} M^q\right] \tag{D.24}$$

where we have explicitly factored out the dependence on $\varphi' - \varphi$ by writing

$$M^q\left(\varphi, \varphi'\right) = e^{2i\left(\varphi' - \varphi\right)} M^q$$

with $M^q$ defined as in Eq. (3.33) of [1],

$$M^q \equiv \tan\theta^q \tau^{qq'} \tan\theta^{q'} \tau^{qq'\dagger}$$

All that remains now is to integrate Eq. (D.24) to obtain the projected norm overlap as in Eq. (D.1),

$$\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger} P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\left(2\pi\right)^2} \int_0^{2\pi} d\varphi \int_0^{2\pi} d\varphi' \, f\left(\varphi' - \varphi\right)$$

where the function

$$f\left(\varphi' - \varphi\right) \equiv e^{-i\left(\varphi' - \varphi\right)N} \left(\prod_{\mu > 0} u_\mu^q u_\mu^{q'}\right) \det\left[1 + e^{2i\left(\varphi' - \varphi\right)} M^q\right]$$

clearly satisfies Eqs. (D.4) and (D.5) for and even number $N = 2p$ of particles. Therefore, we can use Eq. (D.6) to reduce the integral to

$$\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \times \mathrm{Re} \left\{ e^{-i\xi N} \det \left[ 1 + e^{2i\xi} M^q \right] \right\} \tag{D.25}$$

We now assume that $M^q$ can be diagonalized,

$$\boxed{M^q = S D^q S^T} \tag{D.26}$$

where $S$ is an orthogonal matrix and $D^q$ is a diagonal matrix. Then,

$$\det \left[ 1 + e^{2i\xi} M^q \right] = \prod_{\mu>0} \left( 1 + e^{2i\xi} D_{\mu\mu}^q \right) \tag{D.27}$$

It will be convenient to write the complex number $1 + e^{2i\xi} D_{\mu\mu}^q$ in exponential form,

$$1 + e^{2i\xi} D_{\mu\mu}^q = n_\mu (\xi) \, e^{i\Omega_\mu(\xi)}$$

where

$$\boxed{n_\mu (\xi) = \sqrt{1 + 2\cos(2\xi) D_{\mu\mu} + D_{\mu\mu}^2}} \tag{D.28}$$

and[1]

$$\boxed{\Omega_\mu (\xi) = \tan^{-1} \left( 1 + \cos(2\xi) D_{\mu\mu}, \sin(2\xi) D_{\mu\mu} \right)} \tag{D.29}$$

Using these results, we can write the determinant in Eq. (D.27) as

$$\det \left[ 1 + e^{2i\xi} M^q \right] = n(\xi) \, e^{i\Omega(\xi)}$$

where we have defined

$$\boxed{n(\xi) \equiv \prod_{\mu>0} n_\mu (\xi)} \tag{D.30}$$

and

$$\boxed{\Omega(\xi) \equiv \sum_{\mu>0} \Omega_\mu (\xi)} \tag{D.31}$$

Thus we have

$$\left\langle \Phi_q^{(p)} (\varphi) \middle| \Phi_{q'}^{(p)} (\varphi') \right\rangle = \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi) \, e^{i\Omega(\xi)} \tag{D.32}$$

Returning to the overlap integral in Eq. (D.25), we now have

[1] We use the two-argument arctangent function, $\tan^{-1}(x, y)$, which is defined as $\mathrm{atan2}(y, x)$ in some computer languages.

$$\boxed{\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n(\xi) \cos\left[\Omega(\xi) - N\xi\right]} \tag{D.33}$$

and the remaining integral can be evaluated numerically, as discussed in section C.4.

## D.3 Generalized one-body density

### *D.3.1 Preliminary definitions and results*

We introduce the matrix

$$M^{q'}(\varphi, \varphi') \equiv e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \tag{D.34}$$

which is related to the matrix $M^{q'}$ defined in Eq. (3.44) of [1] via

$$M^{q'}(\varphi, \varphi') = e^{2i\left(\varphi'-\varphi\right)} M^{q'}$$

Note that using Eq. (D.19), we have

$$e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} M^q(\varphi, \varphi') = M^{q'}(\varphi, \varphi') \, e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger}$$

and

$$M^q(\varphi, \varphi') \, e^{-2i\varphi} \tan\theta^q \tau^{qq'} = e^{-2i\varphi} \tan\theta^q \tau^{qq'} M^{q'}(\varphi, \varphi')$$

from this, we deduce

$$e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} M^q(\varphi, \varphi') \, e^{-2i\varphi} \tan\theta^q \tau^{qq'} = \left[M^{q'}(\varphi, \varphi')\right]^2$$

More generally, we can show by induction that for any non-negative integer $n$,

$$\boxed{e^{2i\varphi'} \tan\theta^{q'} \tau^{qq'\dagger} \left[M^q(\varphi, \varphi')\right]^n e^{-2i\varphi} \tan\theta^q \tau^{qq'} = \left[M^{q'}(\varphi, \varphi')\right]^{n+1}} \tag{D.35}$$

We now derive some useful equations for the matrices $A(x, \varphi, \varphi')$ and $B(x, \varphi, \varphi')$ defined in Eqs. (D.13) and (D.14), respectively. First, by combining Eqs. (D.17) and (D.22), we get

$$e^{-2i\varphi} \tan\theta^q A(x, \varphi, \varphi') = \left[1 + xM^q(\varphi, \varphi')\right]^{-1} M^q(\varphi, \varphi') \, R(x, \varphi, \varphi') \tag{D.36}$$

Then from Eq. (D.16), we get

$$\begin{aligned} e^{2i\varphi'}\tan\theta^{q'}B(x,\varphi,\varphi') &= xR(x,\varphi,\varphi')\,e^{2i\varphi'}\tan\theta^{q'}\tau^{qq'\dagger}\{1- \\ &\qquad -\left[1+xM^{q}(\varphi,\varphi')\right]^{-1}xM^{q}(\varphi,\varphi')\Big\}\,e^{-2i\varphi}\tan\theta^{q}\tau^{qq'} \\ &= xR(x,\varphi,\varphi')\,e^{2i\varphi'}\tan\theta^{q'}\tau^{qq'\dagger}\left[1+xM^{q}(\varphi,\varphi')\right]^{-1} \\ &\quad\times e^{-2i\varphi}\tan\theta^{q}\tau^{qq'} \end{aligned}$$

Now we can use Eq. (D.35) to obtain the equivalent to Eq. (3.43) in [1],

$$\boxed{e^{2i\varphi'}\tan\theta^{q'}B(x,\varphi,\varphi') = xR(x,\varphi,\varphi')\left[1+xM^{q'}(\varphi,\varphi')\right]^{-1}M^{q'}(\varphi,\varphi')} \tag{D.37}$$

We can also get an equation for $B(x,\varphi,\varphi')$ alone by using Eq. (D.36) in Eq. (D.16), then

$$\begin{aligned} B(x,\varphi,\varphi') &= xR(x,\varphi,\varphi')\,\tau^{qq'\dagger}\left\{I - x\left[1+xM^{q}(\varphi,\varphi')\right]^{-1}M^{q}(\varphi,\varphi')\right\} \\ &\quad\times e^{-2i\varphi}\tan\theta^{q}\tau^{qq'} \\ &= xR(x,\varphi,\varphi')\,\tau^{qq'\dagger}\left[1+xM^{q}(\varphi,\varphi')\right]^{-1}e^{-2i\varphi}\tan\theta^{q}\tau^{qq'} \end{aligned}$$

We will need in particular the equation for $B(1,\varphi,\varphi')$ which we get from this last equation,

$$\boxed{B(1,\varphi,\varphi') = R(1,\varphi,\varphi')\,\tau^{qq'\dagger}\left[1+M^{q}(\varphi,\varphi')\right]^{-1}e^{-2i\varphi}\tan\theta^{q}\tau^{qq'}} \tag{D.38}$$

This is the equivalent to Eq. (3.45) in [1]

### *D.3.2 Projected matrix elements of* $a^\dagger a$

We now consider

$$\begin{aligned} \left\langle \Phi_q^{(p)}\left|P_q^{(N)\dagger}a_\alpha^{q'\dagger}a_\beta^{q'}P_{q'}^{(N)}\right|\Phi_{q'}^{(p)}\right\rangle &= \frac{1}{(2\pi)^2}\int_0^{2\pi}d\varphi\int_0^{2\pi}d\varphi'\,e^{-i(\varphi'-\varphi)N} \\ &\quad\times\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_\alpha^{q'\dagger}a_\beta^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle \end{aligned} \tag{D.39}$$

where we will assume for now $\alpha,\beta>0$. We focus on the matrix element in the integrand,

$$\left\langle \Phi_q^{(p)}\left|e^{-i\hat{N}_q\varphi}a_\alpha^{q'\dagger}a_\beta^{q'}e^{i\hat{N}_{q'}\varphi'}\right|\Phi_{q'}^{(p)}\right\rangle = \left\langle \Phi_q^{(p)}(\varphi)\left|a_\alpha^{q'\dagger}a_\beta^{q'}\right|\Phi_{q'}^{(p)}(\varphi')\right\rangle$$

Then we use Eq. (D.8) to write

$$
\begin{aligned}
&\left\langle \varPhi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \varPhi_{q'}^{(p)} \right\rangle \\
&= \left\langle 0 \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle \left\langle \varPhi_q^{(p)}\left(\varphi\right) \left| e^{\hat{X}_{q'}\left(\varphi'\right)} e^{-\hat{X}_{q'}\left(\varphi'\right)} a_\alpha^{q'\dagger} a_\beta^{q'} e^{\hat{X}_{q'}\left(\varphi'\right)} \right| 0 \right\rangle
\end{aligned}
$$

Then we proceed as in appendix 3 of [1] and expand

$$
\begin{aligned}
e^{-\hat{X}_{q'}\left(\varphi'\right)} a_\alpha^{q'\dagger} a_\beta^{q'} e^{\hat{X}_{q'}\left(\varphi'\right)} = a_\alpha^{q'\dagger} a_\beta^{q'} &- \left[\hat{X}_{q'}\left(\varphi'\right), a_\alpha^{q'\dagger} a_\beta^{q'}\right] \\
&+ \frac{1}{2}\left[\hat{X}_{q'}\left(\varphi'\right), \left[\hat{X}_{q'}\left(\varphi'\right), a_\alpha^{q'\dagger} a_\beta^{q'}\right]\right] + \ldots
\end{aligned}
$$

The first commutator is

$$
\left[\hat{X}_{q'}\left(\varphi'\right), a_\alpha^{q'\dagger} a_\beta^{q'}\right] = -e^{2i\varphi'} \tan\theta_\beta^{q'} a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger}
$$

and the higher-order commutators therefore vanish. Thus we can write

$$
\begin{aligned}
\left\langle \varPhi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \varPhi_{q'}^{(p)} \right\rangle &= \left\langle 0 \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle e^{2i\varphi'} \tan\theta_\beta^{q'} \\
&\quad \times \left\langle \varPhi_q^{(p)}\left(\varphi\right) \left| e^{\hat{X}_{q'}\left(\varphi'\right)} a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| 0 \right\rangle \\
&= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \varPhi_q^{(p)}\left(\varphi\right) \left| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \right\rangle
\end{aligned}
$$

Now going back to the definition of $B$ in Eq. (D.14), we can write this as

$$
\begin{aligned}
\left\langle \varPhi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \varPhi_{q'}^{(p)} \right\rangle &= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \varPhi_q^{(p)}\left(\varphi\right) \right| 0 \Big\rangle \left\langle 0 \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle \\
&\quad \times B_{\beta\alpha}\left(1,\varphi,\varphi'\right)
\end{aligned}
\tag{D.40}
$$

Using Eq. (D.37) with $x = 1$ we can write this as

$$
\begin{aligned}
\left\langle \varPhi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \varPhi_{q'}^{(p)} \right\rangle &= \left\langle \varPhi_q^{(p)}\left(\varphi\right) \right| 0 \Big\rangle \left\langle 0 \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle \\
&\quad \times R\left(1,\varphi,\varphi'\right) \left\{ \left[1 + M^{q'}\left(\varphi,\varphi'\right)\right]^{-1} M^{q'}\left(\varphi,\varphi'\right) \right\}_{\beta\alpha}
\end{aligned}
$$

Next, we use Eq. (D.11) to write this as

$$
\begin{aligned}
&\left\langle \varPhi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \varPhi_{q'}^{(p)} \right\rangle \\
&= \left\langle \varPhi_q^{(p)}\left(\varphi\right) \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle \\
&\quad \times \left\{ \left[1 + M^{q'}\left(\varphi,\varphi'\right)\right]^{-1} M^{q'}\left(\varphi,\varphi'\right) \right\}_{\beta\alpha}
\end{aligned}
\tag{D.41}
$$

We already obtained an explicit form for the overlap $\left\langle \varPhi_q^{(p)}\left(\varphi\right) \right| \varPhi_{q'}^{(p)}\left(\varphi'\right) \Big\rangle$ in Eq. (D.32),

$$\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)}$$

For the remaining term in Eq. (D.41), we assume that $M^{q'}$ can be diagonalized,

$$M^{q'} = S' D^{q'} S'^T \tag{D.42}$$

where $S'$ is an orthogonal matrix and $D^{q'}$ is a diagonal matrix. Then,

$$\left[1 + M^{q'}(\varphi,\varphi')\right]^{-1} M^{q'}(\varphi,\varphi') = S' \left(1 + e^{2i\xi} D^{q'}\right)^{-1} e^{2i\xi} D^{q'} S'^T$$

where we have used $\xi \equiv \varphi' - \varphi$. The matrix $\left(1 + e^{2i\xi} D^{q'}\right)^{-1} e^{2i\xi} D^{q'}$ is diagonal, and its elements are

$$\left[\left(1 + e^{2i\xi} D^{q'}\right)^{-1} e^{2i\xi} D^{q'}\right]_{\mu\mu} = e^{2i\xi} \frac{D_{\mu\mu}^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) - i \sin(2\xi)\right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'}\right)^2}$$

From this we calculate

$$\begin{aligned} &\left\{\left[1 + M^{q'}(\varphi,\varphi')\right]^{-1} M^{q'}(\varphi,\varphi')\right\}_{\beta\alpha} \\ &= e^{2i\xi} \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{D_{\mu\mu}^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi) - i D_{\mu\mu}^{q'} \sin(2\xi)\right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'}\right)^2} \end{aligned}$$

Separating out the real and imaginary parts from the quantity in the summation,

$$W'_{\beta\alpha}(\xi) \equiv \sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{D_{\mu\mu}^{q'} \left[1 + D_{\mu\mu}^{q'} \cos(2\xi)\right]}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'}\right)^2} \tag{D.43}$$

$$Z'_{\beta\alpha}(\xi) \equiv -\sum_{\mu>0} S'_{\beta\mu} S'_{\alpha\mu} \frac{\left(D_{\mu\mu}^{q'}\right)^2 \sin(2\xi)}{1 + 2D_{\mu\mu}^{q'} \cos(2\xi) + \left(D_{\mu\mu}^{q'}\right)^2} \tag{D.44}$$

we can write the matrix element in exponential form

$$\begin{aligned} \left\{\left[1 + M^{q'}(\varphi,\varphi')\right]^{-1} M^{q'}(\varphi,\varphi')\right\}_{\beta\alpha} &= e^{2i\xi} \left[W'_{\beta\alpha}(\xi) + i Z'_{\beta\alpha}(\xi)\right] \\ &\equiv n'_{\beta\alpha}(\xi)\, e^{i\left[\Omega'_{\beta\alpha}(\xi) + 2\xi\right]} \end{aligned} \tag{D.45}$$

where

$$n'_{\beta\alpha}(\xi) = \sqrt{\left[W'_{\beta\alpha}(\xi)\right]^2 + \left[Z'_{\beta\alpha}(\xi)\right]^2}$$
$$\Omega'_{\beta\alpha}(\xi) = \tan^{-1}\left(W'_{\beta\alpha}(\xi), Z'_{\beta\alpha}(\xi)\right)$$

The matrix element in Eq. (D.41) can then be written as

$$\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_\alpha^{q'\dagger} a_\beta^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right) n(\xi)\, e^{i\Omega(\xi)} n'_{\beta\alpha}(\xi) \times e^{i\left[\Omega'_{\beta\alpha}(\xi)+2\xi\right]} \tag{D.46}$$

We can also define the following quantity which will be useful in section D.4,

$$\begin{aligned} S_{\beta\alpha}(\varphi,\varphi') &\equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle} \\ &= e^{2i\xi}\left[W'_{\beta\alpha}(\xi) + iZ'_{\beta\alpha}(\xi)\right] \end{aligned} \tag{D.47}$$

We can now return to Eq. (D.39) and define the function

$$f(\varphi'-\varphi) \equiv e^{-i(\varphi'-\varphi)N}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right) \det\left[1 + e^{2i(\varphi'-\varphi)} M^q\right] \times \left\{\left[1 + e^{2i(\varphi'-\varphi)} M^{q'}\right]^{-1} e^{2i(\varphi'-\varphi)} M^{q'}\right\}_{\beta\alpha}$$

which clearly satisfies Eqs. (D.4) and (D.5) for and even number $N = 2p$ of particles. Therefore, we can use Eq. (D.6) to reduce the integral in Eq. (D.39) to one dimension, and use the exponential forms derived above to simplify Eq. (D.41). The result is

$$\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_\alpha^{q'\dagger} a_\beta^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right) \int_0^\pi d\xi\, \mathrm{Re}\left[e^{-i\xi N} n(\xi)\, e^{i\Omega(\xi)} n'_{\beta\alpha}(\xi)\, e^{i\left[\Omega'_{\beta\alpha}(\xi)+2\xi\right]}\right]$$

or

$$\boxed{\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_\alpha^{q'\dagger} a_\beta^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi}\left(\prod_{\mu>0} u_\mu^q u_\mu^{q'}\right) \int_0^\pi d\xi\, n(\xi)\, n'_{\beta\alpha}(\xi) \times \cos\left[\Omega(\xi) + \Omega'_{\beta\alpha}(\xi) - \xi(N-2)\right]} \tag{D.48}$$

We can proceed along similar lines to derive the projected one-body overlap for the time-reversed states, $\left\langle \Phi_q^{(p)} \middle| P_q^{(N)\dagger} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} P_{q'}^{(N)} \middle| \Phi_{q'}^{(p)} \right\rangle$. We note that

$$\left[\hat{X}_{q'}\left(\varphi'\right), a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'}\right] = -e^{2i\varphi'} \tan\theta_\beta^{q'} a_\beta^{q'\dagger} a_{\bar{\alpha}}^{q'\dagger}$$

and therefore Eq. (D.40) becomes

$$\begin{aligned}
\left\langle \Phi_q^{(p)} \middle| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \middle| \Phi_{q'}^{(p)} \right\rangle &= e^{2i\varphi'} \tan\theta_\beta^{q'} \left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| 0 \right\rangle \left\langle 0 \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle \\
&\quad \times B_{\alpha\beta}\left(1,\varphi,\varphi'\right) \\
&= \left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle \\
&\quad \times \frac{B_{\alpha\beta}\left(1,\varphi,\varphi'\right)}{R\left(1,\varphi,\varphi'\right)} e^{2i\varphi'} \tan\theta_\beta^{q'}
\end{aligned} \tag{D.49}$$

Next, we examine the effect on this result of simultaneously exchanging $\alpha \leftrightarrow \beta$, $\varphi \leftrightarrow \varphi'$, and $q \leftrightarrow q'$. We denote the operation which consists in making those exchanges by the superscript symbol $\leftrightarrow$. Clearly,

$$\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle = \left[\left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle^{\leftrightarrow}\right]^*$$

and from Eq. (D.10),

$$R\left(1,\varphi,\varphi'\right) = \left[\left[R\left(1,\varphi,\varphi'\right)\right]^{\leftrightarrow}\right]^*$$

Then, from Eqs. (D.13) and (D.14),

$$B_{\alpha\beta}\left(1,\varphi,\varphi'\right) = \left[\left[A_{\alpha\beta}\left(1,\varphi,\varphi'\right)\right]^{\leftrightarrow}\right]^*$$

And we can also write

$$e^{2i\varphi'} \tan\theta_\beta^{q'} = \left[\left(e^{-2i\varphi} \tan\theta_\alpha^q\right)^{\leftrightarrow}\right]^*$$

Thus Eq. (D.49) becomes

$$\begin{aligned}
\left\langle \Phi_q^{(p)} \middle| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \middle| \Phi_{q'}^{(p)} \right\rangle = \Bigg\{ \Bigg[ & \left\langle \Phi_q^{(p)}\left(\varphi\right) \middle| \Phi_{q'}^{(p)}\left(\varphi'\right) \right\rangle \\
& \times e^{-2i\varphi} \tan\theta_\alpha^q \frac{A_{\alpha\beta}\left(1,\varphi,\varphi'\right)}{R\left(1,\varphi,\varphi'\right)} \Bigg]^{\leftrightarrow} \Bigg\}^*
\end{aligned}$$

and using Eq. (D.36) with $x = 1$, this simplifies to

$$\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left\{ \left[ \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \right.\right.$$
$$\left.\left. \times \left[ \left[1 + M^q(\varphi,\varphi')\right]^{-1} M^q(\varphi,\varphi') \right]_{\alpha\beta} \right]^{\leftrightarrow} \right\}^*$$
$$= \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$$
$$\times \left[ \left[1 + M^{q'}(\varphi,\varphi')\right]^{-1} M^{q'}(\varphi,\varphi') \right]_{\beta\alpha}$$

where we have used Eq. (D.34) to write

$$\left[M^{q'}(\varphi',\varphi)\right]^* = M^{q'}(\varphi,\varphi')$$

Comparing with Eq. (D.41) it is clear that

$$\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_{\alpha}^{q'\dagger} a_{\beta}^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle \tag{D.50}$$

and therefore

$$\boxed{\left\langle \Phi_q^{(p)} \left| e^{-i\hat{N}_q\varphi} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} e^{i\hat{N}_{q'}\varphi'} \right| \Phi_{q'}^{(p)} \right\rangle = \left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} a_{\alpha}^{q'\dagger} a_{\beta}^{q'} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle} \tag{D.51}$$

### D.3.3 Calculation of the matrix elements $\left\langle \Phi_q^{(p)}(\varphi) \left| a_{\alpha}^{q'} a_{\bar{\beta}}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle$

As usual, we write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| a_{\alpha}^{q'} a_{\bar{\beta}}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left\langle \Phi_q^{(p)}(\varphi) \left| e^{\hat{X}_{q'}(\varphi')} e^{-\hat{X}_{q'}(\varphi')} a_{\alpha}^{q'} a_{\bar{\beta}}^{q'} e^{\hat{X}_{q'}(\varphi')} \right| 0 \right\rangle$$

and expand

$$e^{-\hat{X}_{q'}(\varphi')} a_{\alpha}^{q'} a_{\bar{\beta}}^{q'} e^{\hat{X}_{q'}(\varphi')} = a_{\alpha}^{q'} a_{\bar{\beta}}^{q'} - \left[\hat{X}_{q'}(\varphi'), a_{\alpha}^{q'} a_{\bar{\beta}}^{q'}\right]$$
$$+ \frac{1}{2}\left[\hat{X}_{q'}(\varphi'), \left[\hat{X}_{q'}(\varphi'), a_{\alpha}^{q'} a_{\bar{\beta}}^{q'}\right]\right] + \ldots$$

The first commutator is

$$\left[\hat{X}_{q'}(\varphi'), a_{\alpha}^{q'} a_{\bar{\beta}}^{q'}\right] = e^{2i\varphi'} \left[\delta_{\alpha\beta} \tan\theta_{\beta}^{q'} - \tan\theta_{\alpha}^{q'} a_{\bar{\alpha}}^{q'\dagger} a_{\bar{\beta}}^{q'} - \tan\theta_{\beta}^{q'} a_{\beta}^{q'\dagger} a_{\alpha}^{q'}\right]$$

and the second is

$$\left[\hat{X}_{q'}\left(\varphi'\right),\left[\hat{X}_{q'}\left(\varphi'\right),a_{\alpha}^{q'}a_{\bar{\beta}}^{q'}\right]\right]=2e^{4i\varphi'}\tan\theta_{\alpha}^{q'}\tan\theta_{\beta}^{q'}a_{\beta}^{q'\dagger}a_{\bar{\alpha}}^{q'\dagger}$$

and the expansion therefore stops at the second commutator. Thus we have

$$\begin{aligned}\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\left|a_{\alpha}^{q'}a_{\bar{\beta}}^{q'}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle =&-\delta_{\alpha\beta}e^{2i\varphi'}\tan\theta_{\beta}^{q'}\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle\\&+e^{2i\varphi'}\tan\theta_{\alpha}^{q'}e^{2i\varphi'}\tan\theta_{\beta}^{q'}\\&\times\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\left|a_{\beta}^{q'\dagger}a_{\bar{\alpha}}^{q'\dagger}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle\end{aligned}$$

Now, from Eqs. (D.14) and (D.10) we can write

$$\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\left|a_{\beta}^{q'\dagger}a_{\bar{\alpha}}^{q'\dagger}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle=\frac{\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle}{R\left(1,\varphi,\varphi'\right)}B_{\alpha\beta}\left(1,\varphi,\varphi'\right)$$

and using Eq. (D.37), we finally obtain

$$\begin{aligned}\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\left|a_{\alpha}^{q'}a_{\bar{\beta}}^{q'}\right|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle =&-\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle\\&\times\left\{\left[1+M^{q'}\left(\varphi,\varphi'\right)\right]^{-1}e^{2i\varphi'}\tan\theta^{q'}\right\}_{\alpha\beta}\end{aligned}\tag{D.52}$$

which is the equivalent to Eq. (3.47) in [1]. The explicit expression for $\left\langle \Phi_{q}^{(p)}\left(\varphi\right)\middle|\Phi_{q'}^{(p)}\left(\varphi'\right)\right\rangle$ is given by Eq. (D.32). For the remaining term, we proceed as in section D.3.2 and use the diagonalized form of $M^{q'}$ in Eq. (D.42) to write

$$\begin{aligned}&\left\{\left[1+M^{q'}\left(\varphi,\varphi'\right)\right]^{-1}e^{2i\varphi'}\tan\theta^{q'}\right\}_{\alpha\beta}\\&=e^{2i\varphi'}\sum_{\mu>0}S'_{\beta\mu}S'_{\alpha\mu}\frac{\tan\theta_{\mu}^{q'}\left[1+D_{\mu\mu}^{q'}\cos\left(2\xi\right)-iD_{\mu\mu}^{q'}\sin\left(2\xi\right)\right]}{1+2D_{\mu\mu}^{q'}\cos\left(2\xi\right)+\left(D_{\mu\mu}^{q'}\right)^{2}}\end{aligned}$$

where we have set $\xi=\varphi'-\varphi$. We can then define

$$W_{\beta\alpha}^{(-)}\left(\xi\right)\equiv\sum_{\mu>0}S'_{\beta\mu}S'_{\alpha\mu}\frac{\tan\theta_{\mu}^{q'}\left[1+D_{\mu\mu}^{q'}\cos\left(2\xi\right)\right]}{1+2D_{\mu\mu}^{q'}\cos\left(2\xi\right)+\left(D_{\mu\mu}^{q'}\right)^{2}}\tag{D.53}$$

$$Z_{\beta\alpha}^{(-)}\left(\xi\right)\equiv-\sum_{\mu>0}S'_{\beta\mu}S'_{\alpha\mu}\frac{\tan\theta_{\mu}^{q'}D_{\mu\mu}^{q'}\sin\left(2\xi\right)}{1+2D_{\mu\mu}^{q'}\cos\left(2\xi\right)+\left(D_{\mu\mu}^{q'}\right)^{2}}\tag{D.54}$$

and write the matrix element in exponential form

$$\left\{\left[1+M^{q'}(\varphi,\varphi')\right]^{-1} e^{2i\varphi'}\tan\theta^{q'}\right\}_{\alpha\beta} = e^{2i\varphi'}\left[W^{(-)}_{\beta\alpha}(\xi)+iZ^{(-)}_{\beta\alpha}(\xi)\right]$$
$$\equiv e^{2i\varphi'} n^{(-)}_{\beta\alpha}(\xi)\, e^{i\Omega^{(-)}_{\beta\alpha}(\xi)}$$

where

$$n^{(-)}_{\beta\alpha}(\xi) = \sqrt{\left[W^{(-)}_{\beta\alpha}(\xi)\right]^2+\left[Z^{(-)}_{\beta\alpha}(\xi)\right]^2}$$
$$\Omega^{(-)}_{\beta\alpha}(\xi) = \tan^{-1}\left(W^{(-)}_{\beta\alpha}(\xi), Z^{(-)}_{\beta\alpha}(\xi)\right)$$

Putting all these results together, we find

$$\left\langle \Phi^{(p)}_{q}(\varphi)\left|a^{q'}_{\alpha}a^{q'}_{\bar\beta}\right|\Phi^{(p)}_{q'}(\varphi')\right\rangle = -e^{2i\varphi'}\left(\prod_{\mu>0}u^{q}_{\mu}u^{q'}_{\mu}\right) n(\xi)\, e^{i\Omega(\xi)} \times n^{(-)}_{\beta\alpha}(\xi)\, e^{i\Omega^{(-)}_{\beta\alpha}(\xi)} \tag{D.55}$$

Note that, because of the fact that the operator $a^{q'}_{\alpha}a^{q'}_{\bar\beta}$ does not conserve particle number, this matrix element does not depend on $\xi$ alone, but on $\varphi'$ as well. However, this matrix element will usually be combined with $\left\langle \Phi^{(p)}_{q}\left|P^{(N)\dagger}_{q}a^{q'\dagger}_{\alpha}a^{q'\dagger}_{\bar\beta}P^{(N)}_{q'}\right|\Phi^{(p)}_{q'}\right\rangle$ in calculations of the interaction matrix elements, and the product will again depend on $\xi$ alone, as we will see in section D.3.4. We also define at this point the quantity

$$Y_{\alpha\bar\beta}(\varphi,\varphi') \equiv \frac{\left\langle \Phi^{(p)}_{q}(\varphi)\left|a^{q'}_{\alpha}a^{q'}_{\bar\beta}\right|\Phi^{(p)}_{q'}(\varphi')\right\rangle}{\left\langle \Phi^{(p)}_{q}(\varphi)\middle|\Phi^{(p)}_{q'}(\varphi')\right\rangle} = -e^{2i\varphi'}\left[W^{(-)}_{\beta\alpha}(\xi)+iZ^{(-)}_{\beta\alpha}(\xi)\right] \tag{D.56}$$

which will be useful in section D.4.

### D.3.4 Calculation of the matrix elements $\left\langle \boldsymbol{\Phi^{(p)}_{q}}\left|\boldsymbol{P^{(N)\dagger}_{q}a^{q'\dagger}_{\alpha}a^{q'\dagger}_{\bar\beta}P^{(N)}_{q'}}\right|\boldsymbol{\Phi^{(p)}_{q'}}\right\rangle$

Using Eq. (D.14) we write

$$\left\langle \Phi^{(p)}_{q}(\varphi)\left|a^{q'\dagger}_{\alpha}a^{q'\dagger}_{\bar\beta}\right|\Phi^{(p)}_{q'}(\varphi')\right\rangle = \left\langle \Phi^{(p)}_{q}(\varphi)\middle|0\right\rangle\left\langle 0\middle|\Phi^{(p)}_{q'}(\varphi')\right\rangle B_{\beta\alpha}(x,\varphi,\varphi')$$

Using Eqs. (D.11) and (D.38) (with $x=1$) this becomes

$$\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle \times \left[ \tau^{qq'\dagger} \left[1 + M^q(\varphi, \varphi')\right]^{-1} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \right]_{\beta\alpha} \tag{D.57}$$

which is the equivalent to Eq. (3.48) in [1]. The explicit expression for $\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle$ is given by Eq. (D.32). For the remaining term we can use the diagonalized form of $M^q$ in Eq. (D.26) and write

$$\begin{aligned} &\left[ \tau^{qq'\dagger} \left[1 + M^q(\varphi, \varphi')\right]^{-1} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \right]_{\beta\alpha} \\ &= e^{-2i\varphi} \sum_{\mu,\nu,\sigma>0} \tau_{\mu\beta}^{qq'*} \tau_{\nu\alpha}^{qq'} S_{\mu\sigma} S_{\nu\sigma} \tan\theta_\nu^q \\ &\times \frac{1 + D_{\sigma\sigma}^{q'} \cos(2\xi) - i D_{\sigma\sigma}^{q'} \sin(2\xi)}{1 + 2D_{\sigma\sigma}^{q'} \cos(2\xi) + \left(D_{\sigma\sigma}^{q'}\right)^2} \end{aligned}$$

where we have set $\xi = \varphi' - \varphi$. We can then define

$$W_{\beta\alpha}^{(+)}(\xi) \equiv \sum_{\mu,\nu,\sigma>0} \tau_{\mu\beta}^{qq'*} \tau_{\nu\alpha}^{qq'} S_{\mu\sigma} S_{\nu\sigma} \tan\theta_\nu^q \frac{\left[1 + D_{\sigma\sigma}^{q'} \cos(2\xi)\right]}{1 + 2D_{\sigma\sigma}^{q'} \cos(2\xi) + \left(D_{\sigma\sigma}^{q'}\right)^2} \tag{D.58}$$

$$Z_{\beta\alpha}^{(+)}(\xi) \equiv - \sum_{\mu,\nu,\sigma>0} \tau_{\mu\beta}^{qq'*} \tau_{\nu\alpha}^{qq'} S_{\mu\sigma} S_{\nu\sigma} \tan\theta_\nu^q \frac{D_{\sigma\sigma}^{q'} \sin(2\xi)}{1 + 2D_{\sigma\sigma}^{q'} \cos(2\xi) + \left(D_{\sigma\sigma}^{q'}\right)^2} \tag{D.59}$$

so that we can write the exponential form

$$\left[ \tau^{qq'\dagger} \left[1 + M^q(\varphi, \varphi')\right]^{-1} e^{-2i\varphi} \tan\theta^q \tau^{qq'} \right]_{\beta\alpha} = e^{-2i\varphi} n_{\beta\alpha}^{(+)}(\xi) e^{i\Omega_{\beta\alpha}^{(+)}(\xi)}$$

where

$$\begin{aligned} n_{\beta\alpha}^{(+)}(\xi) &= \sqrt{\left[W_{\beta\alpha}^{(+)}(\xi)\right]^2 + \left[Z_{\beta\alpha}^{(+)}(\xi)\right]^2} \\ \Omega_{\beta\alpha}^{(+)}(\xi) &= \tan^{-1}\left(W_{\beta\alpha}^{(+)}(\xi), Z_{\beta\alpha}^{(+)}(\xi)\right) \end{aligned}$$

Putting all these results together, we find

$$\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = e^{-2i\varphi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi) e^{i\Omega(\xi)} \times n_{\beta\alpha}^{(+)}(\xi) e^{i\Omega_{\beta\alpha}^{(+)}(\xi)} \tag{D.60}$$

As in the case of Eq. (D.55), and again because the operator $a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger}$ does not conserve particle number, we note that the matrix element does not depend on $\xi$ alone. However, when Eqs. (D.55) and (D.60) are multiplied together, e.g. from the Wick-contracted form of a two-body term in the Hamiltonian, the troublesome factors $e^{2i\varphi'}$ and $e^{-2i\varphi}$ combine to give once again a dependence on $\xi$ alone through the factor $e^{2i\xi}$. We also define the quantity

$$\begin{aligned} T_{\alpha\bar{\beta}}(\varphi,\varphi') &\equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_{\bar{\beta}}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle} \\ &= e^{-2i\varphi} \left[ W_{\beta\alpha}^{(+)}(\xi) + i Z_{\beta\alpha}^{(+)}(\xi) \right] \end{aligned} \tag{D.61}$$

which will be useful in section D.4.

## D.4 Application to Hamiltonians

In this section we apply the formalism developed in this appendix to calculate non-diagonal matrix elements for a generic Hamiltonian, expressed in the basis at $q'$

$$\begin{aligned} \hat{H} &= \sum_{\alpha\beta} \left\langle \alpha, q' \left| \hat{T} \right| \beta, q' \right\rangle a_\alpha^{q'\dagger} a_\beta^{q'} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \left\langle \alpha, q'; \beta, q' \left| \hat{V} \right| \gamma, \widetilde{q'; \delta}, q' \right\rangle a_\alpha^{q'\dagger} a_\beta^{q'\dagger} a_\delta^{q'} a_\gamma^{q'} \\ &\equiv \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} V_{\alpha\beta\widetilde{\gamma\delta}}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'\dagger} a_\delta^{q'} a_\gamma^{q'} \end{aligned}$$

For the one-body term, we use Eqs. (D.46) and (D.45) to write

$$\begin{aligned} \left\langle \Phi_q^{(p)}(\varphi) \left| \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle &= \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)} e^{2i\xi} \\ &\times 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} \left[ W'_{\beta\alpha}(\xi) + i Z'_{\beta\alpha}(\xi) \right] \end{aligned}$$

We can then define

$$W^{(0)}(\xi) \equiv 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} W'_{\beta\alpha}(\xi) \tag{D.62}$$

$$Z^{(0)}(\xi) \equiv 2 \sum_{\alpha,\beta>0} T_{\alpha\beta}^{q'} Z'_{\beta\alpha}(\xi) \tag{D.63}$$

and

$$W^{(0)}(\xi) + iZ^{(0)}(\xi) \equiv n^{(0)}(\xi)\, e^{i\Omega^{(0)}(\xi)} \tag{D.64}$$

to write

$$\left\langle \Phi_q^{(p)}(\varphi) \left| \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle = \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) n(\xi)\, e^{i\Omega(\xi)} e^{2i\xi} \times n^{(0)}(\xi)\, e^{i\Omega^{(0)}(\xi)}$$

Then the projected matrix element is

$$\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} \left( \sum_{\alpha\beta} T_{\alpha\beta}^{q'} a_\alpha^{q'\dagger} a_\beta^{q'} \right) P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi\, n(\xi)\, n^{(0)}(\xi) \times \cos\left[ \Omega(\xi) + \Omega^{(0)}(\xi) - \xi(N-2) \right] \tag{D.65}$$

Next we calculate the contribution from the two-body term in the Hamiltonian. For compactness of notation we define the generalized density matrix elements equivalent to those given by Eqs. (4.5)-(4.7) in [1],

$$S_{\beta\alpha}(\varphi,\varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_\beta^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

$$T_{\alpha\bar\beta}(\varphi,\varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'\dagger} a_{\bar\beta}^{q'\dagger} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

$$Y_{\alpha\bar\beta}(\varphi,\varphi') \equiv \frac{\left\langle \Phi_q^{(p)}(\varphi) \left| a_\alpha^{q'} a_{\bar\beta}^{q'} \right| \Phi_{q'}^{(p)}(\varphi') \right\rangle}{\left\langle \Phi_q^{(p)}(\varphi) \middle| \Phi_{q'}^{(p)}(\varphi') \right\rangle}$$

We can use the generalized Wick's theorem given in Eq. (3.17) of [1] and obtain

$$
\begin{aligned}
&\frac{1}{4}\left\langle \Phi_q^{(p)}(\varphi)\left|\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}} a^{q'\dagger}_{\alpha} a^{q'\dagger}_{\beta} a^{q'}_{\delta} a^{q'}_{\gamma}\right| \Phi_{q'}^{(p)}(\varphi')\right\rangle \\
&= \left\langle \Phi_q^{(p)}(\varphi)\middle| \Phi_{q'}^{(p)}(\varphi')\right\rangle \\
&\quad\times\left\{\frac{1}{2}\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}} S_{\gamma\alpha}(\varphi,\varphi') S_{\delta\beta}(\varphi,\varphi')\right. \\
&\quad\left.+\frac{1}{4}\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}} T_{\alpha\bar{\beta}}(\varphi,\varphi') Y_{\bar{\delta}\gamma}(\varphi,\varphi')\right\}
\end{aligned}
$$

Next, we use Eq. (D.47) to write

$$
\begin{aligned}
\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}} S_{\gamma\alpha}(\varphi,\varphi') S_{\delta\beta}(\varphi,\varphi') &= e^{4i\xi}\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}}\left[W'_{\gamma\alpha}(\xi)+iZ'_{\gamma\alpha}(\xi)\right]\left[W'_{\delta\beta}(\xi)+iZ'_{\delta\beta}(\xi)\right] \\
&= e^{4i\xi}\left[W'(\xi)+iZ'(\xi)\right]
\end{aligned}
$$

where we have defined

$$
W'(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}}\left[W'_{\gamma\alpha}(\xi) W'_{\delta\beta}(\xi) - Z'_{\gamma\alpha}(\xi) Z'_{\delta\beta}(\xi)\right] \tag{D.66}
$$

$$
Z'(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\beta\widetilde{\gamma\delta}}\left[W'_{\gamma\alpha}(\xi) Z'_{\delta\beta}(\xi) + Z'_{\gamma\alpha}(\xi) W'_{\delta\beta}(\xi)\right] \tag{D.67}
$$

For the remaining term in the two-body contribution, we use Eqs. (D.61) and (D.56) to write[2]

$$
\begin{aligned}
\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}} T_{\alpha\bar{\beta}}(\varphi,\varphi') Y_{\bar{\delta}\gamma}(\varphi,\varphi') &= e^{2i\xi}\sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}}\left[W^{(+)}_{\beta\alpha}(\xi)+iZ^{(+)}_{\beta\alpha}(\xi)\right] \\
&\quad\times\left[W^{(-)}_{\gamma\delta}(\xi)+iZ^{(-)}_{\gamma\delta}(\xi)\right] \\
&= e^{2i\xi}\left[W^{(\pm)}(\xi)+iZ^{(\pm)}(\xi)\right]
\end{aligned}
$$

where we have defined

$$
W^{(\pm)}(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}}\left[W^{(+)}_{\beta\alpha}(\xi) W^{(-)}_{\gamma\delta}(\xi) - Z^{(+)}_{\beta\alpha}(\xi) Z^{(-)}_{\gamma\delta}(\xi)\right] \tag{D.68}
$$

$$
Z^{(\pm)}(\xi) \equiv \sum_{\alpha\beta\gamma\delta} V^{q'}_{\alpha\bar{\beta}\widetilde{\gamma\bar{\delta}}}\left[W^{(+)}_{\beta\alpha}(\xi) Z^{(-)}_{\gamma\delta}(\xi) + Z^{(+)}_{\beta\alpha}(\xi) W^{(-)}_{\gamma\delta}(\xi)\right] \tag{D.69}
$$

[2] The sign in Eq. (D.56) does not appear because the order of indices is reversed in $Y_{\bar{\delta}\gamma}(\varphi,\varphi')$.

We are now ready to combine all the terms and project onto particle number for the Hamiltonian matrix elements,

$$\begin{aligned}\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} \hat{H} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, \mathrm{Re} \Big\{ & e^{-i\xi N} n(\xi)\, e^{i\Omega(\xi)} \\ & \times \Big\{ e^{2i\xi} \left[ W^{(0)}(\xi) + iZ^{(0)}(\xi) \right] \\ & + \frac{e^{4i\xi}}{2} \left[ W'(\xi) + iZ'(\xi) \right] \\ & + \frac{e^{2i\xi}}{4} \left[ W^{(\pm)}(\xi) + iZ^{(\pm)}(\xi) \right] \Big\} \Big\}\end{aligned}$$

We can then define

$$\begin{aligned}n_H(\xi)\, e^{i\Omega_H(\xi)} \equiv e^{2i\xi} \left[ W^{(0)}(\xi) + iZ^{(0)}(\xi) \right] + \frac{e^{4i\xi}}{2} \left[ W'(\xi) + iZ'(\xi) \right] \\ + \frac{e^{2i\xi}}{4} \left[ W^{(\pm)}(\xi) + iZ^{(\pm)}(\xi) \right]\end{aligned} \quad \text{(D.70)}$$

and obtain finally

$$\begin{aligned}\left\langle \Phi_q^{(p)} \left| P_q^{(N)\dagger} \hat{H} P_{q'}^{(N)} \right| \Phi_{q'}^{(p)} \right\rangle = \frac{1}{\pi} \left( \prod_{\mu>0} u_\mu^q u_\mu^{q'} \right) \int_0^\pi d\xi \, n(\xi)\, n_H(\xi) \\ \times \cos\left[ \Omega(\xi) + \Omega_H(\xi) - N\xi \right]\end{aligned} \quad \text{(D.71)}$$

which can be evaluated numerically.

# References

1. Q. Haider and D. Gogny, J. Phys. G 18, 993 (1992).

## Appendix E
# Symmetric Ordered Products of Operators

# .1 Pedestrian derivation of the SME

## *.1.1 Basic formula*

Consider the integral

$$N(q) = \int_{-\infty}^{\infty} dq'\, N(q, q')\, f(q')$$

We change integration variable to $s = q - q'$,

$$N(q) = \int_{-\infty}^{\infty} ds\, N(q, q-s)\, f(q-s)$$

We expand $f(q-s)$ about $q$,

$$f(q-s) = \sum_{m=0}^{\infty} \frac{(-1)^m s^m}{m!} f^{(m)}(q)$$

and we expand

$$g(q) \equiv N(q, q-s)$$

about $q + s/2$,

$$\begin{aligned} g(q) &= g\left(q + \frac{s}{2} - \frac{s}{2}\right) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n s^n}{2^n n!} g^{(n)}\left(q + \frac{s}{2}\right) \\ &= \sum_{n=0}^{\infty} \frac{(-1)^n s^n}{2^n n!} N^{(n)}\left(q + \frac{s}{2}, q - \frac{s}{2}\right) \end{aligned}$$

Then we have

$$\begin{aligned} N(q) &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{2^n m! n!} f^{(m)}(q) \int_{-\infty}^{\infty} ds\, s^{m+n} N^{(n)}\left(q + \frac{s}{2}, q - \frac{s}{2}\right) \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(-1)^{m+n}}{2^n m! n!} \left[\frac{\partial^m}{\partial q^m} f(q)\right] \left[\frac{\partial^n}{\partial q^n} \int_{-\infty}^{\infty} ds\, s^{m+n} N\left(q + \frac{s}{2}, q - \frac{s}{2}\right)\right] \end{aligned}$$

Next, we gather terms with the same value of $m + n$. For this we define$p = m + n$ and write

$$\begin{aligned}
N(q) &= \sum_{p=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \delta_{m+n,p} \frac{(-1)^{m+n}}{2^n m! n!} \\
&\quad \times \left[\frac{\partial^m}{\partial q^m} f(q)\right] \left[\frac{\partial^n}{\partial q^n} \int_{-\infty}^{\infty} ds\, s^{m+n} N\left(q+\frac{s}{2}, q-\frac{s}{2}\right)\right] \\
&= \sum_{p=0}^{\infty} \sum_{m=0}^{p} \frac{(-1)^p}{2^{p-m} m! (p-m)!} \\
&\quad \times \left[\frac{\partial^m}{\partial q^m} f(q)\right] \left[\frac{\partial^{p-m}}{\partial q^{p-m}} \int_{-\infty}^{\infty} ds\, s^{p} N\left(q+\frac{s}{2}, q-\frac{s}{2}\right)\right] \\
&= \sum_{p=0}^{\infty} \frac{1}{p!} \frac{1}{2^p} \sum_{m=0}^{p} 2^m \binom{p}{m} \\
&\quad \times \left[i^m \frac{\partial^m}{\partial q^m} f(q)\right] \left[i^{p-m} \frac{\partial^{p-m}}{\partial q^{p-m}} i^p \int_{-\infty}^{\infty} ds\, s^{p} N\left(q+\frac{s}{2}, q-\frac{s}{2}\right)\right]
\end{aligned}$$

We then define

$$\hat{P} \equiv i \frac{\partial}{\partial q}$$

and

$$N_p(q) \equiv i^p \int_{-\infty}^{\infty} ds\, s^p N\left(q+\frac{s}{2}, q-\frac{s}{2}\right)$$

and

$$\left[N_p(q)\, \hat{P}\right]^{(p)} f(q) \equiv \frac{1}{2^p} \sum_{m=0}^{p} 2^m \binom{p}{m} \left[\hat{P}^m f(q)\right] \left[\hat{P}^{p-m} N_p(q)\right] \qquad (.1)$$

so that

$$N(q) = \sum_{p=0}^{\infty} \frac{1}{p!} \left[N_p(q)\, \hat{P}\right]^{(p)}$$

We can check these results against for example the operator form in Eq. (3.180) for the order-2 case. From Eq. (3.180) we have

$$\begin{aligned}
\left[N^{(2)}(q)\,\hat{P}\right]^{(2)} f(q) &\equiv \frac{1}{2^2}\sum_{k=0}^{2}\binom{2}{k}\hat{P}^{2-k}N^{(2)}(q)\,\hat{P}^k f(q) \\
&= \frac{1}{4}\left\{\hat{P}^2 N^{(2)}(q) + 2\hat{P}N^{(2)}(q)\,\hat{P} + N^{(2)}(q)\,\hat{P}^2\right\} f(q) \\
&= \frac{1}{4}\left\{2^0 \times \left[\hat{P}^2 N^{(2)}(q)\right] + 2^1 \times 2\left[\hat{P}N^{(2)}(q)\right]\hat{P}\right. \\
&\quad \left. +2^2 \times N^{(2)}(q)\,\hat{P}^2\right\} f(q)
\end{aligned}$$

where the square brackets have been added to make it clear that the operator $\hat{P}$ only acts within the brackets. Also the $2^m$ factor, which appears in Eq. (.1) also appears here after combining common terms.

### *.1.2 Derivatives of SOPOs*

We derive a compact expression for

$$\begin{aligned}
\hat{P}^m\left\{\left[A(q)\,\hat{P}\right]^{(n)} f(q)\right\} &= \hat{P}^m \frac{1}{2^n}\sum_{k=0}^{n} 2^k \binom{n}{k}\left[\hat{P}^k f(q)\right]\left[\hat{P}^{n-k}A(q)\right] \\
&= \frac{1}{2^n}\sum_{k=0}^{n} 2^k \binom{n}{k}\sum_{l=0}^{m}\binom{m}{l} \\
&\quad \times \left[\hat{P}^{k+l} f(q)\right]\left[\hat{P}^{m+n-(k+l)}A(q)\right] \\
&= \frac{1}{2^n}\sum_{r=0}^{\infty}\left[\sum_{k=0}^{n} 2^k \binom{n}{k}\binom{m}{r-k}\right] \\
&\quad \times \left[\hat{P}^r f(q)\right]\left[\hat{P}^{m+n-r}A(q)\right]
\end{aligned}$$

Next, we wish to simplify the coefficient

$$C_{m,n,r} \equiv \sum_{k=0}^{n} 2^k \binom{n}{k}\binom{m}{r-k}$$

We use Mathematica to simplify this sum. If $m+1-r>0$, then

$$C_{m,n,r} = \binom{m}{r}\,{}_2F_1\left(-n,-r;m+1-r;2\right)$$

Otherwise, if $m+1-r \leq 0$,

$$C_{m,n,r} = 2^{r-m}\binom{n}{r-m}\,{}_2F_1\left(-m,-m-n-r;1-m+r;2\right)$$

In either case,

$$\boxed{\hat{P}^m \left\{ \left[ A(q)\,\hat{P} \right]^{(n)} f(q) \right\} = \frac{1}{2^n} \sum_{r=0}^{\infty} C_{m,n,r} \left[ \hat{P}^r f(q) \right] \left[ \hat{P}^{m+n-r} A(q) \right]} \quad (.2)$$

For example, for $m = 0$, we find for $r = 0$

$$C_{0,n,0} = 1$$

and for $r > 0$,

$$\begin{aligned} C_{0,n,r} &= 2^{r-m} \binom{n}{r-m} {}_2F_1(-m, -m-n-r; 1-m+r; 2) \\ &= 2^r \binom{n}{r} {}_2F_1(0, -n-r; 1+r; 2) \\ &= 2^r \binom{n}{r} \end{aligned}$$

and therefore,

$$\begin{aligned} \hat{P}^0 \left\{ \left[ A(q)\,\hat{P} \right]^{(n)} f(q) \right\} &= \frac{1}{2^n} \sum_{r=0}^{\infty} 2^r \binom{n}{r} \left[ \hat{P}^r f(q) \right] \left[ \hat{P}^{n-r} A(q) \right] \\ &= \left[ A(q)\,\hat{P} \right]^{(n)} f(q) \end{aligned}$$

as expected.

### .1.2.1 Properties of the coefficient $C_{m,n,r}$

We recall the definition,

$$C_{m,n,r} \equiv \sum_{k=0}^{n} 2^k \binom{n}{k} \binom{m}{r-k}$$

which reduces to

$$C_{m,n,r} = \begin{cases} \binom{m}{r} {}_2F_1(-n, -r; m+1-r; 2) & m+1-r > 0 \\ 2^{r-m} \binom{n}{r-m} {}_2F_1(-m, -m-n-r; 1-m+r; 2) & m+1-r \leq 0 \end{cases}$$

Therefore we always have

$$C_{m,n,0} = \sum_{k=0}^{n} 2^k \binom{n}{k} \binom{m}{-k}$$

or,

$$\boxed{C_{m,n,0} = 1}$$

### .1.3 Useful identities for SOPOs

First, for a generic operator $A$ we write

$$\hat{P}A = A^{(1)} + A\hat{P}$$

or,

$$\boxed{A^{(1)} = \left[\hat{P}, A\right]} \tag{.3}$$

Be careful not to confuse notations:

$$\begin{aligned} A^{(1)} &= \left(\hat{P}A\right) \\ &\neq \hat{P}A \end{aligned}$$

In general, we can show by induction

$$\hat{P}^s A = \sum_{k=0}^{s} \binom{s}{k} A^{(s-k)} \hat{P}^k \tag{.4}$$

For a generic operator $A$ and and integers $m \geq 0$ and $n \geq 0$ we next show that

$$\left(A\hat{P}^{(m)}\right)^{(n)} = A^{(n)} \hat{P}^{(m)}$$

We show this first for $n = 0$:

$$\begin{aligned} \left(A\hat{P}^{(m)}\right)^{(0)} &= A\hat{P}^{(m)} \\ &= A^{(0)} \hat{P}^{(m)} \end{aligned}$$

Next, we show that if the identity is true for $n$, then it is also true for $n+1$ by using Eq. (.3) to calculate

$$
\begin{aligned}
\left(A\hat{P}^{(m)}\right)^{(n+1)} &= \left(\left(A\hat{P}^{(m)}\right)^{(n)}\right)^{(1)} \\
&= \hat{P}\left(A^{(n)}\hat{P}^{(m)}\right) - \left(A^{(n)}\hat{P}^{(m)}\right)\hat{P} \\
&= A^{(n+1)}\hat{P}^{(m)}
\end{aligned}
$$

Therefore, by induction, we deduce

$$
\boxed{\left(A\hat{P}^{(m)}\right)^{(n)} = A^{(n)}\hat{P}^{(m)}} \tag{.5}
$$

Next, we show that

$$
\left(\hat{P}^{(m)}A\right)^{(n)} = \hat{P}^{(m)}A^{(n)}
$$

Again, we start with the $n = 0$ case,

$$
\begin{aligned}
\left(\hat{P}^{(m)}A\right)^{(0)} &= \hat{P}^{(m)}A \\
&= \hat{P}^{(m)}A^{(0)}
\end{aligned}
$$

Next, we show that if the identity is true for $n$, then it is also true for $n+1$ by using Eq. (.3) to calculate

$$
\begin{aligned}
\left(\hat{P}^{(m)}A\right)^{(n+1)} &= \left(\left(\hat{P}^{(m)}A\right)^{(n)}\right)^{(1)} \\
&= \hat{P}\left(\hat{P}^{(m)}A^{(n)}\right) - \left(\hat{P}^{(m)}A^{(n)}\right)\hat{P} \\
&= \hat{P}^{(m)}A^{(n+1)}
\end{aligned}
$$

Then, by induction, we deduce

$$
\boxed{\left(\hat{P}^{(m)}A\right)^{(n)} = \hat{P}^{(m)}A^{(n)}} \tag{.6}
$$

Next we show that

$$
A\hat{P}^{(n)} = \sum_{m=0}^{n} (-1)^{n-m} \binom{n}{m} \hat{P}^m A^{(n-m)}
$$

First we show this for $n = 0$. Trivially the LHS is

$$
A\hat{P}^{(0)} = A
$$

while the RHS is

$$\sum_{m=0}^{0}(-1)^{0-m}\binom{0}{m}\hat{P}^m A^{(0-m)} = A$$

as well. Then we assume the identity is true for $n$ and deduce its validity for $n+1$ by calculating

$$A\hat{P}^{(n+1)} = \left[\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^m A^{(n-m)}\right]\hat{P}$$

We then use Eq. (.3) to write

$$\begin{aligned} A\hat{P}^{(n+1)} = &\left[\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m+1} A^{(n-m)}\right] \\ &-\left(\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m} A^{(n-m)}\right)^{(1)} \end{aligned}$$

and using Eq. (.6) in the second term, this becomes

$$\begin{aligned} A\hat{P}^{(n+1)} &= \sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m+1} A^{(n-m)} \\ &\quad -\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m} A^{(n-m+1)} \\ &= \sum_{m=1}^{n+1}(-1)^{n-m+1}\binom{n}{m-1}\hat{P}^{m} A^{(n-m+1)} \\ &\quad -\sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m} A^{(n-m+1)} \\ &= \sum_{m=0}^{n+1}(-1)^{n+1-m}\left[\binom{n}{m-1}+\binom{n}{m}\right]\hat{P}^{m} A^{(n+1-m)} \end{aligned}$$

We can then use Pascal's rule for the binomial coefficients to write

$$A\hat{P}^{(n+1)} = \sum_{m=0}^{n+1}(-1)^{n+1-m}\binom{n+1}{m}\hat{P}^{m} A^{(n+1-m)}$$

which proves the induction step. Therefore we have established

$$\boxed{A\hat{P}^{(n)} = \sum_{m=0}^{n}(-1)^{n-m}\binom{n}{m}\hat{P}^{m} A^{(n-m)}} \tag{.7}$$

Returning to SOPOs, we show that

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \left[B^{(s)}\hat{P}\right]^{(q)}$$

To prove this, we write

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \left(\frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\hat{P}^{q-i}B\hat{P}^{i}\right)^{(s)}$$

Using Eq. (.5), this becomes

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\left(\hat{P}^{q-i}B\right)^{(s)}\hat{P}^{i}$$

and using Eq. (.6), this reduces to

$$\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \frac{1}{2^q}\sum_{i=0}^{q}\binom{q}{i}\hat{P}^{q-i}B^{(s)}\hat{P}^{i}$$

or,

$$\boxed{\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)} = \left[B^{(s)}\hat{P}\right]^{(q)}} \tag{.8}$$

Next, we simplify the expression for

$$A\left[B\hat{P}\right]^{(q)} = A\frac{1}{2^q}\sum_{s=0}^{q}\binom{q}{s}\hat{P}^{q-s}B\hat{P}^{s}$$

Using Eq. (.7), we write

$$\begin{aligned} A\left[B\hat{P}\right]^{(q)} &= \frac{1}{2^q}\sum_{s=0}^{q}\binom{q}{s}\left[\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q-s}{m}\hat{P}^{m}A^{(q-s-m)}\right]B\hat{P}^{s} \\ &= \frac{1}{2^q}\sum_{s=0}^{q}\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q}{s}\binom{q-s}{m}\hat{P}^{m}A^{(q-s-m)}B\hat{P}^{s} \end{aligned}$$

We introduce an index $t = q - s - m$, and use it to eliminate the sum over $m$,

$$A\left[B\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{t=0}^{\infty}\delta_{t,q-s-m}\sum_{s=0}^{q}\sum_{m=0}^{q-s}(-1)^{q-s-m}\binom{q}{s}\binom{q-s}{m}$$
$$\times\hat{P}^m A^{(q-s-m)}B\hat{P}^s$$
$$= \frac{1}{2^q}\sum_{t=0}^{\infty}\sum_{s=0}^{q}(-1)^t\binom{q}{s}\binom{q-s}{q-s-t}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s$$

The product of the two binomial coefficients can be re-written

$$A\left[B\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{t=0}^{\infty}\sum_{s=0}^{q}(-1)^t\binom{q}{t}\binom{q-t}{s}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s$$
$$= \frac{1}{2^q}\sum_{t=0}^{q}(-1)^t\binom{q}{t}\left[\sum_{s=0}^{q-t}\binom{q-t}{s}\hat{P}^{q-s-t}A^{(t)}B\hat{P}^s\right]$$

Using Eq. (3.180), the term in brackets can be written as a SOPO, and we get

$$A\left[B\hat{P}\right]^{(q)} = \frac{1}{2^q}\sum_{t=0}^{q}(-1)^t\binom{q}{t}2^{q-t}\left[A^{(t)}B\hat{P}\right]^{(q-t)}$$

or,

$$\boxed{A\left[B\hat{P}\right]^{(q)} = \sum_{t=0}^{q}\left(-\frac{1}{2}\right)^t\binom{q}{t}\left[A^{(t)}B\hat{P}\right]^{(q-t)}} \tag{.9}$$

We can also show that

$$\left[A\hat{P}\right]^{(n)}B = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[AB^{(s)}P\right]^{(n-s)}$$

To prove this, we start with Eq. (3.180) and write

$$\left[A\hat{P}\right]^{(n)}B = \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\hat{P}^{n-r}A\hat{P}^rB$$

Then we use Eq. (.4),

$$\left[A\hat{P}\right]^{(n)}B = \frac{1}{2^n}\sum_{r=0}^{n}\binom{n}{r}\hat{P}^{n-r}A\sum_{i=0}^{r}\binom{r}{i}B^{(r-i)}P^i$$
$$= \frac{1}{2^n}\sum_{r=0}^{n}\sum_{i=0}^{r}\binom{n}{r}\binom{r}{i}\hat{P}^{n-r}AB^{(r-i)}P^i$$

We introduce the summing index $s = r - i$, and use it to replace the sum over $r$

$$\left[A\hat{P}\right]^{(n)} B = \frac{1}{2^n} \sum_{s=0}^{\infty} \sum_{r=0}^{n} \sum_{i=0}^{r} \binom{n}{r} \binom{r}{i} \delta_{s,r-i} \hat{P}^{n-r} A B^{(r-i)} P^i$$
$$= \frac{1}{2^n} \sum_{s=0}^{\infty} \sum_{i=0}^{n} \binom{n}{s+i} \binom{s+i}{i} \hat{P}^{n-s-i} A B^{(s)} P^i$$

Writing out the binomial coefficients in terms of factorials, we can readily show

$$\binom{n}{s+i} \binom{s+i}{i} = \binom{n}{s} \binom{n-s}{i}$$

so that

$$\left[A\hat{P}\right]^{(n)} B = \frac{1}{2^n} \sum_{s=0}^{\infty} \sum_{i=0}^{n} \binom{n}{s} \binom{n-s}{i} \hat{P}^{n-s-i} A B^{(s)} P^i$$
$$= \frac{1}{2^n} \sum_{s=0}^{n} \binom{n}{s} 2^{n-s} \frac{1}{2^{n-s}} \sum_{i=0}^{n} \binom{n-s}{i} \hat{P}^{n-s-i} A B^{(s)} P^i$$

and using Eq. (3.180) again, we can write this as

$$\boxed{\left[A\hat{P}\right]^{(n)} B = \sum_{s=0}^{n} \frac{1}{2^s} \binom{n}{s} \left[A B^{(s)} P\right]^{(n-s)}} \tag{.10}$$

Next, we show that

$$\left[\left[A\hat{P}\right]^{(n)} \hat{P}\right]^{(q)} = \left[A\hat{P}\right]^{(n+q)}$$

Using Eq. (3.180) we write

$$\left[\left[A\hat{P}\right]^{(n)} \hat{P}\right]^{(q)} = \frac{1}{2^q} \sum_{i=0}^{q} \binom{q}{i} \hat{P}^{q-i} \left[A\hat{P}\right]^{(n)} \hat{P}^i$$

and use Eq. (3.180) again to write

$$\left[\left[A\hat{P}\right]^{(n)} \hat{P}\right]^{(q)} = \frac{1}{2^q} \sum_{i=0}^{q} \binom{q}{i} \hat{P}^{q-i} \left[\frac{1}{2^n} \sum_{j=0}^{n} \binom{n}{j} \hat{P}^{n-j} A \hat{P}^j\right] \hat{P}^i$$
$$= \frac{1}{2^{n+q}} \sum_{i=0}^{q} \sum_{j=0}^{n} \binom{q}{i} \binom{n}{j} \hat{P}^{q-i+n-j} A \hat{P}^{i+j}$$

We introduce a new summation index $s = i + j$ and use it to replace the summation over $j$,

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^{n+q}}\sum_{s=0}^{\infty}\delta_{s,i+j}\sum_{i=0}^{q}\sum_{j=0}^{n}\binom{q}{i}\binom{n}{j}\hat{P}^{q-i+n-j}A\hat{P}^{i+j}$$
$$= \frac{1}{2^{n+q}}\sum_{s=0}^{n+q}\sum_{i=0}^{s}\binom{q}{i}\binom{n}{s-i}\hat{P}^{q+n-s}A\hat{P}^{s}$$

Where the sum over $s$ stops at $n+q$ since that is the largest possible value of $i+j$, and the upper limit of the sum over $i$ has been changed to $s$ since the maximum value of $s$ is $n+q$, which includes $q$. The sum over $i$ can be further simplified using the Chu-Vandermonde identity,

$$\sum_{i=0}^{s}\binom{q}{i}\binom{n}{s-i} = \binom{n+q}{s}$$

Therefore,

$$\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \frac{1}{2^{n+q}}\sum_{s=0}^{n+q}\binom{n+q}{s}\hat{P}^{q+n-s}A\hat{P}^{s}$$

Using Eq. (3.180) one final time, we get

$$\boxed{\left[\left[A\hat{P}\right]^{(n)}\hat{P}\right]^{(q)} = \left[A\hat{P}\right]^{(n+q)}} \qquad (.11)$$

### .1.4 Composition of two SOPOs

We use Eq. (.10) to write

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[A\left(\left[B\hat{P}\right]^{(q)}\right)^{(s)}P\right]^{(n-s)}$$

and use Eq. (.8),

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\left[A\left[B^{(s)}\hat{P}\right]^{(q)}P\right]^{(n-s)}$$

Next, we use Eq. (.9),

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\frac{1}{2^s}\binom{n}{s}\sum_{t=0}^{q}\left(-\frac{1}{2}\right)^{t}\binom{q}{t}\left[\left[A^{(t)}B^{(s)}\hat{P}\right]^{(q-t)}P\right]^{(n-s)}$$

Using Eq. (.11), this becomes

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{s=0}^{n}\sum_{t=0}^{q}\frac{(-1)^{t}}{2^{s+t}}\binom{n}{s}\binom{q}{t}\left[A^{(t)}B^{(s)}\hat{P}\right]^{(n+q-s-t)}$$

At this point, we introduce a new summation variable $i = s + t$, and use it to eliminate the sum over $t$:

$$\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} &= \sum_{i=0}^{\infty}\delta_{i,s+t}\sum_{s=0}^{n}\sum_{t=0}^{q}\frac{(-1)^{t}}{2^{s+t}}\binom{n}{s}\binom{q}{t}\left[A^{(t)}B^{(s)}\hat{P}\right]^{(n+q-s-t)}\\ &= \sum_{i=0}^{\infty}\sum_{s=0}^{n}\frac{(-1)^{i-s}}{2^{i}}\binom{n}{s}\binom{q}{i-s}\left[A^{(i-s)}B^{(s)}\hat{P}\right]^{(n+q-i)}\end{aligned}$$

To complete the derivation, we give more stringent limits for the summation indices $i$ and $s$. The binomial coefficients impose the conditions

$$\begin{aligned}0 \leq \quad s \quad &\leq n\\ 0 \leq i - s &\leq q\end{aligned}$$

Thus we have

$$i \leq s + q \leq n + q$$

while for $s$, we have the two inequality relations

$$\begin{aligned}0 \leq s &\leq n\\ i - q \leq s &\leq i\end{aligned}$$

which we can combine into a single one,

$$\max(0, i-q) \leq s \leq \min(i, n)$$

Therefore, we have shown

$$\boxed{\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)} = \sum_{i=0}^{n+q}\sum_{s=\max(0,i-q)}^{\min(i,n)}\frac{(-1)^{i-s}}{2^{i}}\binom{n}{s}\binom{q}{i-s}\\ \times\left[A^{(i-s)}B^{(s)}\hat{P}\right]^{(n+q-i)}\end{aligned}} \tag{.12}$$

which gives the composition of two SOPO's as a linear combination of SOPO's.

### *.1.5 Composition of three SOPO's*

Using Eq. (.12) we write

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)}=\left[A\hat{P}\right]^{(n)}\sum_{i=0}^{q+r}\sum_{s=\max(0,i-r)}^{\min(i,q)}\frac{(-1)^{i-s}}{2^i}\binom{q}{s}\binom{r}{i-s}\times\left[B^{(i-s)}C^{(s)}\hat{P}\right]^{(q+r-i)}$$

and we use Eq. (.12) again to write

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)}=\sum_{i=0}^{q+r}\sum_{s=\max(0,i-r)}^{\min(i,q)}\frac{(-1)^{i-s}}{2^i}\binom{q}{s}\binom{r}{i-s}\sum_{j=0}^{n+q+r-i}\sum_{t=\max(0,j-(q+r-i))}^{\min(j,n)}\frac{(-1)^{j-t}}{2^j}\binom{n}{t}\times\binom{q+r-i}{j-t}\left[A^{(j-t)}\left(B^{(i-s)}C^{(s)}\right)^{(t)}\hat{P}\right]^{(n+q+r-i-j)}$$

To simplify the notation, we collect all the terms that depend on $s$ into a single term

$$F\left(B,C,r,i,t\right)\equiv\sum_{s=\max(0,i-r)}^{\min(i,q)}(-1)^s\binom{q}{s}\binom{r}{i-s}\left(B^{(i-s)}C^{(s)}\right)^{(t)} \qquad (.13)$$

so that

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)}=\sum_{i=0}^{q+r}\frac{(-1)^i}{2^i}\sum_{j=0}^{n+q+r-i}\sum_{t=\max(0,j-(q+r-i))}^{\min(j,n)}\frac{(-1)^{j-t}}{2^j}\times\binom{n}{t}\binom{q+r-i}{j-t}\times\left[A^{(j-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-i-j)}$$

Next, we introduce a sum over $p=i+j$ to eliminate the sum over $j$,

$$\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)} = \sum_{p=0}^{\infty}\sum_{i=0}^{q+r}\frac{(-1)^i}{2^i}\sum_{t=\max(0,p-(q+r))}^{\min(p-i,n)}\frac{(-1)^{p-i-t}}{2^{p-i}}\binom{n}{t}$$
$$\times\binom{q+r-i}{p-i-t}\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}$$
$$= \sum_{p=0}^{\infty}\sum_{i=0}^{q+r}\frac{(-1)^p}{2^p}\sum_{t=\max(0,p-(q+r))}^{\min(p-i,n)}(-1)^t\binom{n}{t}$$
$$\times\binom{q+r-i}{p-i-t}\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}$$

To complete the derivation, we give more stringent limits for the summation indices $p$ and $i$. From the binomial coefficients we see that

$$i \leq q+r$$

but also

$$i \leq p-t \leq p$$

and therefore,

$$i \leq \min\left(p, q+r\right)$$

Finally,

$$p-i-t \leq q+r-i$$
$$\Rightarrow p \leq q+r+t$$

but since $t \leq n$, then we must have

$$p \leq q+r+n$$

In summary, we have shown

$$\boxed{\begin{aligned}\left[A\hat{P}\right]^{(n)}\left[B\hat{P}\right]^{(q)}\left[C\hat{P}\right]^{(r)} = &\sum_{p=0}^{n+q+r}\sum_{i=0}^{\min(p,q+r)}\frac{(-1)^p}{2^p}\sum_{t=\max(0,p-q-r)}^{\min(p-i,n)}(-1)^t\\ &\times\binom{n}{t}\binom{q+r-i}{p-i-t}\\ &\times\left[A^{(p-i-t)}F\left(B,C,r,i,t\right)\hat{P}\right]^{(n+q+r-p)}\end{aligned}} \tag{.14}$$

which gives the composition of three SOPO's as a linear combination of SOPO's.

### .1.5.1 Special cases

We derive here Eqs. (A5) and (A6) in [1]. Using Eq. (.14) with $n = r = 0$ and $q = 1$ we get

$$\begin{aligned} A\left[B\hat{P}\right]^{(1)} C &= \sum_{p=0}^{1}\sum_{i=0}^{p} \frac{(-1)^p}{2^p}\binom{1-i}{p-i}\left[A^{(p-i)}F\left(B,C,0,i,0\right)\hat{P}\right]^{(1-p)} \\ &= \left[AF\left(B,C,0,0,0\right)\hat{P}\right]^{(1)} - \frac{1}{2}\left\{A^{(1)}F\left(B,C,0,0,0\right)\right. \\ &\quad \left. +AF\left(B,C,0,1,0\right)\right\} \end{aligned}$$

Now, using Eq. (.13),

$$F\left(B,C,0,i,0\right) = (-1)^i\binom{q}{i}BC^{(i)}$$

and in particular,

$$F\left(B,C,0,0,0\right) = BC$$

and

$$F\left(B,C,0,1,0\right) = -BC^{(1)}$$

and therefore

$$\boxed{A\left[B\hat{P}\right]^{(1)} C = \left[ABC\hat{P}\right]^{(1)} + \frac{1}{2}\left(ABC^{(1)} - A^{(1)}BC\right)} \tag{.15}$$

Next, using Eq. (.14) with $n = r = 0$ and $q = 2$ we get

$$\begin{aligned} A\left[B\hat{P}\right]^{(2)} C &= \sum_{p=0}^{2}\sum_{i=0}^{p} \frac{(-1)^p}{2^p}\binom{2-i}{p-i}\left[A^{(p-i)}F\left(B,C,0,i,0\right)\hat{P}\right]^{(2-p)} \\ &= \left[AF\left(B,C,0,0,0\right)\hat{P}\right]^{(2)} - \frac{1}{2}\left\{2\left[A^{(1)}F\left(B,C,0,0,0\right)\hat{P}\right]^{(1)}\right. \\ &\quad \left. + \left[AF\left(B,C,0,1,0\right)\hat{P}\right]^{(1)}\right\} + \frac{1}{4}\left\{A^{(2)}F\left(B,C,0,0,0\right)\right. \\ &\quad \left. +A^{(1)}F\left(B,C,0,1,0\right) + AF\left(B,C,0,2,0\right)\right\} \end{aligned}$$

or,

$$\boxed{\begin{aligned} A\left[B\hat{P}\right]^{(2)}C = \left[ABC\hat{P}\right]^{(2)} &+ \left[\left(ABC^{(1)} - A^{(1)}BC\right)\hat{P}\right]^{(1)} \\ &+ \frac{1}{4}\left(A^{(2)}BC - 2A^{(1)}BC^{(1)} + ABC^{(2)}\right) \end{aligned}} \tag{.16}$$

Next, we look at the special case where

$$A = C = \frac{1}{\sqrt{N^{(0)}}}$$

Then, using Eq. (.15) we get

$$\frac{1}{\sqrt{N^{(0)}}}\left[B\hat{P}\right]^{(1)}\frac{1}{\sqrt{N^{(0)}}} = \left[\bar{B}\hat{P}\right]^{(1)} + \frac{i}{2}C^{(1)}\left(B, N^{(0)}\right) \tag{.17}$$

where

$$\begin{aligned} \bar{B} &\equiv \frac{1}{\sqrt{N^{(0)}}}B\frac{1}{\sqrt{N^{(0)}}} \\ C^{(1)}\left(B, N^{(0)}\right) &\equiv \frac{1}{\sqrt{N^{(0)}}}B\left(\frac{1}{\sqrt{N^{(0)}}}\right)' - \left(\frac{1}{\sqrt{N^{(0)}}}\right)'B\frac{1}{\sqrt{N^{(0)}}} \end{aligned}$$

Next, using Eq. (.16),

$$\begin{aligned} \frac{1}{\sqrt{N^{(0)}}}\left[B\hat{P}\right]^{(2)}\frac{1}{\sqrt{N^{(0)}}} = \left[\bar{B}\hat{P}\right]^{(2)} &+ \left[iC^{(1)}\left(B, N^{(0)}\right)\hat{P}\right]^{(1)} \\ &- C^{(2)}\left(B, N^{(0)}\right) \end{aligned} \tag{.18}$$

where

$$\begin{aligned} C^{(2)}\left(B, N^{(0)}\right) \equiv \frac{1}{4}\Bigg[&\left(\frac{1}{\sqrt{N^{(0)}}}\right)''B\frac{1}{\sqrt{N^{(0)}}} - 2\left(\frac{1}{\sqrt{N^{(0)}}}\right)'B\left(\frac{1}{\sqrt{N^{(0)}}}\right)' \\ &+ \frac{1}{\sqrt{N^{(0)}}}B\left(\frac{1}{\sqrt{N^{(0)}}}\right)''\Bigg] \end{aligned}$$

# References

1. R. Bernard, H. Goutte, D. Gogny, W. Younes, Phys. Rev. C 84, 044308 (2011).

## Appendix A

# Algorithm for the TDGCM in the Gaussian overlap approximation

The algorithm used in this manuscript for the time-dependent generator-coordinate method in the Gaussian overlap approximation was discussed in [1, 2], and continues to be improved upon [3]. We give the broad outline of the algorithm here for convenience, and direct the reader to [2] in particular for more details.

Table 2 gives the pseudocode for the main algorithm, and the Crank-Nicholson algorithm [2, 4] used to evolve the wave function in time is given in Table 3. The main algorithm in Table 2 begins by reading in the potential energy surface with zero-point energy corrections ($V(q_{20}, q_{30})$, if the HFB calculations are constrained by the quadrupole and octupole moments, for example) in step 1 and the components of the inertia tensor ($B_{22}(q_{20}, q_{30})$, $B_{23}(q_{20}, q_{30})$, $B_{33}(q_{20}, q_{30})$) in step 2. The collective Hamiltonian on the discretized $(q_{20}, q_{30})$ grid, $K(q_{20}, q_{30})$, is constructed in step 3. The construction of $K(q_{20}, q_{30})$ involves replacing the derivatives in the expression for the collective Hamiltonian (see section 3.2.1),

$$H_{\mathrm{coll}} = -\frac{\hbar^2}{2} \sum_{i,j=2}^{3} \frac{\partial}{\partial q_{i0}} B_{ij}(q_{20}, q_{30}) \frac{\partial}{\partial q_{i0}} + V(q_{20}, q_{30}) \tag{A.1}$$

with their finite difference approximations. Explicit expressions for $K(q_{20}, q_{30})$ can be found in the appendix of [2]. The initial wave function, $g(t=0)$, usually generated by the solution to the static GCM equation, is read into memory in step 4. At this point, the time evolution loop of the TDGCM algorithm begins. At each time increment $\Delta t$, the Crank-Nicholson algorithm given in Table 3 is applied to evolve $g(t)$ into $g(t+\Delta t)$ at step 6. In order to avoid reflections of the wave function at the far end of the $(q_{20}, q_{30})$ grid (i.e., at very large values of $q_{20}$) the wave function $g(t+\Delta t)$ is multiplied by a damping damping factor with a Woods-Saxon form (see, e.g., Eq. (24) in [2]) in step 7. The loop repeats until the user-supplied termination time $t_{\mathrm{max}}$.

**Algorithm 2** pseudocode for the TDGCM algorithm.

```
1: Read PES
2: Read inertia tensor
3: Construct collective Hamiltonian K
4: Read initial wave function
5: for t = 0 to t_max by Δt do
6:     Apply Crank-Nicholson algorithm to wave function
7:     Damp wave function
8: end for
```

**Algorithm 3** Crank-Nicholson algorithm.

Initialize wave function gn0 $\leftarrow g(t)$
**repeat**
    gn1 $\leftarrow g(t) - \frac{i\Delta t}{2\hbar} K g(t) - \frac{i\Delta t}{2\hbar} K\mathrm{gn0}$
    $\epsilon \leftarrow \sup|\mathrm{gn1} - \mathrm{gn0}|$
    gn0 $\leftarrow$ gn1
**until** $\epsilon > \epsilon_{\mathrm{max}}$ or too many iterations

# References


1. J. F. Berger, M. Girod, and D. Gogny, Comp. Phys. Comm. 63, 365 (1991).
2. H. Goutte, J. F. Berger, P. Casoli, and D. Gogny, Phys. Rev. C 71, 024316 (2005).
3. D. Regnier, N. Dubray, M. Verrière, and N. Schunck, Comp. Phys. Comm. 225, 180 (2018).
4. W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, “Numerical Recipes: The Art of Scientific Computing”, Cambridge University Press, Cambridge, 1992.

Appendix B
# Mathematica script for calculating the coefficients of the Schrodinger-like equation

The following Mathematica (Wolfram Research [1]) script implements the SOPO algebra used to simplify expressions in chapter 3.

```
Unprotect[NonCommutativeMultiply];
(* zero element *)
0**A_ := 0; A_**0 := 0;
(* unit element *)
1**A_ := A; A_**1 := A;
(* distributivity *)
A_**(B_+C_) := A**B + A**C; (B_+C_)**A_ := B**A + C**A;
(* product with a scalar *)
number3Q[x_,y_,n_] := NumberQ[x]&&NumberQ[y]&&NumberQ[n
    ];
A_**(B_(x_.y_^n_./;number3Q[x,y,n])) := ((x*y^n)A**B);
    (A_(x_.y_^n_./;number3Q[x,y,n]))**B_ := ((x*y^n)A**B
    );
(* Composition of three SOPO's *)
sopo[n_][A_]**sopo[q_][B_]**sopo[r_][C_] := Module[ {
    i,imax,p,t,tmin,tmax,F,s,smin,smax,val}, val = 0;
For[p = 0, p <= n+q+r, p++,
      imax = Min[p,q+r];
      For[i = 0, i <= imax, i++,
        tmin = Max[0,p-q-r];
        tmax = Min[p-i,n];
        For[t = tmin, t <= tmax, t++,
          F = 0;
          smin = Max[0,i-r];
          smax = Min[i,q];
          For[s = smin, s <= smax, s++,
            F += I^(i+t)*(-1)^s*Binomial[q,s]*Binomial[r,
                i-s]*Derivative[t][Derivative[i-s][B]**
                Derivative[s][C]];          ];
          val += I^(p-i-t)*(-1)^(p+t)/2^p*Binomial[n,t]*
              Binomial[q+r-i,p-i-t]*sopo[n+q+r-p][
              Derivative[p-i-t][A]**F];          ];
      ];
   ];
   val ];
(* Composition of two SOPO's *)
sopo[n_][A_]**sopo[q_][B_] := Module[ {i,s,smin,smax,
    val}, val = 0; For[i = 0, i <= n+q, i++,
    smin = Max[0,i-q]; smax = Min[i,n]; For[s =
    smin, s <= smax, s++, val += I^i*(-1)^(i-s)/2^
    i*Binomial[n,s]*Binomial[q,i-s]*sopo[n+q-i][
    Derivative[i-s][A]**Derivative[s][B]]; ]; ];
   val ];
```

```
Protect[NonCommutativeMultiply];
(* Derivatives of SOPO's *)
Unprotect[Derivative];
Derivative[q_][sopo[n_][A_]] := I^q*sopo[n][Derivative[
    q][A]];
Unprotect[NonCommutativeMultiply];
Derivative[q_][A_**B_] := Sum[Binomial[q,i]*Derivative[
    i][A]**Derivative[q-i][B],{i,0,q}];
Protect[NonCommutativeMultiply];
Protect[Derivative];
(* Some additional identities for SOPO's *)
sopo[n_][0] := 0;
sopo[q_][sopo[n_][A_]] := sopo[n+q][A];
sopo[n_][A_+B_] := sopo[n][A] + sopo[n][B];
sopo[q_][(x_.y_^n_./;number3Q[x,y,n])A_] := (x*y^n)sopo
    [q][A];
getcoeff[n_,expr_] := Module[    {terml,terml1,terml2,
    terml3,outl},     terml = Cases[expr,x_.sopo[n][A_]:>{
    x,A}];
  terml1 = Cases[terml,{_,A_/;FreeQ[A,_**_]}];     terml2
      = Cases[terml,{_,A_**B_/;(FreeQ[A,_**_]&&FreeQ[B,
      _**_])}];     terml3 = Cases[terml,{_,A_**B_**X_/;(
      FreeQ[A,_**_]&&FreeQ[B,_**_]&&FreeQ[X,_**_])}];
  outl = terml1;     ];
(*****)
jop = 1 + sopo[1][j1] + sopo[2][j2]; hop = sopo[0][h0]
    + sopo[1][h1] + sopo[2][h2];
res = jop**hop**jop;
res1 = res; res1 = res1/.(sopo[n_][_]/;n>=3)->0
res1 = Collect[Simplify[res1],sopo[_][_]];
coeff0 = Plus@@Cases[res1,x_.sopo[0][A_]:>(x)A]; coeff1
     = Plus@@Cases[res1,x_.sopo[1][A_]:>(x)A]; coeff2 =
    Plus@@Cases[res1,x_.sopo[2][A_]:>(x)A];
(* Rules for making the notation more compact using:
    CP[A,B] = AB + BA    CM[A,B] = AB - BA    CP[A,B,C] =
    ABC + CBA    CM[A,B,C] = ABC - CBA *)
compactify = { y_.A_**B_ + z_.B_**A_/;z == y :> (y)CP[A
    ,B], y_.A_**B_ + z_.B_**A_/;z == -y :> (y)CM[A,B],
    y_.A_**B_**F_ + z_.F_**B_**A_/;z == y :> (y)CP[A,B,F
    ], y_.A_**B_**F_ + z_.F_**B_**A_/;z == -y :> (y)CM[A
    ,B,F] };
coeffS = coeff0//.compactify; coeffT = coeff1//.
    compactify; coeffU = coeff2//.compactify;
```

# References

1. Wolfram Research, Inc., Mathematica Version 9.0, Wolfram Research Inc., Champaign, Illinois, 2012.