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COMPUTATION OF THE REACTION MATRIX, G*

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I. Definition and Some Properties of G

Brueckner's reaction operator[1] for the interaction of two identical Fermions in a medium of the same kind of Fermions is defined by

$$G(E_s) = v + v \frac{Q}{E_s - H^o} G(E_s). \qquad (1)$$

Here v is the two-body interaction, the Pauli operator Q forbids either Fermion from being scattered into a normally occupied single-particle (SP) state, and H^o is the unperturbed pair Hamiltonian

$$H^o(12) = T(1) + U(1) + T(2) + U(2),$$

where U is the SP potential which should be determined self-consistently in terms of G. In the early work the energy E_s was regarded as determined by the state (ket vector) on which G operated (to the right). Then, effectively, E_s is an operator, and in $G^+(E_s)$ E_s would have to operate to the left in order to avoid making the G-matrix non-Hermition.[2] This complication is removed and greater generality is attained by regarding E_s as a parameter held constant for all matrix elements. We thus deal with a continuous family of reaction operators, parametrized by the "starting energy",[3] E_s.

Brandow[4] has shown that the generalized-time-ordered form of perturbation theory for finite systems leads most directly to a non-Hermitian U. However, we shall assume that U is Hermitian, as it is in all shell-model and self-consistent field calculations known to us. The full interaction and Q are invariably Hermitian, so we expect that $G(E_s)$ is Hermitian. This is the case because Eq. (1) implies

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$$G(E_s) = v + v \frac{1}{Q(E_s - H^0 - v)Q} v \tag{2a}$$

$$= v + G(E_s) \frac{Q}{E_s - H^0} v \tag{2b}$$

and from Eq. (1) $G^+(E_s)$ also satisfies (2b). Thus, if

$$v^+ = v,\ Q^+ = Q,\ U^+ = U,\ E_s = \text{real parameter} \tag{3a}$$

then

$$G^+(E_s) = G(E_s). \tag{3b}$$

In the Moszkowski-Scott[5] separation method $v = v_s + v_\ell$ where the separation distance, d, dividing the short- from the long-ranged part of the interaction, depends on the state (ket vector) on which v acts. In G_s^+ (calculated from v_s) d would have to act to the left in order for G_s to be Hermitian. Alternatively, d may be regarded as a parameter.

Tobocman[6] has shown that basing many-body perturbation theory on a related reaction operator

$$\bar{G}(E_s) = (v - U_2) + (v - U_2) \frac{Q}{E_s - H^0} \bar{G}(E_s)$$

or on even more general ones, has certain formal advantages. But $\bar{G}$ would be more difficult to calculate than G because U_2 depends separately on r_1 and r_2, whereas v depends on r_{12}. Thus, although $\bar{G}$ has been discussed occasionally,[7] no calculations of it have been reported. Also, the Coulomb interaction is almost always omitted from v in Eq. (1) because its long range would cause calculational difficulties, and it can be treated adequately as a perturbation.

Initially the greatest problem in computing G had to do with the strong short-range repulsive core. But this was quickly overcome by several methods. Much of the remaining difficulty arises from the Pauli operator. In degenerate perturbation theory, in which the unperturbed ("model") wave function consists of more than one configuration, there are three classes of SP states: normally occupied or "hole" states (h) with model occupation numbers $n_h = 1$; "valence" or "active" states (v) with $0 \leq n_v \leq 1$; and normally empty or "particle" states (p) with $n_p = 0$. There is great latitude in the choice of the active subspace in which the shell-model diagonalizations are carried out.

In the non-degenerate (closed shell) theory, in which there are no valence SP states, the Pauli operator is defined by

$$Q^{ND}(12) = Q_1(1)Q_1(2) \quad , \quad Q_1 = \sum_p^{emp} |p><p|. \tag{4a}$$

We shall also define

$$P_1 = \sum_h^{occ} |h><h| = I_1 - Q_1 \tag{4b}$$

and

$$P^{ND}(12) = I(12) - Q^{ND}(12) = P_1(1)P_1(2) + P_1(1)Q_1(2) + Q_1(1)P_1(2). \tag{4c}$$

Q_1 and P_1 are Hermitian projection operators, i.e.

$$Q_1 = Q_1^+ = Q_1^2 \quad , \quad P_1 = P_1^+ = P_1^2 \tag{4d}$$

and these properties carry over to Q^{ND} and P^{ND}.

In the degenerate (open shell) theory with valence "particles" only (no valence holes) we let Q_1 and P_1 be defined as above, and

$$A_1 = \sum_{v_p}^{val.} |v_p><v_p| \tag{5a}$$

so that

$$P_1 + A_1 + Q_1 = I_1. \tag{5b}$$

Then Q^D is defined[8] by

$$Q^D(12) = Q_1(1)Q_1(2) + A_1(1)Q_1(2) + Q_1(1)A_1(2) \tag{6a}$$

$$= [A_1(1) + Q_1(1)][A_1(2) + Q_1(2)] - A_1(1)A_1(2) \tag{6b}$$

and

$$P^D(12) = I(12) - Q^D(12) \tag{6c}$$

$$= P_1(1)P_1(2) + P_1(1)[I(2)-P_1(2)] + [I(1)-P_1(1)]P_1(2) + A_1(1)A_1(2). \tag{6d}$$

These regions are shown in Fig. 1, from Ref. 7. The definition (6a) is most appropriate to the case in which there are few valence particles relative to the number of valence states, so that scattering into pair states of the form $|vp>$ is seldom blocked by the normal occupancy of state $|v>$. When there are more than two valence particles, the effective interaction differs from the G-matrix by valence-blocking corrections in addition to other corrections.

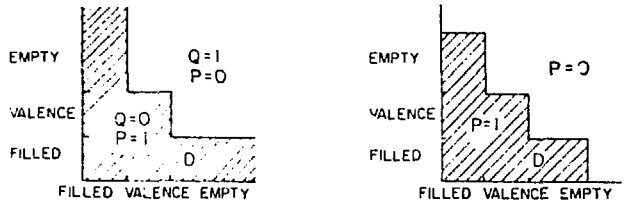

Fig. 1. Pauli projection operator P before and after truncation.

In the seldom discussed degenerate theory with valence holes only, the non-

degenerate Pauli operator (4a) can be used, because only particle-particle ladders are summed by the G-matrix. However, because of (5b), the P's in (4c) must be replaced by (P+A)'s. Finally, if there are both valence particles and holes, we define

$$A_1^h = \sum_{v_h} |v_h><v_h| \quad , \quad A_1^p = \sum_{v_p} |v_p><v_p| \tag{7a}$$

so that

$$P_1 + A_1^h + A_1^p + Q_1 = I. \tag{7b}$$

Then Q^D may be defined by (6) with A_1 replaced by A_1^p and P_1 by $P_1 + A_1^h$.

The Pauli operator may be regarded as providing a dependence of G on the particle density near the interacting particles. In the non-degenerate case

$$(\vec{r}_1,\vec{r}_2|Q^{ND}|\vec{r}_1',\vec{r}_2') = [\delta(\vec{r}_1-\vec{r}_1') - \rho_1(\vec{r}_1,\vec{r}_1')\ [\delta(\vec{r}_2-\vec{r}_2') - \rho_1(\vec{r}_2,\vec{r}_2')] \tag{8a}$$

where ρ_1 is the SP density matrix (in position space) of the model ground state,

$$\rho_1(\vec{r}_1,\vec{r}_1') = <\Phi|\psi^+(\vec{r}_1')\psi(\vec{r}_1)|\Phi> = <\vec{r}_1'|P_1|\vec{r}_1> = \sum_h^{occ} <\vec{r}_1|h><h|\vec{r}_1'>, \tag{8b}$$

often called the "mixed density" as distinguished from its diagonal part, $\rho(\vec{r}_1)$, the particle density at $\vec{r}_1$. An expansion about the mixed density of nuclear matter has been given.[9] Approximating the entire propagator, $Q/(E-H^o)$, by that of nuclear matter of density $\rho(\frac{1}{2}[r_1+r_2])$ is called the local density approximation (LDA).[10]

The reaction operator, as defined so far, has singularities[11] as a function of E_s. In the non-degenerate case

$$\frac{Q^{ND}}{E_s-H^o} = \sum_{p_1p_2}^{emp} \frac{|p_1p_2><p_1p_2|}{E_s-e_{p_1p_2}} \tag{9}$$

where $e_{p_1p_2} = e_{p_1} + e_{p_2}$, with e_p the SP energy of state $|p>$. It is clear from (9) that the perturbative expansion of G has singularities for E_s equal to any $e_{p_1p_2}$. Similarly, from (2a), it is seen that a non-perturbative solution has a singularity at the eigenvalues of $Q(H_2^o + v)Q$, which lie near the $e_{p_1p_2}$. In the Brueckner-Goldstone[12] non-degenerate perturbation expansion, in its rearrangement by generalized-time-ordering,[13,3,4] and in the degenerate perturbation expansions,[8] the self-consistent E_s is always less than the lowest singularity (for non-superfluid systems). But in the SP Green's function approach to nuclear structure[14] and in the calculation of the optical potential, a transition operator is needed. The Brueckner reaction matrix must then be analytically continued to higher E_s as a Heitler reaction matrix containing a principal value operator as well as the

below the lowest $e_{p_1p_2}$, which is the case for interactions far off the energy shell where $E_s = e_{k_1} + e_{k_2} - \delta E$ with δE the excitation of the medium. However, for on-shell interactions between valence particles or high-lying holes, E_s is just below the lowest singularity and there is a strong energy dependence.[15] This is seen clearly in the G-matrix elements for the s-d shell valence nucleons in ^{18}F shown in Fig. 2, taken from Barrett, Hewitt, and McCarthy.[16]

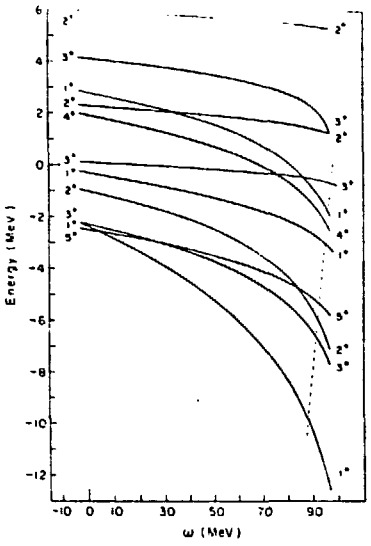

Fig. 2. T=0 spectrum in ^{18}F calculated (Ref. 16) with the G-matrix as effective interaction. The dashed line indicates the self-consistent value of the starting energy, ω,

In summary, unlike the bare interaction v, the reaction operator is dependent on the medium through Q (density dependence) and through the self-energy U (dispersive or spectral dependence), and is energy (or velocity or momentum) dependent through E_s. The latter gives rise to a "state" dependence of the effective interaction because the self-consistent E_s for a particular matrix element depends on the pair states involved in the matrix element.

II. The Bethe-Goldstone Wave Function

If v contains a hard core, Eq. (1) is singular. This difficulty is overcome by working with the equation for the Moller wave operator Ω associated with G by

$$G(E_s) = v\,\Omega(E_s), \tag{10a}$$

which satisfies

$$\Omega(E_s) = 1 + \frac{Q}{E_s - H^0}\, v\,\Omega(E_s). \tag{10b}$$

Acting to the right on an unperturbed pair state ϕ it yields the correlated Bethe-Goldstone[17] pair state ψ,

$$\psi(E_s) = \Omega(E_s)\phi = \phi + \frac{Q}{E_s - H^0}\, v\,\psi(E_s) \tag{10c}$$

which vanishes inside the hard core. A weak singularity of $v\psi$ remains, but gives no trouble as it is integrable. In relative coordinates, for the L^{th} partial wave

$$v_L\psi_L = \lambda_L\delta(r-c) + f_L(r) \tag{11}$$

where $f_L(r)$ is finite.[17]

It is convenient also to define the defect operator

$$\chi(E_s) = I - \Omega(E_s) = \frac{Q}{H^0 - E_s}\, v\,\Omega(E_s) \tag{12a}$$

and the defect wave function

$$\zeta(E_s) = \chi(E_s)\phi = \phi - \psi(E_s) = \frac{Q}{H^o - E_s} v\, \psi(E_s). \tag{12b}$$

In infinite nuclear matter the "small parameter" κ of the compact cluster expansion[4] is

$$\kappa = \rho W \tag{13a}$$

where ρ is the nuclear density and W is the "wound integral"[18]

$$W = \int |\zeta(\vec{r})|^2 \, d^3r, \tag{13b}$$

which is a very characteristic quantity for the interaction, v.[19] The transformation from G to Q is very useful even if v does not have a hard core.

In infinite matter where the hole state spectrum is continuous and the unperturbed pair states are taken to be plane waves, it follows from (10b) that the BG wave function for two normally occupied states and for $E_s = e_{h_1 h_2}$ has no phase shift. It "heals"[18] to the unperturbed wave function because the final states permitted by Q are of higher unperturbed energy than E_s. In fact the defect function in the L^{th} partial wave decays as

$$\zeta_L \sim \frac{\text{const}}{r} \cos(k_F r + \cdots)$$

where k_F is the Fermi wave number.[17] In a harmonic potential, U, the BG wave function oscillates about ϕ and "heals" to it before Q becomes negligible beyond the nuclear surface where it tunnels into the potential. This rapid decay is the most important property which any approximate defect function must have.

In their calculations for infinite nuclear matter, Brueckner and Gammel[20] solved the integral equation (10c) numerically after approximating the Green's function for a fixed average momentum of the pair, $\vec{K}$,

$$\langle \vec{r},\vec{K} \left| \frac{Q}{H^o - E} \right| \vec{r}',\vec{K} \rangle = \int d^3k \; Q(\vec{K}+\vec{k},\vec{K}-\vec{k};k_F) \; \frac{e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}}{e_{\vec{K}+\vec{k}} + e_{\vec{K}-\vec{k}} - E}$$

first by "angle-averaging" over the angle between $\vec{K}$ and $\vec{k}$,[21] which restores spherical symmetry and uncouples different partial waves, and second by truncating at some k_{max}. The angle-averaged, nuclear-matter Pauli operator is[21]

$$Q^{AANM}(k,K;k_F) = \begin{cases} 0 \text{ if } k^2+K^2 < k_F^2 \text{ and } 1 \text{ if } k > k_F+K \\ (k^2+K^2-k_F^2)/2kK, \text{ otherwise} \end{cases} \tag{14a}$$

where

$$\vec{k} = \tfrac{1}{2}(\vec{p}_1 - \vec{p}_2) \quad \text{and} \quad \vec{K} = \tfrac{1}{2}(\vec{p}_1 + \vec{p}_2). \tag{14b}$$

It has been found to be a quite accurate approximation.[22] In their excellent review of methods (through 1967) for calculating G in nuclear matter Dahll, Ostgaard,

and Brandow[23] found Brueckner's method could be very accurate, and found ways to improve it.

III. Representations of G in Terms of P Rather than Q

The operator Q is of infinite dimensionality for both particles, whereas each term of P is of infinite dimensionality for at most one particle. Two ways of expressing G or Ω in terms of P rather than Q are known. The first is to multiply Eq. (10c) by H^o-E_s, which leads to the Bethe-Goldstone integro-differential equation[17]

$$(H^o+v-E_s)\psi = (H^o-E_s)\phi + P\,v\psi. \tag{15}$$

Several ways of solving this equation, when P is truncated, will be described below.

A second, more complicated formulation,[7] can be derived from a familiar identity[24] for a matrix partitioned by the projection operators P and Q:

$$(M^{-1})_{QQ} = [M_{QQ} - M_{QP}(M_{PP})^{-1} M_{PQ}]^{-1} = [M-MP(M_{PP})^{-1}PM]^{-1}. \tag{16}$$

With $M = (E-h)^{-1}$, where h is H^o or H^o+v, the inverse of (16) is

$$\frac{Q}{Q(E-h)Q} = \mathcal{P}\frac{I}{E-h} - \mathcal{P}\frac{I}{E-h}P\left[P\frac{\mathcal{P}}{E-h}P\right]^{-1}P\,\mathcal{P}\frac{I}{E-h} \tag{17}$$

where once again $\mathcal{P}$ stands for the Cauchy principal value. The equation for G in terms of the full Green's function, Eq. (2a), becomes

$$G(E) = G^I(E) - \chi^{I\dagger}(E)\;P\,A(E)P\,\chi^I(E) \tag{18}$$

where we have let $G^I(E)$ denote the reaction matrix for two interacting particles in the potential U but isolated from the medium ($Q \to I$), which satisfies

$$\begin{aligned} G^I(E_s) &= v + v\,\mathcal{P}\frac{I}{E-H^o-v}v = v + v\,\mathcal{P}\frac{I}{E-H^o}G^I(E_s) \\ &= v[I-\chi^I(E_s)] = [I-\chi^{I\dagger}(E_s)]v, \end{aligned} \tag{19}$$

and where

$$A(E_s) = \left[\left(\mathcal{P}\frac{I}{E_s-H^o-v}\right)_{PP}\right]^{-1}. \tag{20}$$

The inversion in Eq. (20) can be done easily because the space P is of finite dimension. However, the evaluation of $\left(\mathcal{P}\frac{I}{E_s-H^o-v}\right)_{PP}$ can be done only approximately, in terms of a truncated set of eigenfunctions of the two-particle Schroedinger equation.

IV. The Integral Equation Relating Two Reaction Operators

As it is not possible to solve for G or ψ exactly, various approximation methods have been developed. These involve simplifying the interaction or the propagator. We should like to know in principle how the exact G is related to an approximate one so we can estimate correction terms. Fortunately, different reaction matrices are related exactly by identities. If the spectrum is continuous, these identities are integral equations. The rigorous version of a comprehensive identity of Moszkowski and Scott,[5] which allows all quantities to vary, can be derived as follows:[2,3]

$$\Omega_A(E_A) - I - \frac{Q_A}{E_A-H_A^o} G_A(E_A) = 0 \tag{21a}$$

$$\Omega_B^\dagger(E_B) - I - G_B^\dagger(E_B)\left[\frac{Q_B}{E_B-H_B^o}\right]^\dagger = 0. \tag{21b}$$

Multiplying (21a) on the left by $G_B^\dagger(E_B)$, subtracting it from (21b) multiplied on the right by $G_A(E_A)$, and using (10a), one obtains

$$G_A(E_A) = G_B^\dagger(E_B) + \Omega_B^\dagger(E_B)(v_A-v_B^\dagger)\Omega_A(E_A) + G_B^\dagger(E_B)\left\{\frac{Q_A}{E_A-H_A^o} - \frac{Q_B}{E_B-H_B^{o\dagger}}\right\}G_A(E_A). \tag{22}$$

Incidentally, a special case of this in which only E_s varies yields[25,13,26]

$$\frac{dG(E)}{dE} = -G(E)\left(\frac{Q}{E-H^o}\right)^2 G(E) = -\chi^\dagger(E)\chi(E). \tag{23}$$

One sees that the diagonal matrix elements of G are non-positive. The propagator-correction term in (22) sometimes is split[5] into a Pauli and a spectral (dispersion) term:

$$\frac{Q}{E-H^o} - \frac{Q_A}{E-H_A} = \frac{Q-Q_A}{E-H^o} + Q_A\left[\frac{I}{E-H^o} - \frac{I}{E-H_A}\right], \text{ if } [Q_A,H^o] = 0 \tag{24a}$$

$$= \frac{Q-Q_A}{E-H_A} + Q\left[\frac{I}{E-H^o} - \frac{I}{E-H_A}\right], \text{ if } [Q,H_A] = 0. \tag{24b}$$

V. Two Simple Approximations Which Provide Insight

A. The Moszkowski-Scott Separation of the Interaction. Different parts of the interaction produce quite different effects. The strong repulsive core must be treated to all orders, whereas a weak interaction need be kept only to low orders. Regions of rapid variation induce high Fourier components in the defect function, whereas slowly varying parts induce only low components. Eden and Emery,[27] Gomes, Walecka, and Weisskopf,[18] and others considered separation of the

hard core, the tensor force, etc. In the Moszkowski-Scott[5] separation method, with

$$v = v_s + v_\ell, \tag{25}$$

the short-ranged part, v_s, includes, along with the repulsive core (which may be soft), the strong, rapidly varying attraction just beyond the core. The remaining long-ranged part, v_ℓ, is weak and slowly varying. A reaction matrix, G_s, obtained from v_s is defined. Since v_s produces the short-range correlation in the BG wave function, which involves primarily admixtures of high-lying unperturbed states, it is a good approximation to replace Q by I in the equation for G_s, so that

$$G_s^I(E) = v_s + v_s \, \mathcal{P}\frac{I}{E-H^o} G_s^I(E). \tag{26}$$

The especially clever feature of the method is that the separation distance, d, is chosen in principal such that each diagonal element of G_s, proportional to tan δ, is zero for the self-consistent value of the starting energy. The BG wave function, ψ_s, then heals to ϕ at the separation distance (see Fig. 3, from Ref. 5).

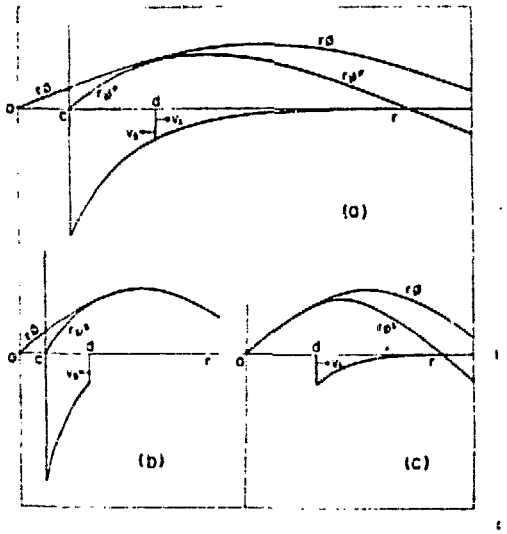

Fig. 3. Illustration of the MS separation method (Ref. 5).

Since v_ℓ is too weak to produce much wave distortion, ψ_s may be used as a good approximation to the correct ψ. The identity (22) yields

$$G(E) = G_s^I(E,d) + \Omega_s^I(E,d)^\dagger v_\ell(d)\Omega(E) + G_s^I(E,d) \, \mathcal{P}\frac{P}{H^o-E} G(E) \tag{27a}$$

with diagonal elements (for the self-consistent values E_α and d_α, where α labels the pair state)

$$\langle\alpha|G(E_\alpha)|\alpha\rangle = \langle\alpha|v_\ell(d_\alpha) + v_\ell(d_\alpha)\frac{Q}{E_\alpha-H^o} v_\ell(d_\alpha) + 2v_\ell(d_\alpha)\frac{Q}{E_\alpha-H^o} G_s^I(E_\alpha,d_\alpha) + \ldots|\alpha\rangle. \tag{27b}$$

For simplicity in the evaluation of G_s^I the free particle Hamiltonian, T, was used, and corresponding dispersion corrections were included in the formulation:

$$G_s^F(E) = v_s + v_s \, \mathcal{P}\frac{I}{E-T} G_s^F(E) \tag{28a}$$

and

$$G(E) = G_s^F(E) + \Omega_s^F(E)^\dagger v_\ell(E)\Omega_s(E)$$
$$+ G_s^F(E)\, Q \frac{P}{H^o-E}\, G(E) + G_s^F(E)\, Q\left[\frac{I}{E-H^o} - \frac{I}{E-T}\right] G(E). \tag{28b}$$

In triplet even states Scott and Moszkowski[5] found a large contribution in (27b) from the quadratic term in the long-range tensor force,

$$v_{T\ell} = v_T(r)\ \theta(r-d)\ S_{12}, \tag{29}$$

where S_{12} is the tensor operator. In their calculations with the separation method for finite nuclei, Kuo and Brown[28] used the free-particle spectrum and the angle-averaged, nuclear-matter, Pauli operator, $Q^{AANM}(k_F)$, with a fixed Fermi wave number, $k_F = 1.36$ fm^{-1}, appropriate to the saturation density. Because Q^{AANM} commutes with T

$$v_{T\ell} \frac{Q}{E_s-H^o} v_{T\ell} \to \int d^3k\, d^3K\, v_{T\ell}|\vec{k}\vec{K}\rangle \frac{Q(k,K,k_F)}{E_s-\frac{\hbar^2}{2m}(k^2+K^2)} \langle\vec{k}\vec{K}|v_{T\ell}. \tag{29a}$$

They found that this could be fairly accurately approximated in a closure approximation

$$v_{T\ell} \frac{Q^{AANM}(1.36)}{E_s-T} v_{T\ell} \approx v_{T\ell} \frac{I}{E_s-\langle T\rangle_{eff}} v_{T\ell} = (8+2S_{12}) \frac{[v_T(r)]^2\theta(r-d)}{E_s-\langle T\rangle_{eff}}. \tag{29b}$$

In a later paper Kuo[29] evaluated

$$\langle\psi_s^F|V_{T\ell} \frac{Q^{AANM}}{E_s-T} V_{T\ell}|\psi_s^F\rangle,$$

again finding closure to be accurate. However, Dahll, et al.[23] showed that in nuclear matter the infinite series of terms in the tensor force converges slowly, because there is no separation distance beyond which the coupled distortions in the $^3S_1$ and $^3D_1$ partial waves both vanish, and Köhler[5] discovered that the MS expansion does not treat the large dispersion effect adequately. In the "modified separation method" (MMS)[3] the equation for G_s contains Q, and Eq. (28b) is modified accordingly.

B. The Reference Spectrum. We have seen that the exact BG wave function heals to the unperturbed function because the Pauli operator keeps the intermediate state spectrum above the self-consistent values of E_s, i.e. above twice the Fermi energy, e_F. If Q is replaced by I, the intermediate spectrum extends further downward, overlapping the self-consistent E_s, and the "healing" property is lost. But if E_s is chosen off-shell, below the hole-pair spectrum, the healing property is regained. Alternatively, the healing property is regained if the hole-pair spectrum is replaced by an upward-shifted auxiliary spectrum, lying above

$2\,e_F$ (Ref. 30 and page 111 of Ref. 5). In the "reference spectrum" (RS) method of Bethe, Brandow, and Petschek,[3] such an auxiliary spectrum is introduced. Then Ω^{RS}, which satisfies

$$\Omega^{RS}(E) = I + \frac{I}{E-H^{RS}} v\, \Omega^{RS}(E), \tag{30a}$$

can have the main qualitative behavior of the correct Ω, while being much easier to calculate because it lacks Q. Then

$$G(E) = G^{RS}(E) + G^{RS}(E) \left[\frac{I}{H^{RS}-E} - \frac{Q}{H^{o}-E}\right] v\, \Omega(E). \tag{30b}$$

The RS method works for all partial waves, unlike the separation method. It shows very simply that the repulsive core contribution grows rapidly as E_s goes off shell. For example, in nuclear matter with an interaction containing a hard core of radius c, for the L^{th} partial wave

$$\langle \phi_{\vec{k}} | v_L | \psi^{RS}_{\vec{k}_o} \rangle = \frac{\hbar^2}{m^*} \{(\gamma^2+k_o^2) \int_o^c \mathcal{J}_L(kr)\, \mathcal{J}_L(k_o r)dr$$

$$+ \mathcal{J}_L(kc)\frac{d}{dr}(\mathcal{J}_L - \mathcal{H}_L)_c\} + \int_c^\infty [\mathcal{J}_L(kr) - \mathcal{H}_L(\gamma r;k)]v_L(r)u_L^{RS}(r)dr \tag{31}$$

where $\mathcal{J}_L$ and $\mathcal{H}_L$ are Riccati-Bessel and Riccati-Hankel functions, and u_L^{RS} is the RS radial wave function. The matrix element contains contributions from inside the core, the core edge, and outside the core. The inner core contribution is proportional to $\frac{\hbar^2}{m^*}\gamma^2$, which is the negative of the relative-state starting energy plus a constant.

Bethe, et al. carefully worked out the parameters of a reference spectrum in nuclear matter of the form

$$e^R_{p_1} = A^R + p_1^2/2m^* \tag{32}$$

which would approximate closely the off-energy-shell Brueckner-Hartree-Fock spectrum for $2k_F < k < 4k_F$ where the Fourier transform of the defect function is large. A similar reference spectrum is illustrated in Fig. 4, taken from Ref. 31. In the "compact cluster" expansion of Brandow,[4] in which U contains only self-energies which are placed on the energy shell by generalized time ordering, the SP potential of "particles" is nearly zero, so that $Q\,H^{gto}\,Q \tilde{=} QTQ$. Then G^{RS} becomes just the reaction matrix for free, isolated particles, similar to G^F_s, Eq. (28a),

$$G^F(E) = v + v\, \mathcal{P}\frac{I}{E-T} G^F(E). \tag{33}$$

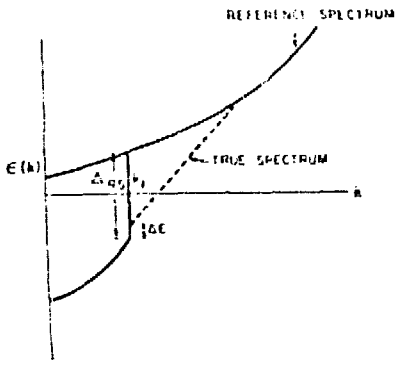

Fig. 4. The BBP (Ref. 3) reference spectrum in nuclear matter. The dashed line is an interpolation. From Ref. 31.

Sprung, et al.[32] have made many calculations of nuclear matter with the RS method.

The earliest calculations of G^{RS} for finite nuclei were those of Day, of Brandow, and of C. W. Wong.[33] Kuo and Brown[28] evaluated G^{RS} for relative p-states (where v is not attractive enough for the separation method to be used) in ^{18}O. Later Wong[34] calculated Pauli and spectral corrections, which can be expressed as

$$\Delta G(E) = G^{RS}(E)\left[\frac{I}{H^{RS}-E} - \frac{Q}{H^{o}-E}\right]\left[G^{RS}(E) + \Delta G(E)\right] = -\left[\Delta_1\chi(E)\right]^{+}\left[G^{RS}(E) + \Delta G(E)\right], \tag{34}$$

$$\Delta\chi(E) = \frac{-I}{H^{RS}-E}G^{RS}(E) + \frac{Q}{H^{o}-E}G(E) = \Delta_1\chi(E) + \frac{Q}{H^{o}-E}\Delta G(E). \tag{35}$$

Here the leading correction to the defect operator, $\Delta_1\chi$, can be separated into Pauli and spectral parts as

$$\Delta_1\chi(E) = \left[\frac{-I}{H^{RS}-E} + \frac{Q}{H^{o}-E}\right]G^{RS}(E) = \Delta_1^{P}\chi(E) + \Delta_1^{S}\chi(E) \tag{36}$$

with

$$\Delta_1^{P}\chi(E) = -P\,\frac{I}{H^{RS}-E}G^{RS}(E) = -P\,\chi^{RS}(E) \tag{37}$$

and

$$\Delta_1^{S}\chi(E) = \frac{Q}{H^{o}-E}G^{RS}(E) - Q\,\chi^{RS}(E). \tag{38}$$

Wong used the free-particle reference spectrum and a local, angle-averaged, nuclear-matter Pauli operator

$$Q(k,R) = Q^{AANM}(k,K_{eff}(R);k_F(R)) \tag{39a}$$

with

$$k_F^3(R) = \frac{3\pi^2}{2}\rho(R) \quad , \quad K_{eff}^2(R) \approx 0.3\,k_F^2(R). \tag{39b}$$

This Q commutes with the relative kinetic energy, and its variation with R gives a distinct improvement in the nuclear surface. Wong also introduced another approximate Pauli operator (denoted by Q^{W} below), defined in the relative and center-of-mass (rel-cm) oscillator representation. It is an approximation to the single-oscillator-configuration, two-particle Q. He found that his local Q gave results similar to the more accurate shell model one, thereby justifying his

somewhat refined version, Eq. (39), of the local density approximation.[10]

VI. Accurate Calculations with an Approximate Q in Oscillator Relative States

For finite nuclei one would like to calculate a G-matrix for which Q and U correspond to the self-consistent orbitals. In light nuclei the orbitals correspond closely (except in the surface) to those of the harmonic oscillator potential. Moreover, the harmonic potential contains the only spatial dependence which separates in both 2-particle and rel-cm coordinates. For these reasons the oscillator basis is a preferred basis in which to calculate a finite-nuclear G. It is special in comparison with more realistic potentials such as the Woods-Saxon in having no continuous spectrum. A two-particle harmonic-oscillator state $|n_1\ell_1 m_1, n_2\ell_2 m_2\rangle$ is expressible[35] as a linear combination of rel-cm states $|n\ell m, NLM\rangle$ with

$$\rho \equiv \bar{n}_1+\bar{n}_2 = \bar{n}+\bar{N} \quad , \quad \bar{n} \equiv 2n+\ell. \tag{40}$$

The states of given ρ lie on a line of angle -45° in a plot such as Fig. 1. Moshinsky and Brody[36] have tabulated the coefficients of this transformation with the angular momenta coupled to total orbital angular momentum, λ. For the reduction of G to relative states we need a propagator which is both a good approximation to the self-consistent (SC) propagator and diagonal in N, L, and ℓ.

There are two common choices of approximate Hamiltonian. One is the shifted oscillator (SO),[37,38] which can be generalized to include an effective mass,[39]

$$H^{SO} = \frac{-\hbar^2\nabla^2}{2m^*} - C + \frac{Kr^2}{2}. \tag{41}$$

The other approximate Hamiltonian, H^{QTQ}, is defined such that[40,41,4]

$$Q^{SOC}\,\frac{I}{H^{QTQ}-E}\,Q^{SOC} = Q^{SOC}\,\frac{I}{Q^{SOC}TQ^{SOC}-E}\,Q^{SOC} \tag{42}$$

where SOC stands for "single oscillator configuration". It is based on two assumptions: that U = 0 for virtual particles, a good approximation for the compact cluster expansion;[4] and that $Q_1^{SC} = Q_1^{SOC}$. Unlike the cruder approximation[28,34]

$$Q^{SOC}\,\frac{I}{T-E}\,Q^{SOC}, \tag{42a}$$

Eq. (42a) preserves the orthogonality of the particle and hole states (similar to the orthogonalized-plane-wave approximation in solid state theory); and unlike Köhler's approximation,[42]

$$Q^{SOC}\,\frac{I}{\frac{1}{2}H^{OSC}-E}\,Q^{SOC}, \tag{42b}$$

Eq. (42) allows for the non-diagonality of T in the oscillator basis. However, the additional approximation of keeping only diagonal elements of T_{cm},

$$\langle NL|Q[QTQ-E]^{-1}\,Q|N'L'\rangle = \delta_{NN'}\delta_{LL'}\,\langle NL|Q[QT_{rel}\,Q + \tfrac{1}{2}e^{osc}_{NL}-E]^{-1}\,Q|NL\rangle, \quad (42c)$$

is still made in the calculations.

Two approximations to P^{SOC} have been widely used. Eden and Emery[27] proposed

$$P^{EE}(\rho) = \begin{cases} 1, & \rho \le \rho_{max} \\ 0, & \rho > \rho_{max}. \end{cases} \quad (43)$$

It is diagonal both in 2-body and in rel-cm oscillator states. Wong's[34] approximation is defined in the rel-cm oscillator basis for closed L-shell configurations, by

$$(n\ell NL|P^{W}|n'\ell'N'L') = \frac{\delta_{\ell\ell'}\delta_{LL'}}{(2L+1)(2\ell+1)} \sum_{\lambda} (2\lambda+1) \sum_{n_1\ell_1 n_2\ell_2} M^{n\ell NL}_{n_1\ell_1 n_2\ell_2}(\lambda)\, M^{n'\ell N'L}_{n_1\ell_1 n_2\ell_2}(\lambda) \quad (44)$$

where M is a Moshinsky coefficient and the sum is over pair states $|n_1\ell_1, n_2\ell_2\rangle$ for which (see Fig. 1) P^{SOC} is unity. The averaging over λ is just an angle-averaging in the classical (vector model) limit. P^{W} is more accurate than P^{EE} and is preferable if one is not going to calculate "residual Pauli corrections"[38] involving $P\text{-}P^{rel\text{-}cm}$. Moreover, P^{W} can be easily generalized to j-j coupling, to non-oscillator radial functions, and to fractional occupancy.[34] However, P^{W} should not be used if residual Pauli corrections are to be made, because P^{W} is not defined in the 2-body oscillator representation; whereas P_{EE} is defined there, and by Eq. (40) takes the same simple form, Eq. (43). A related difficulty with P^{W} is that it is not a projection, i.e. is not idempotent, $(P^{W})^2 \neq P^{W}$, because of the dropping of the off-diagonal elements.

In (44) $N'+n' = N+n$. Köhler and McCarthy[42,43] have made the additional truncation in which $N' = N$:

$$(n\ell NL|P^{KM}|n'\ell'N'L') = \delta_{nn'}\delta_{NN'}\delta_{\ell\ell'}P^{W}(NLn\ell). \quad (45)$$

Kallio and Day[44] also have required full diagonality, but have kept a dependence on λ by omitting the average over λ:

$$(n\ell NL|P^{KD}(\lambda)|n'\ell'N'L') = \delta_{nn'}\delta_{\ell\ell'}\delta_{NN'}\delta_{LL'} \sum_{n_1\ell_1 n_2\ell_2} \left[M^{n\ell NL}_{n_1\ell_1 n_2\ell_2}(\lambda)\right]^2. \quad (46)$$

They show that even small differences in the Pauli operator significantly affect the asymptotic behavior of the defect function and hence such quantities as U insertions and the rms radius.

Next we turn to the methods for calculating G with a propagator diagonal in N and L. We let $g = \langle NL|G|NL\rangle$. All the methods involve truncating the projection operator P (as in Fig. 1) or Q to a finite number of states. As the oscillator pair-energy parameter ρ increases, the fraction of the line ρ=const for which

$P = 1$ decreases rapidly. Moreover, Wong[34] has shown that $P^W(\ell L,\rho)$ falls off, as ρ increases, even more rapidly than this geometrical argument would suggest. Sauer[45] found that g-matrix elements calculated with the maximum relative radial quantum number equal to 5 agreed with the matrix elements for $n_{max} = 15$ to within 1%.

We shall describe four nearly exact methods for solving for g with a truncated P or Q: two for solving the BG equation, one involving g^I and the reaction matrix identity, Eq. (22), and one involving expansion in eigenfunctions of the Schroedinger equation for an isolated pair.

The BG equation (15) may be regarded as an inhomogeneous equation in which the inhomogeneity is a linear combination of oscillator orbitals. Eden and Emery[27] suggested calculating Green's functions for each of these inhomogeneities and taking that linear combination which satisfies the boundary conditions. MacKellar and Becker[37,38] further developed this Green's function method, including the first exact treatment of the tensor force through coupled partial waves. Figure 5 shows the $^3S_1$ - D_1 defect function for several values of the starting energy.[46]

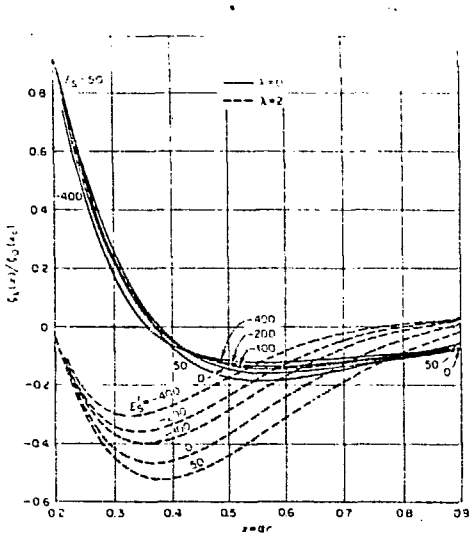

Fig. 5. Triplet relative defect functions for N=L=ℓ=0, n=5 for the Hamada-Johnston interaction for several values of the shifted starting energy $E_s' \equiv E_s + 2C$, $\alpha=(m\omega/2\hbar)^{1/2}=0.4$ fm^{-1}, and $\rho_{max}=5$. From Ref. 46.

Kallio and Day[44] solved the BG equation by iterating the inhomogeneity, $P^{KD}(\lambda)v$. They also applied this inhomogeneity-iteration method to nuclear matter. Siemens[47] has done extensive calculations of nuclear-matter matrix elements with the iteration method. Its only drawback is that convergence becomes slower as k_F increases and is not efficient for calculations at high density.

Köhler and McCarthy[42,43] first calculate the reference matrix

$$g^I(E) = v + v\,\frac{I_{rel}}{E-\langle H^o_{cm}\rangle_{NL}-H^o_{rel}}\,g^I(E) \quad (47a)$$

and then solve either in perturbation theory[42] or more accurately by matrix inversion,[43] in a truncated basis of relative oscillator states,

$$\left[I_{rel}-g^I(E)\,\frac{P^{KM}_{trunc}}{\langle H^o_{cm}\rangle_{NL}+H^o_{rel}-E}\right]g(E) = g^I(E). \quad (47b)$$

Here P^{KM}_{trunc} is the approximation of (45) in which the sum over $(n_1\ell_1,n_2\ell_2)$ in (44)

is truncated. By energy conservation (40) this implies a truncation of n and ℓ. In Ref. 42 they have used, instead of the QTQ prescription, $\frac{1}{2} H^{osc}$ (42b); and in the other papers[43] an oscillator spectrum. Both of these are diagonal in relative oscillator states, so the propagator is

$$\sum_{n\ell} |n\ell)\ P^{W}_{trunc}(NLn\ell)\,[\langle H^{o}_{cm}\rangle_{NL} + \langle n\ell|H^{o}_{rel}|n\ell\rangle - E]^{-1}(n\ell|. \tag{48}$$

The reference matrix has singularities in the desired range of starting energies, so one must be careful to calculate $g^{I}(E)$ for values of E well removed from these singularities in order to avoid loss of numerical accuracy in the matrix inversion. The method is mathematically equivalent to the method of Green's functions described above; however, the work is arranged differently.

Sauer[45] has applied the matrix inversion method to the QTQ problem,

$$G(E) = v + v\,\frac{Q^{SOC}}{Q^{SOC}(E-T)Q^{SOC}}\,\overline{QC}\,G(E) \tag{49}$$

where it involves additional approximations, because T_{rel} is not quite diagonal in relative oscillator states, and some arbitrarines s, because after truncation Q is no longer a projection operator. In terms of the reference matrix,

$$g^{I}(E) = v + v\,\frac{I_{rel}}{E-\frac{1}{2}e_{NL}-T_{rel}}\,\overline{1}\,g^{I}(E), \tag{50}$$

Sauer's approximation is to solve in a truncated space of (nℓ) states

$$\sum_{\bar{\ell}=\ell,2j-\ell}\ \sum_{\bar{n}'}^{n_{max}} \{\delta^{n\ell}_{\bar{n}'\bar{\ell}} - \sum_{\bar{n}}^{n_{max}} (n\ell|g^{I}|\bar{n}\bar{\ell})(\bar{n}|\Delta_{\bar{\ell}}|\bar{n}'\}(\bar{n}'\bar{\ell}|g|n'\ell') = (n\ell|g^{I}|n'\ell') \tag{51}$$

where the Pauli-correction kernel is

$$(\bar{n}|\Delta_{\bar{\ell}}|\bar{n}') = Q^{W}(NL\bar{n}\bar{\ell})\ \langle\bar{n}|A^{-1}_{\bar{\ell}}|\bar{n}'\rangle\ Q^{W}(NL\bar{n}'\bar{\ell}) - \langle\bar{n}|B^{-1}_{\bar{\ell}}|\bar{n}'\rangle$$

with

$$(n|A_{\ell}|n') = E - \tfrac{1}{2}e_{NL} - Q^{W}(NLn\ell)\,(n\ell|T_{rel}|n'\ell)Q^{W}(NLn'\ell) \tag{52a}$$

$$(n|B_{\ell}|n') = E - \tfrac{1}{2}e_{NL} - (n\ell|T_{rel}|n'\ell). \tag{52b}$$

Notice that as $\bar{n} \to \infty$, $Q^{W}(NL\bar{n}\bar{\ell}) \to 1$ and $(n|A_{\ell}|n') \to (n|B_{\ell}|n')$ fairly rapidly.

Butler, et al.[48] have suggested that an expansion of a BG wave function in terms of eigenfunctions of the Schroedinger equation[49]

$$[H^{osc}_{cm} + H^{osc}_{rel} + v]\psi_{NL,i} = (e^{osc}_{NL} + E^{rel}_{i})\psi_{NL,i} \tag{53}$$

should converge rapidly. Barrett, Hewitt, and McCarthy[16] have implemented this

idea by expanding the reference BG wave function in ψ_i's and then using the matrix inversion method. The reference BG equation corresponding to (53) is

$$[H^{osc}_{cm} + H^{osc}_{rel} + v - E]\psi^{I}_{NLn\ell}(E) = (e^{osc}_{NLn\ell}-E)\phi_{NL,n\ell} = (e^{osc}_{n\ell}-E^{rel})\phi_{NL,n\ell}. \quad (54)$$

Then

$$\psi^{I}_{NLn\ell}(E) = (e^{osc}_{n\ell}-E^{rel}) \sum_i \frac{\psi_{NL,i}\,(\psi_{NL,i}|\phi_{NL,n\ell})}{E^{rel}_i-E^{rel}} \quad (55)$$

and

$$(n'\ell'|G^{I}_{NL}(E)|n\ell) = (e^{osc}_{n\ell}-E^{rel}) \sum_i \frac{(E^{rel}_i-e^{osc}_{n'\ell'})}{(E^{rel}_i-E^{rel})} (\phi_{NL,n'\ell'}|\psi_{NL,i})(\psi_{NL,i}|\phi_{NL,n\ell})$$

$$= (e^{osc}_{n\ell}-E^{rel})\left[\delta_{n',n}\delta_{\ell',\ell} - (e^{osc}_{n'\ell'}-E^{rel}) \sum_i \frac{(\phi_{NL,n'\ell'}|\psi_{NL,i})(\psi_{NL,i}|\psi_{NL,n\ell})}{E^{rel}_i-E^{rel}}\right]. \quad (56)$$

In practice one truncates the sum over eigenfunctions i. Equation (56) has the advantage that the dependence on the starting energy is explicit. It can provide a very accurate energy derivative.

VII. Accurate Calculations in the Two-Particle Oscillator Basis

Finally, we discuss the case in which a propagator defined in terms of individual particle states is used. The only known method is to use Eq. (22) again in a truncated basis, i.e. the matrix inversion method. The equation to be solved is

$$G(E) = G^{RCM}(E) + G^{RCM}(E)\left[\frac{Q}{E-H^{o}} - \frac{Q^{RCM}}{E-H^{RCM}}\right]G(E) \quad (57)$$

where RCM labels the approximate quantities defined in terms of rel-cm states. In (57) these quantities are assumed to be re-expressed in terms of two-particle oscillator states. We recall that I and Q^{EE} can be expressed in two-particle states, but Q^{W} cannot.

The first use of (57) was with $Q^{RCM} = Q^{EE}$, $H^{RCM} = H^{SO}$, $Q = Q^{SOC}$ and G(E) on the right-hand side approximated by G^{RCM}.[38] Later the full matrix inversion was used.[50] The case $Q = Q^{SOC}$ has also been treated by calculating G^{RCM} with $Q^{RCM} = I$ and $H^{RCM} = H^{osc}$ by the eigenfunction expansion method.[16] Equation (56) transforms to the two-particle oscillator basis $\alpha,\beta,\ldots$ as

$$G^{I}_{\beta\alpha}(E) = (e^{osc}_{\alpha}-E)\left[\delta_{\beta\alpha} - (e^{osc}_{\beta}-E) \sum_i^{i_{max}} \frac{b_{i\beta}\, b_{i\alpha}}{E_i-E}\right] \quad (58a)$$

where

$$b_{i\alpha} = (\psi_i|\phi_\alpha). \quad (58b)$$

The H^{o} in (57) can be allowed to contain level-shifts,[27,38,16]

$$H^0 = H^{SO} + \sum_\alpha (e_\alpha - e_\alpha^{osc}) |\phi_\alpha><\phi_\alpha|, \tag{59}$$

so as to have self-consistent energies of the low-lying "particle" states.

Self-consistency of the Pauli operator with the orbitals of a self-consistent field calculation can be obtained by expanding the SC orbitals in a truncated basis of oscillator states and then solving (57) with $Q = Q^{SC}$, or, if G^{SOC} has already been obtained from (57), by solving

$$G(E) = G^{SOC}(E) + G^{SOC}(E) \left[\frac{Q^{SC}}{E-T-U^{SC}} - \frac{Q^{SOC}}{E-H^{SO}} \right] G(E). \tag{60}$$

MacKellar[51] initiated the first residual Pauli corrections from Eq. (60) with $U^{SC} = U^{SO}$. This refinement of G made enough difference in the saturation properties of ^{16}O to warrant its inclusion in other calculations.[52,53] It is expected to become more important the heavier the nucleus. Spectral corrections, $U^{SC} \neq U^{SO}$, were also included in Ref. 53. Equation (58) could be applied easily, with ϕ_α in (58b) becoming a self-consistent pair state expanded in oscillator pair states.

We have now reached the stage where G is essentially exact, limited only by the truncation of the oscillator basis and the uncertainty in the best definition of the potential U for virtual particles.

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