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Abstract

Scaling the system size of the interacting boson model-1 (IBM-1) into the realm of hundreds of bosons has many interesting applications in the field of nuclear structure, most notably quantum phase transitions in nuclei. We introduce `ibar`, a new software package for calculating the eigenvalues and eigenvectors of the IBM-1 Hamiltonian, for large numbers of bosons. Energies and wavefunctions of the nuclear states, as well as transition strengths between them are calculated using these values. Numerical errors in the recursive calculation of coefficients of fractional parentage are reduced by using an arbitrary precision mathematical library. This software has been tested for up to 400 bosons, which is 25 times larger than the standard IBM-1 code PHINT.

Keywords:
Interacting boson model, Quantum phase transitions, Coefficients of fractional parentage, Nuclear structure

1. Introduction

One topic that has recently been of interest in nuclear structure is the study of quantum phase transitions in nuclei [1–10], and the interacting boson model-1 with s and d bosons (sd-IBM-1)[11] is useful framework for studying such behavior. The sd-IBM-1, which can be treated as a vast truncation of the nuclear shell model [12–14], is an algebraic model that can be used to describe collective motion in even-even nuclei. It is primarily successful at low energies, where states are less likely to be influenced by single-particle excitations. The states are constructed from s and d-bosons, which correspond to pairs of valence nucleons coupling to $L = 0$ and $L = 2$ respectively [15]. Higher angular momentum excitations are possible, but are assumed to only play a role in higher-energy states.

The number of bosons included in an sd-IBM-1 calcuation is defined by how many valence particles or holes the nucleus is away from proton and neutron shell closures. The standard proton and neutron shell closures occur at 2, 8, 20, 28, 50, 82, and 126 nucleons. Knowing these numbers, it might be difficult to imagine why a calculation should ever require more than 22 bosons in total. The answer to this is that large boson calculations are not intended to generate spectra for comparing to experimental data, but rather to understand the behavior of certain observables as the system scales up to mesoscopic sizes. If such behavior is characteristic of a first or second order quantum phase transition, which can only be determined by looking at how the behavior evolves into an equivalent infinite-sized system, then the system can be scaled back down to a realistic number of particles to see if any experimentally observed behavior in nuclei could be characteristic of such a phase transition.

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The code `PHINT` has been used for many years to perform sd-IBM-1 calculations with up to 16 bosons [16], but it is unable to calculate systems with a larger size. Other software has been written to extend calculations to higher numbers of particles [17], but precision loss in the calculation of angular momentum coupling coefficients limits the number of bosons to 80. In specific subsets of the IBM-1 Hamiltonian, certain symmetries can be exploited to allow calculations for several thousands of bosons [18], but for the general Hamiltonian this is not possible.

The software `ibar` was recently written to perform precise sd-IBM-1 calculations with large numbers of particles, and it has already been used in a number of investigations into the characteristics of quantum phase transitions in nuclei [19–25]. It is currently capable of calculating wavefunctions, energies, and transition matrix elements for systems with up to 400 bosons. In addition, significant progress has been made towards scaling the software even further, up to 1000 bosons. Scaling up to such a large number of particles presents numerous computational challenges, and a few such challenges will be addressed in later sections of this paper. In Section 2 the sd-IBM-1 will be briefly introduced. In Sections 3 through 5, details about the calculation of Hamiltonian matrix elements, and diagonalization of the Hamiltonian will be presented. Section 6 details some simple tests of the software, and gives some discussion about energy degeneracy breaking.

2. The interacting boson model

2.1. Operators

States and operators in the sd-IBM-1 are constructed from s and d-boson creation and annihilation operators. The s-bosons have angular momentum $L = 0$, and have one magnetic substate. The d-bosons have $L = 2$, so they have five magnetic substates. The model constructed from these particles therefore

has six dimensions, and the algebraic group that describes them is U(6). The operators are $s^\dagger$, $d^\dagger_\mu$, s, and d_μ, where $\mu = -2 \ldots 2$, and they satisfy the Bose commutation relations. In order to calculate matrix elements in the sd-IBM-1, the operators should be spherical tensors, so the annihilation operators need to be modified in the following way [11]:

$$\tilde{s} = s \qquad \tilde{d}_\mu = (-1)^\mu d_{-\mu} \tag{1}$$

Tensor products of these spherical tensors can be used to construct a Hamiltonian for the model. The number of bosons in the model space is defined by the total number of pairs of valence particles and holes in the nucleus, and that number of bosons is conserved by the Hamiltonian. Although the relative numbers of s and d-bosons can change, the total number remains the same. Another common restriction on the Hamiltonian is that it contains only one and two-body terms. Higher order terms are possible, but typically are not necessary, and as such, are removed from the Hamiltonian. One last restriction is that terms in the Hamiltonian couple to a total angular momentum of 0, so that angular momentum is conserved, and the Hamiltonian can be written in block diagonal form with respect to L.

2.2. Phase transitional Hamiltonian

Calculations performed in the sd-IBM-1 to probe the characteristics of quantum phase transitions in nuclei typically use a Hamiltonian that can be varied between spherical and deformed by adjusting an order parameter. As previously mentioned, the sd-IBM-1 is described by the U(6) group algebra. The subgroups of particular interest, U(5), O(6), and SU(3), are called dynamical symmetries, and are physically relevant to the discussion of quantum phase transitions. The following is a simple Hamiltonian that can be used to describe a form of all three dynamical symmetries [26, 27]:

$$\hat{H}_{\mathrm{ECQF}} = c\left((1-\zeta)\hat{n}_d - \frac{\zeta}{4N}\hat{Q}^\chi \cdot \hat{Q}^\chi\right) \tag{2}$$

where c is a scale factor, $\hat{n}_d = d^\dagger \cdot \tilde{d}$ is the d-boson number operator, and $\hat{Q}^\chi = [s^\dagger \tilde{d}]^{(2)} + [d^\dagger \tilde{s}]^{(2)} + \chi[d^\dagger \tilde{d}]^{(2)}$ is the quadrupole operator. The Hamiltonian is labelled ECQF [26], as it refers to the extended consistent-Q formalism, which means that the E2 transition operator is defined in terms of the same quadrupole operator:

$$\hat{T}(E2) = e_B \hat{Q}^\chi \tag{3}$$

where e_B refers to the effective boson charge. In the Hamiltonian, ζ can take on values from 0 to 1, and χ can have values from $\pm\frac{\sqrt{7}}{2}$ to 0. The factor of $4N$ in front of the quadrupole term causes the transition from vibrational to rotational structure to occur at approximately $\zeta = \frac{1}{2}$. In terms of the geometric shape transition, the parameter ζ transitions the Hamiltonian from spherical ($\zeta = 0$) to deformed ($\zeta = 1$), and χ transitions the Hamiltonian from gamma-soft ($\chi = 0$) to rigid ($\chi = \pm\frac{\sqrt{7}}{2}$).

To identify the critical point of first and second order phase transitions, several numerical derivatives of the observables are needed, which requires the coefficients and overall calculations to be performed in high-precision and with minimal precision loss. In some cases, the parameter space in which dramatic changes are occuring cannot even be described in single-precision. In all phases of the design and creation of `ibar`, precision was carefully kept in mind.

2.3. Basis states

The matrix elements of the Hamiltonian are calculated in the U(5) basis, which is the most natural form for expanding in terms of reduced matrix elements of the $d^\dagger$ operator. The U(5) basis states can be enumerated using the quantum numbers of the following group chain:

$$U(6) \supset U(5) \supset O(5) \supset O(3) \supset O(2) \tag{4}$$

U(6) is characterized by the total boson quantum number N, U(5) by the number of d-bosons in a state n_d, O(5) by the seniority v, O(3) by the angular momentum L, and O(2) by the magnetic substate quantum number m_L. The seniority quantum number v can also be represented by n_β, which is the number of pairs of d-bosons, where the pairs couple to angular momentum 0. O(5) is not fully reducible with respect to O(3), so an additional quantum number is needed to fully characterize the chain, and this quantum number will be n_Δ. It refers to the number of d-boson triplets, where the triplets couple to angular momentum 0, but it could be defined in many other ways.

When constructing the set of basis states to be used for computing matrix elements of an sd-IBM-1 Hamiltonian, it is convenient to examine a single angular momentum L at a time. The number of d-bosons, n_d can take on all integer values from 0 to N. The seniority quantum number v represents the seniority of the state and can have the following values: [28]

$$v = n_d,\ n_d - 2,\ n_d - 4,\ \ldots,\ 0 \text{ if } n_d \text{ is even.}$$

$$v = n_d,\ n_d - 2,\ n_d - 4,\ \ldots,\ 1 \text{ if } n_d \text{ is odd.} \tag{5}$$

Using v and n_d, an alternate quantum number n_β is defined: $n_\beta = \frac{1}{2}(n_d - v)$. In order to find the allowed values for the additional quantum number n_Δ, the index λ is used, which takes on values between $\lfloor\frac{L+1}{2}\rfloor$ and L. One additional restriction on λ is that $L = 2\lambda - 1$ is not allowed [29]. Using the allowed values of λ, n_Δ is defined by the following.

$$n_\Delta = \frac{1}{3}(n_d - 2n_\beta - \lambda) \tag{6}$$

After calculating the possible values for n_Δ, two final checks are made for every state in the basis: $n_\Delta \geq 0$ and $n_d = 2n_\beta + 3n_\Delta + \lambda$ [11].

3. Calculating matrix elements of the Hamiltonian

3.1. Wigner-Eckart theorem

Before getting into the details of calculating matrix elements of the Hamiltonian, it is important to remark on the calculation of matrix elements of tensor products in general. All operators

in the sd-IBM-1 are constructed from s and d-boson operators. One of the benefits of these operators being spherical tensors is that the Wigner-Eckart theorem can be applied to matrix elements of tensor products of the operators. The Wigner-Eckart theorem separates matrix elements into two parts: a reduced matrix element which contains all physical information, and a 3-j symbol which contains the geometric information.

$$\langle n_d n_\beta n_\Delta L m | T^{(k)}_\kappa | n'_d n'_\beta n'_\Delta L' m' \rangle = (-1)^{L-M} \times \begin{pmatrix} L & k & L' \\ -m & \kappa & m' \end{pmatrix} \langle n_d n_\beta n_\Delta L || T^{(k)}_\kappa || n'_d n'_\beta n'_\Delta L' \rangle \quad (7)$$

The tensor products of boson operators that make up the Hamiltonian can then be decoupled in to sums of reduced matrix elements of the operators that the tensor product was constructed from. In the sd-IBM-1, all terms in the Hamiltonian couple to angular momentum 0, which is why there are no cross terms between states of different L. This makes both k and the projection quantum number κ equal to 0, and Eq. 7 reduces to the following:

$$\langle n_d n_\beta n_\Delta L m | T^{(0)}_0 | n'_d n'_\beta n'_\Delta L m \rangle = \frac{1}{\sqrt{2L+1}} \times \langle n_d n_\beta n_\Delta L || T^{(0)}_0 || n'_d n'_\beta n'_\Delta L \rangle \quad (8)$$

3.2. Matrix elements of a general sd-IBM-1 Hamiltonian

One form of the sd-IBM-1 Hamiltonian which is often referred to as the ECQF Hamiltonian was given in Eq. 2. That Hamiltonian was constructed specifically to transition between vibrational and rotational structure at approximately $\zeta = \frac{1}{2}$, but the following is a more general form that includes additional multipole terms:

$$\hat{H} = e_0 + \epsilon \hat{n}_d + \kappa \hat{Q}^\chi \cdot \hat{Q}^\chi + a_1 \hat{L} \cdot \hat{L} + a_3 \hat{T}^{(3)} \cdot \hat{T}^{(3)} + a_4 \hat{T}^{(4)} \cdot \hat{T}^{(4)} \quad (9)$$

where κ is sometimes referred to as a_2. The operators in this Hamiltonian are defined in terms of s and d-boson creation and annihilation operators:

$$\begin{aligned} \hat{n}_d &= d^\dagger \cdot \tilde{d} \\ \hat{Q}^\chi \cdot \hat{Q}^\chi &= \left([s^\dagger \tilde{d}]^{(2)} + [d^\dagger \tilde{s}]^{(2)} + \chi [d^\dagger \tilde{d}]^{(2)} \right) \\ &\quad \cdot \left([s^\dagger \tilde{d}]^{(2)} + [d^\dagger \tilde{s}]^{(2)} + \chi [d^\dagger \tilde{d}]^{(2)} \right) \\ \hat{L} \cdot \hat{L} &= 10 [d^\dagger \tilde{d}]^{(1)} \cdot [d^\dagger \tilde{d}]^{(1)} \\ \hat{T}^{(3)} \cdot \hat{T}^{(3)} &= [d^\dagger \tilde{d}]^{(3)} \cdot [d^\dagger \tilde{d}]^{(3)} \\ \hat{T}^{(4)} \cdot \hat{T}^{(4)} &= [d^\dagger \tilde{d}]^{(4)} \cdot [d^\dagger \tilde{d}]^{(4)} \end{aligned} \quad (10)$$

The alternate parameter ζ and the scale factor c from Eq. 2 can be reintroduced into the Hamiltonian:

$$\epsilon = c(1-\zeta) \qquad \kappa = -\frac{c\zeta}{4N} \quad (11)$$

The scalar products in the Hamiltonian can be represented as tensor products using the following equation: [29]

$$U^{(K)} \cdot V^{(K)} = (-1)^K \sqrt{2K+1} (U^{(K)} \times V^{(K)})^{(0)} \quad (12)$$

It is important to note that the d-boson creation and annihilation operators have angular momentum 2. A tensor product of two $d^\dagger$ or $\tilde{d}$ operators can couple up to angular momentum 4, and a scalar product implies a coupling to 0 angular momentum. The d-boson number operator can be rewritten as

$$n_d = d^\dagger \cdot \tilde{d} = \sqrt{5} [d^\dagger \tilde{d}]^{(0)}. \quad (13)$$

The s-boson operators have angular momentum 0, so a tensor product with two $\tilde{s}$ or $s^\dagger$ operators will only couple to 0, and can be represented as a scalar product.

$$s^\dagger \cdot \tilde{s} = [s^\dagger \tilde{s}]^{(0)} \quad (14)$$

A tensor product of an s-boson operator $\tilde{s}$ or $s^\dagger$ with a d-boson operator $\tilde{d}$ or $d^\dagger$ must couple to angular momentum 2, and there can be no scalar product between the two. The Hamiltonian shown in Eq. 9 can be converted into normal order form, which is more convenient for the eventual evaluation of Hamiltonian matrix elements. Normal ordering simply means that all creation operators are on the left side in the tensor product, and all annihilation operators are on the right [30]. The following formula for recoupling angular momentum can be used to do this:

$$[d^\dagger \tilde{d}]^{(k)} \cdot [d^\dagger \tilde{d}]^{(k)} = \frac{2k+1}{\sqrt{5}} [d^\dagger \tilde{d}]^{(0)} + (2k+1) \times \sum_{L=0,2,4} \begin{Bmatrix} 2 & 2 & k \\ 2 & 2 & L \end{Bmatrix} [d^\dagger d^\dagger]^{(L)} \cdot [\tilde{d}\tilde{d}]^{(L)} \quad (15)$$

The normal order Hamiltonian can be written as

$$\begin{aligned} \hat{H} &= c_0 + c_1 [s^\dagger \tilde{s}]^{(0)} + c_2 \sqrt{5} [d^\dagger \tilde{d}]^{(0)} + c_3 [d^\dagger d^\dagger]^{(0)} \cdot [\tilde{d}\tilde{d}]^{(0)} \\ &\quad + c_4 [d^\dagger d^\dagger]^{(2)} \cdot [\tilde{d}\tilde{d}]^{(2)} + c_5 [d^\dagger d^\dagger]^{(4)} \cdot [\tilde{d}\tilde{d}]^{(4)} \\ &\quad + c_6 \left([d^\dagger d^\dagger]^{(2)} \cdot [\tilde{d}\tilde{s}]^{(2)} + [d^\dagger s^\dagger]^{(2)} \cdot [\tilde{d}\tilde{d}]^{(2)} \right) \\ &\quad + c_7 \sqrt{5} \left([d^\dagger d^\dagger]^{(0)} \cdot [\tilde{s}\tilde{s}]^{(0)} + [s^\dagger s^\dagger]^{(0)} \cdot [\tilde{d}\tilde{d}]^{(0)} \right) \\ &\quad + c_8 [d^\dagger s^\dagger]^{(2)} \cdot [\tilde{d}\tilde{s}]^{(2)} + c_9 [s^\dagger s^\dagger]^{(0)} \cdot [\tilde{s}\tilde{s}]^{(0)}. \end{aligned} \quad (16)$$

Once the Hamiltonian in Eq. 9 is converted to normal order form, the coefficients of the Hamiltonian will be

$$\begin{aligned} c_0 &= e_0 \\ c_1 &= 5a_2 \\ c_2 &= \epsilon + 6a_1 + (1+\chi^2)a_2 + \frac{7}{5}a_3 + \frac{9}{5}a_4 \\ c_3 &= -6a_1 + \chi^2 a_2 - \frac{7}{5}a_3 + \frac{9}{5}a_4 \\ c_4 &= -3a_1 - \frac{3}{14}\chi^2 a_2 + \frac{4}{5}a_3 + \frac{18}{35}a_4 \\ c_5 &= 4a_1 + \frac{2}{7}\chi^2 a_2 + \frac{1}{10}a_3 + \frac{1}{70}a_4 \\ c_6 &= 2\chi a_2 \\ c_7 &= a_2 \\ c_8 &= 2a_2 \\ c_9 &= 0. \end{aligned} \quad (17)$$

This is the Hamiltonian form used in calculations, as the U(5) basis states can be applied to calculate the matrix elements of this Hamiltonian [29].

$$
\begin{aligned}
&\langle n_s n_d n_\beta n_\Delta|\ [s^\dagger s]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = n_s \\
&\langle n_s n_d n_\beta n_\Delta|\ \sqrt{5}[d^\dagger \tilde{d}]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = n_d \\
&\langle n_s n_d n_\beta n_\Delta|\ 5[d^\dagger d^\dagger]^{(0)} \cdot [\tilde{d}\tilde{d}]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = \\
&\qquad n_d(n_d+3) - v(v+3) \\
&\langle (n_s+2)(n_d-2)(n_\beta-1)n_\Delta|\ \sqrt{5}[\tilde{d}\tilde{d}]^{(0)} \cdot [s^\dagger s^\dagger]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = \\
&\qquad \sqrt{n_d(n_d+3) - v(v+3)}\,\sqrt{n_s+1}\,\sqrt{n_s+2} \\
&\langle n_s n_d n_\beta n_\Delta|\ \sqrt{5}[d^\dagger \tilde{d}]^{(0)} \cdot [s^\dagger s]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = n_d n_s \\
&\langle n_s n_d n_\beta n_\Delta|\ [s^\dagger s^\dagger]^{(0)} \cdot [ss]^{(0)}\ |n_s n_d n_\beta n_\Delta\rangle = n_s(n_s-1)
\end{aligned}
\tag{18}
$$

The matrix elements of the three Hamiltonian terms associated with the parameters c_3, c_4, and c_5 can be found by relating those terms to the following Hamiltonian, written in terms of Casimir operators:

$$
\begin{aligned}
\hat{H} = E_0 &+ \epsilon' \hat{C}_1(U(5)) + \alpha' \left(\frac{1}{2}\hat{C}_2(U(5)) - \frac{5}{2}\hat{C}_1(U(5)) \right) \\
&+ \beta' \left(-\frac{1}{2}\hat{C}_2(O(5)) + \hat{C}_2(U(5)) - \hat{C}_1(U(5)) \right) \\
&+ \gamma' \left(\frac{1}{2}\hat{C}_2(O(3)) - 6\hat{C}_1(U(5)) \right)
\end{aligned}
\tag{19}
$$

The eigenvalues of this Hamiltonian are

$$
\begin{aligned}
E_0 &+ \epsilon' n_d + \alpha' \frac{1}{2} n_d(n_d-1) + \beta'\,(n_d(n_d+3) - v(v+3)) \\
&+ \gamma'(L(L+1) - 6n_d).
\end{aligned}
\tag{20}
$$

The parameters α', β', and γ' are related to the parameters c_3, c_4, and c_5 by the following transformation [11]:

$$
\begin{aligned}
\alpha' &= \frac{4}{7}c_4 + \frac{3}{7}c_5 \\
\beta' &= \frac{1}{5}c_3 - \frac{2}{7}c_4 + \frac{3}{35}c_5 \\
\gamma' &= -\frac{1}{7}c_4 + \frac{1}{7}c_5
\end{aligned}
\tag{21}
$$

By transforming the three $[d^\dagger d^\dagger]^{(k)} \cdot [\tilde{d}\tilde{d}]^{(k)}$ terms of the normal order Hamiltonian into Casimir form, the matrix elements of the Casimir terms can be used in place of the matrix elements of those three normal order terms.

The remaining matrix element of the normal order Hamiltonian is $\langle n_s n_d n_\beta n_\Delta L||[d^\dagger s^\dagger]^{(2)} \cdot [\tilde{d}\tilde{d}]^{(2)}||n'_s n'_d n'_\beta n'_\Delta L\rangle$, which is calculated by fully decoupling the reduced matrix element. The first step is decoupling the scalar product [29]:

$$
\begin{aligned}
\langle n_d n_\beta n_\Delta L||T^{(k)} \cdot U^{(k)}||n'_d n'_\beta n'_\Delta L\rangle = &\frac{1}{\sqrt{2L+1}} \sum_{n''_d, n''_\beta, n''_\Delta, L''} (-1)^{L''-L} \\
&\times \langle n_d n_\beta n_\Delta L||T^{(k)}||n''_d n''_\beta n''_\Delta L''\rangle \langle n''_d n''_\beta n''_\Delta L''||U^{(k)}||n'_d n'_\beta n'_\Delta L\rangle
\end{aligned}
\tag{22}
$$

where $T^{(k)}$ and $U^{(k)}$ are generic tensor operators that couple to angular momentum k. The next step is to decouple the remaining $[\tilde{d}\tilde{d}]^{(2)}$ reduced matrix element:

$$
\begin{aligned}
\langle n_d n_\beta n_\Delta L||\left(T^{(k_1)} \times U^{(k_2)}\right)^{(k)}||n'_d n'_\beta n'_\Delta L'\rangle = &(-1)^{(L+L'+k)}\sqrt{2k+1} \\
&\times \sum_{n''_d, n''_\beta, n''_\Delta, L''} \langle n_d n_\beta n_\Delta L||T^{(k_1)}||n''_d n''_\beta n''_\Delta L''\rangle \\
&\times \langle n''_d n''_\beta n''_\Delta L''||U^{(k_2)}||n'_d n'_\beta n'_\Delta L'\rangle \begin{Bmatrix} k_1 & k_2 & k \\ L' & L & L'' \end{Bmatrix}
\end{aligned}
\tag{23}
$$

At this point, the reduced matrix element $\langle n_s n_d n_\beta n_\Delta L||[d^\dagger s^\dagger]^{(2)} \cdot [\tilde{d}\tilde{d}]^{(2)}||n'_s n'_d n'_\beta n'_\Delta L\rangle$ has been decoupled into a sum of products of reduced matrix elements of the individual boson operators, and 6-j symbols. The reduced matrix elements of the boson operators can be related to the coefficients of fractional parentage of identical bosons.

4. Reduced Matrix Elements

The reduced matrix element $\langle n_s n_d n_\beta n_\Delta L||d^\dagger||n'_s n'_d n'_\beta n'_\Delta L'\rangle$ is found using a recursion formula. An efficient algorithm that uses isoscalar factors for calculating these coefficients is particularly well suited for identical boson systems with well-defined seniority [31, 32]. The procedure begins by first calculating the multiplicity of states for a given angular momentum L and seniority v. These can be found by solving for the coefficients of Gaussian polynomials [33].

4.1. Multiplicity of States

The first step in calculating the multiplicity of states for a given angular momentum L and seniority v is to solve for the coefficients p_m of Gaussian polynomials [33]. The allowed values of m range from 1 to nl, where n is the number of bosons, and l is the angular momentum of each boson.

$$
p_m = \sum_{\substack{s=1 \\ s \mid m}}^{min(r,p-r)} s - \sum_{\substack{s=max(r,p-r)+1 \\ s \mid m}}^{p} s
\tag{24}
$$

where $p = 2l+1$, $r = n$, and $s \mid m$ means that only terms where s is divisible by m are included. Next, the coefficients c_m are calculated recursively using p_m.

$$
c_m = \frac{1}{m} \sum_{s=0}^{m-1} p_{m-s} c_s
\tag{25}
$$

where $c_0 = 1$. The multiplicity of states for n bosons and angular momentum L is $c_{(nl-L)} - c_{(nl-L-1)}$. The orthogonalization procedure used during the calculation of reduced matrix elements requires the multiplicity of states for a seniority v and angular momentum L, which is calculated by $c_{(vl-L)} - c_{(vl-L-1)} - c_{((v-2)l-L)} + c_{((v-2)l-L-1)}$, assuming $v \geq 2$. For $v < 2$, the multiplicity is simply $c_{(vl-L)} - c_{(vl-L-1)}$. For a d-boson system, l should be set to 2.

4.2. Isoscalar factors

Isoscalar factors (ISFs) are closely related to the required reduced matrix elements of the single d-boson creation operator, and can be solved for using the following recursive formula [31, 32]:

$$\left\langle \begin{array}{cc|c} (1) & (v-1) & (v) \\ l & \alpha_1 L_1 & (\alpha_1' L_1') L \end{array} \right\rangle = \frac{P(\alpha_1' \; L_1' \; \alpha_1 \; L_1 \; L)}{\sqrt{vP(\alpha_1' \; L_1' \; \alpha_1' \; L_1' \; L)}} \tag{26}$$

where $P(\alpha_1' \; L_1' \; \alpha_1 \; L_1 \; L)$ is defined by

$$\begin{aligned} P(\alpha_1' \; L_1' \; \alpha_1 \; L_1 \; L) &= \delta_{\alpha_1',\alpha_1}\delta_{L_1',L_1} + (-1)^{L+L_1'}(v-1) \\ &\times \sqrt{(2L_1'+1)(2L_1+1)} \sum_{\alpha_2,L_2} \left(\left\{ \begin{array}{ccc} l & L_2 & L_1' \\ l & L & L_1 \end{array} \right\} \right. \\ &\left. - \frac{2\delta_{L_2,L}}{(2L+1)(N-4+2v)} \right) \left\langle \begin{array}{cc|c} (1) & (v-2) & (v-1) \\ l & \alpha_2 L_2 & \alpha_1 L_1 \end{array} \right\rangle \\ &\times \left\langle \begin{array}{cc|c} (1) & (v-2) & (v-1) \\ l & \alpha_2 L_2 & \alpha_1' L_1' \end{array} \right\rangle \end{aligned} \tag{27}$$

assuming the following initial values:

$$\left\langle \begin{array}{cc|c} (1) & (1) & (2) \\ l & l & L \end{array} \right\rangle = 1 \qquad (L = 0, 2, 4, \ldots, 2l)$$

This set of coefficients will be overcomplete, so Gram-Schmidt orthogonalization is used to calculate the orthogonal ISFs. The $\alpha = 0$ set of coefficients for a given L and v is accepted without orthogonalization. For the $\alpha > 0$ sets of coefficients, all previous sets of coefficients with the same L and v must be projected out. If only zeros are left after projecting out sets of coefficients, then the new set was not unique, and should be ignored. If non-zero values are left, then a new set of ISFs has been found, and the whole set should be normalized [31, 32].

This procedure uses the multiplicity of states to identify when all sets of ISFs have been calculated. The relationship between reduced matrix elements of the d-boson creation operator and ISFs is the following:

$$\langle v v \alpha L \| d^\dagger \| (v-1)(v-1)\alpha' L' \rangle = \sqrt{v} \left\langle \begin{array}{cc|c} (1) & (v-1) & (v) \\ 2 & \alpha' L' & \alpha L \end{array} \right\rangle \tag{28}$$

4.3. Arbitrary precision

When using standard double-precision floating point arithmetic for calculating these reduced matrix elements, numerical errors begin to dominate in the coefficients beyond 50 bosons, due to the procedure being recursive. At each recursion, the ISFs will have fractionally less precision than the previous recursion, and eventually, not enough precision will be left to orthogonalize the set. Long before that point, the coefficients cease to be useful. For the preparation of reduced matrix elements for the program `ibar`, an arbitrary precision arithmetic library called GMP was used to perform arithmetic to a user-defined precision [34].

During the process of calculating sets of reduced matrix elements, it became apparent that approximately one digit of decimal precision is lost for every three particles added to the system. This value was determined by taking the largest remainder from orthogonalization in each iteration. With the expectation of calculating up to 1000 bosons, 400 decimal digits of precision were used. Near 400 bosons, several computational bottlenecks became apparent: storing a high precision set of ISFs for a single seniority uses an enormous amount of RAM, loading the full set of ISFs in double-precision for 400 bosons requires more than 500 MB of RAM, and the calculation of ISFs can take weeks on a modern desktop computer.

To address the RAM concern for storing the 400-digit ISFs, the relevant ISFs from the previous seniority are actively loaded and released based on which new coefficients require them. Although it is natural to calculate a single seniority at a time, restructuring the double-precision coefficient files such that they are ordered by angular momentum L rather than seniority v significantly reduces the amount of memory required to store them. This file format is functional in `ibar` due to the block diagonal nature of the Hamiltonian, and the fact that the Hamiltonian matrix elements do not require ISFs with significantly different angular momentum than the current L.

Beyond the precision loss from using a recursive formula, the calculation of 6-j symbols, which are essential ingredients in angular momentum coupling, can result in significant precision loss. They can be calculated in the following way [29]:

$$\begin{aligned} \left\{ \begin{array}{ccc} J_1 & J_2 & J_3 \\ j_1 & j_2 & j_3 \end{array} \right\} &= \Delta(J_1 J_2 J_3)\Delta(J_1 j_2 j_3)\Delta(j_1 J_2 j_3) \\ &\times \Delta(j_1 j_2 J_3) \sum_t \frac{(-1)^t (t+1)!}{f(t)} \end{aligned} \tag{29}$$

where $\Delta(j_1 j_2 j_3)$ are the triangle coefficients:

$$\Delta(j_1 j_2 j_3) = \sqrt{\frac{(j_1 + j_2 - j_3)!(j_1 - j_2 + j_3)!(-j_1 + j_2 + j_3)!}{(j_1 + j_2 + j_3 + 1)!}} \tag{30}$$

The factor $f(t)$ in the denominator of Eq. 29 is a large product of factorials:

$$\begin{aligned} f(t) &= (t - J_1 - J_2 - J_3)!(t - J_1 - j_2 - j_3)!(t - j_1 - J_2 - j_3)! \\ &\times (t - j_1 - j_2 - J_3)!(j_1 + j_2 + J_1 + J_2 - t)! \\ &\times (j_2 + j_3 + J_2 + J_3 - t)!(j_1 + j_3 + J_1 + J_3 - t)! \end{aligned} \tag{31}$$

where t takes on all integer values where the factorials have non-negative arguments. Double-precision floating point numbers can have exponents that range from approximately 10^{-308} to 10^{308}. A system with 400 d-bosons can couple to angular momentum 800, and 800! has about 1977 decimal digits, so beyond precision loss from alternating signs in the t sum, there is some risk of overflow when multiplying the factorials. This is resolved by taking the natural logarithm of the factorials, and adding those together, instead of multiplying the factorials. As a simple example of this process:

$$\ln\left(\frac{a!b!}{c!d!}\right) = \ln(a!) + \ln(b!) - \ln(c!) - \ln(d!) \tag{32}$$

Also, the calculation of the factorial itself can be rewritten:

$$\ln(a!) = \ln\left(\prod_{k=1}^{a} k\right) = \sum_{k=1}^{a} \ln(k) \tag{33}$$

Once the factorials in the numerator and denominator of the sum in Eq. 29 have been combined in the logarithm, an exponential is taken, and the terms are added together. There is precision loss from the alternating signs, so calculating these coefficients with high-precision is helpful. Logarithms and exponentials have not yet been added to GMP at the time of this writing, so the exponentials were calculated in the form of a Taylor expansion. The logarithms were calculated as the inverse of the exponential using the Newton-Raphson method. To avoid precision loss from these 6-j symbols in `ibar`, a lookup table is calculated in high precision using GMP and is saved as double-precision in a coefficient file.

The reduced matrix elements calculated by the described algorithm are ordered by a quantum number α rather than n_Δ. In order to use these elements in a calculation, the discussion about allowed values of n_Δ in Section 2.3 is used to define the relationship between n_Δ and α: the first allowed n_Δ is $\alpha = 0$, the second allowed n_Δ is $\alpha = 1$, and so on. Also, rather than storing every possible reduced matrix element $\langle n_d v \alpha L \| d^\dagger \| n'_d v' \alpha' L' \rangle$, it is adequate to keep only $\langle v v \alpha L \| d^\dagger \| (v-1)(v-1) \alpha' L' \rangle$. The following relation defines the reduced matrix elements in terms of those where $n_d = v$ [29]:

$$\langle n_d v \alpha L \| d^\dagger \| (n_d - 1)(v-1) \alpha' L' \rangle = \sqrt{\frac{n_d + v + 1}{2v + 1}} \times \langle v v \alpha L \| d^\dagger \| (v-1)(v-1) \alpha' L' \rangle \tag{34}$$

5. Diagonalization and transition matrix elements

5.1. Matrix diagonalization

With a procedure known for calculating all Hamiltonian matrix elements, the full Hamiltonian can be calculated. The basis can get quite large for system with a large number of bosons. For example, the $L = 20$ Hamiltonian for 400 bosons is a 138007×138007 matrix, and this would require 145.3 GB of storage to simply save the matrix if it was not compressed. The Hamiltonian matrix is sparse, so `ibar` compresses the matrix in a way that leaves out all zero matrix elements.

The next step is diagonalizing the Hamiltonian, and the library ARPACK is used to iteratively perform the diagonalization [35]. ARPACK uses an implicitly restarted Lanczos method for diagonalization, and the library asks `ibar` to perform the matrix multiplication manually. This is fortunate, as there would be no way for ARPACK to know about the custom matrix compression used in `ibar`.

An iterative method like Lanczos is desirable when calculating only a few eigenvectors, as it is significantly faster than fully diagonalizing the matrix and calculating all eigenvalues. If all eigenvalues were desired, then a full diagonalization would be the best option. The memory required to store the matrix, and the time required to diagonalize the matrix are the limiting factors for this method, but storing the Hamiltonian as a band matrix would help significantly. The basis is ordered by boson number, and the Hamiltonian terms cannot change the number of d-bosons by more than two, so the matrix elements should tend towards the diagonal. The option to fully diagonalize a band structured matrix using the library LAPACK may be added to a future version of `ibar`, but beyond a certain system size, storing the eigenvectors will be impractical [36].

5.2. Transition matrix elements

The E2 transition operator in `ibar` is defined in the following way:

$$\hat{T}(E2) = e_B \left([d^\dagger \tilde{s}]^{(2)} + [s^\dagger \tilde{d}]^{(2)} + \chi [d^\dagger \tilde{d}]^{(2)} \right) \tag{35}$$

In the consistent Q-formalism, χ of this operator is defined to be the same as the χ that appears in the Hamiltonian. Changing χ to a different value is an option, however, so this operator has up to two parameters. The reduced matrix elements of the operator are calculated in a similar way to how the Hamiltonian reduced matrix elements were calculated. The difference is that the Hamiltonian matrix elements used basis states, where transition operators use eigenstates of the Hamiltonian. This results in the evaluation of a large sum of cross terms between basis states for each transition matrix element.

Labeling the eigenstates by $|L\alpha\rangle$ allows us to define the R(E2) and B(E2) in terms of reduced matrix elements of the E2 operator:

$$R(E2; L_\alpha \to L'_{\alpha'}) = \langle L' \alpha' \| T^{(E2)} \| L \alpha \rangle$$
$$B(E2; L_\alpha \to L'_{\alpha'}) = \frac{1}{2L+1} \langle L' \alpha' \| T^{(E2)} \| L \alpha \rangle^2 \tag{36}$$

Electric monopole transitions can also be calculated, and the operator is defined in terms of the d-boson number operator:

$$\hat{T}(E0) = \beta_0 n_d \tag{37}$$

The n_d operator does not change any U(5) quantum numbers, so the only terms in the evaluation that can be nonzero have the same basis state on either side of the reduced matrix elements.

6. Results

6.1. Testing the software

In the previous sections, the algorithms used to generate reduced matrix elements and Hamiltonian matrix elements in `ibar` were explained in detail. One useful way to test whether the software gives the correct result is to select a Hamiltonian that is part of a dynamical symmetry, and compare the calculations to analytic expressions for those symmetries. The following SU(3) Hamiltonian is useful for testing this sd-IBM-1 software, as the Hamiltonian matrix elements require reduced matrix elements from the lookup table, and there are well known expressions for testing the eigenvalues and transition matrix elements:

$$\hat{H} = \kappa \hat{Q}^{-\sqrt{7}/2} \cdot \hat{Q}^{-\sqrt{7}/2}$$
$$\hat{Q}^{-\sqrt{7}/2} = [s^\dagger \tilde{d}]^{(2)} + [d^\dagger \tilde{s}]^{(2)} - \frac{\sqrt{7}}{2} [d^\dagger \tilde{d}]^{(2)} \tag{38}$$

where κ is a negative parameter. One feature of this Hamiltonian is that the ratio of energies $R_{4/2} = E(4_1^+)/E(2_1^+)$ is equal to 10/3 for all system sizes. A calculation performed in `ibar` for

400 bosons with this Hamiltonian deviates from this value by about 2×10^{-9}. When listing energy information about real nuclei, the binding energy is typically subtracted from the ground state, and the ground state is assigned an energy of 0. The eigenvalues of the $L = 0$ portion of an SU(3) Hamiltonian like Eq. 38 begin at an extremely negative value, and the ground state is then shifted up to 0 energy. For the 400 boson calculation where $\kappa = -\frac{1}{4N}$, the $R_{4/2}$ is actually calculated in the following way:

$$\frac{E(4_1^+)}{E(2_1^+)} = \frac{-200.7453125000006 + 200.7500000000011}{-200.7485937500001 + 200.7500000000011} \quad (39)$$

where the -200.75 value is the lowest energy eigenvalue from the $L = 0$ calculation, and can be subtracted out, as if it were a binding energy. This ratio of differences inherently has several digits of precision loss, which explains why the `ibar` value deviates from the analytical value by 2×10^{-9}, rather than something like 10^{-14}, which one might have expected in a double-precision calculation with a well-conditioned matrix. Another observable to test `ibar` with is a ratio of $B(E2)$s, such as $\frac{B(E2;4_1^+ \to 2_1^+)}{B(E2;2_1^+ \to 0_1^+)}$. The analytic expression for this ratio for the Hamiltonian given in Eq. 38 is the following:

$$\frac{B(E2; 4_1^+ \to 2_1^+)}{B(E2; 2_1^+ \to 0_1^+)} = \frac{10(2N-2)(2N+5)}{7(2N)(2N+3)}. \quad (40)$$

Transition strengths like this are calculated from sums of the eigenvectors and the relevant reduced matrix elements of the boson operators, and the calculated ratio deviates from the analytic expression by only 3×10^{-14}.

6.2. Degeneracy breaking

The Hamiltonian in Eq. 38 has several energy degeneracies, and the eigenvectors for these degenerate states have components in common. This creates a problem where the states become artificially mixed during diagonalization. If the Hamiltonian was written in terms of the SU(3) basis, there would be no interaction terms between such degenerate states, so the artificial mixing will yield incorrect results in the eigenvectors. To get around a problem like this, it is common to break the degeneracy with an extra term, like in the following Hamiltonian:

$$\hat{H} = \epsilon d^\dagger \cdot \tilde{d} + \kappa \hat{Q}^{-\sqrt{7}/2} \cdot \hat{Q}^{-\sqrt{7}/2}$$
$$\hat{Q}^{-\sqrt{7}/2} = [s^\dagger \tilde{d}]^{(2)} + [d^\dagger \tilde{s}]^{(2)} - \frac{\sqrt{7}}{2}[d^\dagger \tilde{d}]^{(2)} \quad (41)$$

where ϵ is extremely small. If $\epsilon = 0$, the 2_2^+ and 2_3^+ states are degenerate. Taking the limit as $\epsilon \to 0$, and setting $\kappa = -\frac{1}{4N}$ and $N = 400$, the transition strength $B(E2; 2_2^+ \to 0_2^+)$ should be exactly 63760. The B(E2) in Table 1 deviates from the analytic value of 63760 by a relative error of about 3×10^{-8} at $\epsilon = 10^{-6}$, and begins to diverge as ϵ is decreased further. It is extremely important to break the degeneracies in the SU(3) limit, if the observables of interest involve the eigenvectors of degenerate states. Setting $\epsilon = 10^{-6}$ should break the degeneracy in as safe a way as possible.

Table 1: Evolution of the transition strength $B(E2; 2_2^+ \to 0_2^+)$ as ϵ from Eq. 41 is decreased to 0.

ϵ	$B(E2; 2_2^+ \to 0_2^+)$
10^{-2}	63758.07223259
10^{-4}	63760.00207527
10^{-6}	63760.00211314
10^{-8}	63759.99585572
10^{-10}	63760.46962882
10^{-12}	34391.69107325
10^{-14}	20104.10125927

In contrast to the degeneracies of the SU(3) limit, the degeneracies that span the O(5) symmetry from U(5) to O(6) do not always create the same problems, as the eigenvectors frequently do not have components in common. However, care should also be taken with these degenerate states, as they can numerically create problems along the O(5) symmetry when calculating transition strengths between them. Although the degenerate states along the O(5) symmetry do not consistently mix, it can be safer to slightly break the degeneracy by adding in a small, but non-zero χ.

7. Conclusions

The software `ibar` has been developed and extensively tested for up to 400 bosons, and has been used successfully in a number of investigations into the behavior of quantum phase transitions in nuclei. The number of particles available in `ibar` is many times greater than what was previously available, and the generation of precise coefficients created numerous numerical challenges. Reduced matrix elements of the $d^\dagger$ operator, as well as 6-j symbols were calculated to high-precision using an arbitrary precision library. These coefficients are used to construct the Hamiltonian in `ibar`, and precise values for energies, wavefunctions, and transition strengths are found by diagonalizing the Hamiltonian. The software `ibar` and the coefficients it uses can be found at `http://www.nscodes.com`.

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