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MICROSCOPIC CALCULATION OF THE PARAMETERS OF THE INTERACTING BOSE-FERMI APPROXIMATION FOR NONDEGENERATE ORBITS

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Microscopic calculations of the parameters of the quadrupole operator of the Interacting Bose-Fermi Approximation are reported for the realistic case in which the valence orbits are nondegenerate. The results of these exact calculations are compared with those of an approximate formalism and in general reasonable agreement is found.

In this letter, we present the results of a fully microscopic calculation of the parameters of the Interacting Bose-Fermi Approximation (IBFA) [1] model for the realistic case in which the valence nucleons occupy nondegenerate single-particle orbitals. We focus on the quadrupole operator, which plays a central role in the model. In both the Interacting Boson Approximation (IBA) [2] model of even-even nuclei and the IBFA model of odd- A nuclei, the strength and structure of the quadrupole-quadrupole interaction dictate whether the nucleus is spherical, axially symmetric deformed or γ -unstable. In previous approaches to determine the form of the quadrupole operator for odd- A nuclei [3], the nondegeneracy of the valence nucleon orbits was treated approximately, using the Number Operator Approximation (NOA) [4] of Otsuka and Arima. In our calculations, the nondegeneracy of the valence orbits is treated exactly and our results are then compared with those of the earlier approximate treatment. We find that the approximate

formalism leads to results in fairly close agreement with our exact results.

The procedure we use is closely related to earlier work on the IBA [5]. As in that work we use a multinomial expansion to relate the matrix elements of the multi-orbit problem to matrix elements for individual orbits. We have, however, simplified the earlier formalism to facilitate its extension to the higher generalized seniority matrix elements required in the IBFA.

The IBFA model of odd- A nuclei is an approximation to the nuclear shell model. The states of the model are built up out of s and d boson creation operators and single fermion creation operators. The s and d boson creation operators correspond to the fermion operators S and D which create the energetically lowest pairs of like nucleons. The fermion pair creation operators can be expressed in terms of single-fermion creation operators c_j^+ according to

$$S^+ = \sum_j \alpha_j (\Omega_j/2)^{1/2} (c_j^+ c_j^+)^{(0)} \quad (1)$$

$$D^+ = \sum_{j_1 \leq j_2} \beta_{j_1 j_2} (1 + \delta_{j_1 j_2})^{-1/2} (c_{j_1}^+ c_{j_2}^+)^{(2)}, \quad (2)$$

where

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$$\Omega_j = j + 1/2. \quad (3)$$

For even-even nuclei, for which the IBA model applies, the correspondence between fermion and boson state vectors (for like nucleons) is expressed by [6,7]

$$(s^+)^N |0\rangle_B \Leftrightarrow (S^+) |\tilde{0}\rangle_F, \quad (4)$$

$$d^+(s^+)^{N-1} |0\rangle_B \Leftrightarrow D^+(S^+)^{N-1} |\tilde{0}\rangle_F. \quad (5)$$

Here we only indicate the correspondence through states with generalized-seniority [8] $v = 2$. Consideration of these state vectors is enough to generate the zeroth-order hamiltonian of the IBA [7]. We also introduce subscripts B and F to denote the closed shell vacua for bosons and fermions, respectively.

Introducing the single-fermion creation operators a_j^+ for the IBFA model space, we can extend the above correspondence (4), (5) to odd- A nuclei according to [3]

$$a_j^+ (s^+)^N |0\rangle_{\text{IBF}} \Leftrightarrow c_j^+ (S^+)^N |\tilde{0}\rangle_F, \quad (6)$$

$$(a_j^+ d^+)^{(J)} (s^+)^{N-1} |0\rangle_{\text{IBF}} \Leftrightarrow P_{v=3} (c_j^+ D^+)^{(J)} (S^+)^{N-1} |\tilde{0}\rangle_F. \quad (7)$$

In eq. (7), the projection operator $P_{v=3}$ is introduced to guarantee that the fermion state vector has $v = 3$ only. Also the subscript IBF denotes the vacuum of the boson-fermion space.

We can similarly impose a correspondence between the fermion quadrupole operator

$$Q_F^{(2)} = \sum_{j_1 j_2} q_{j_1 j_2} (c_{j_1}^+ \tilde{c}_{j_2})^{(2)}, \quad (8)$$

where

$$q_{j_1 j_2} = 5^{-1/2} \langle j_1 \| r^2 Y^{(2)} \| j_2 \rangle, \quad (9)$$

and the quadrupole operator $Q_{\text{IBFA}}^{(2)}$ of the IBFA.

As discussed in ref. [3], the IBFA quadrupole operator can be decomposed into a pure boson quadrupole operator $Q_B^{(2)}$ and a boson-fermion operator $Q_{\text{BF}}^{(2)}$, viz.

$$Q_{\text{IBFA}}^{(2)} = Q_B^{(2)} + Q_{\text{BF}}^{(2)}, \quad (10)$$

where

$$Q_B^{(2)} = \kappa (s^+ \tilde{d} + d^+ \tilde{s})^{(2)} + \chi (d^+ \tilde{d})^{(2)}, \quad (11)$$

$$\begin{aligned} Q_{\text{BF}}^{(2)} = & \sum_{j_1, j_2} \Gamma_{j_1, j_2} (a_{j_1}^+ \tilde{a}_{j_2})^{(2)} \\ & + \sum_{j_1, j_2, j_3} \Lambda_{j_1 j_2 j_3} : [(d^+ \tilde{a}_{j_1})^{(j_3)} (\tilde{s} a_{j_2}^+)^{(j_2)}]^{(2)} : \\ & + \text{h.c.} \end{aligned} \quad (12)$$

The normal ordering notation $(: :)$ indicates that in calculating the matrix elements of this operator contributions arising from the commutation of a_j^+ and $\tilde{a}_j$ are neglected. The operator $Q_{\text{BF}}^{(2)}$ can in principle include an additional term involving one d^+ operator and one $\tilde{d}$ operator. However, this term is expected to be less important than the two that are given in (12) and will not be considered in this work^{*1}.

The correspondence between the pure fermion quadrupole operator and the IBFA quadrupole operator is expressed by the requirement that the matrix elements of $Q_F^{(2)}$ between pure fermion states equal those of $Q_{\text{IBFA}}^{(2)}$ between the corresponding IBFA states.

Under the assumption that the structure coefficients α_j and $\beta_{j_1 j_2}$ of the S and D pair creation operators do not change with the addition of an odd fermion, the operator $Q_B^{(2)}$ is identical to the IBA quadrupole operator for the neighboring even-even nucleus. Microscopic calculations of the IBA quadrupole operator in a nondegenerate orbit formalism have already been reported elsewhere [5]. Thus, we report here only the results for the parameters $\Gamma_{j_1 j_2}$ and $\Lambda_{j_1 j_2 j_3}$ of $Q_{\text{BF}}^{(2)}$.

To obtain the parameters of $Q_{\text{BF}}^{(2)}$, it is necessary to evaluate the reduced matrix elements of the one-body operator $(c_{j_1}^+ \tilde{c}_{j_2})^{(2)}$ between fermion state vectors with generalized seniorities $v \leq 3$. In ref. [5], expressions for reduced one-body matrix elements through $v = 2$ were presented. To facilitate their extension to $v = 3$ states, we found it useful to first simplify these expressions. As an example, we now obtain for the reduced matrix element of $(c_{j_1}^+ \tilde{c}_{j_2})^{(2)}$ between $v = 2$ states the result

^{*1} Calculations of the IBF image of the fermion operator c_j^+ confirm that this term is less important than the others.

Table 1

Multi-orbit predictions for the parameters $\Gamma_{j_1 j_2}$ of the IBFA model neutron quadrupole operator for 13 valence neutrons outside an $N = 50$ core. The two sets of results presented are explained in the text.

j_2	Exact		Approx.					
	$j_1 = 7/2$		5/2	11/2	3/2	1/2	7/2	1/2
7/2	0.4842	0.1527	0	0	0.3393	0	0.3757	0.1137
5/2	-0.1527	0.3356	0	0	-0.1593	0.3518	-0.1137	0.2373
11/2	0	0	-0.6606	0	0	0	0	0
3/2	0.3393	0.1593	0	0	-0.5379	-0.5494	0.3603	0.1670
1/2	0	0.3518	0	0	0.5494	0	0	0.3584

$$\begin{aligned}
 & {}_F \langle \tilde{0} | S^{N-1} D \| (c_{j_1}^+ \tilde{c}_{j_2})^{(2)} \| D^+ (S^+)^{N-1} | \tilde{0} \rangle_F \\
 & = (-)^{j_1-j_2} 5^{3/2} \sum_{j_b} \beta_{j_1 j_b} \beta_{j_2 j_b} \begin{Bmatrix} j_2 & j_1 & 2 \\ 2 & 2 & j_b \end{Bmatrix} \\
 & \times [(1 + \delta_{j_1 j_b})(1 + \delta_{j_2 j_b})]^{1/2} \\
 & \times [S_{33}(j_1, j_b, j_2) - (\alpha_{j_2}/\alpha_{j_1}) S_{32}(j_b, j_2, j_1)], \quad (13)
 \end{aligned}$$

where

$$\begin{aligned}
 S_{33}(j_1, j_2, j_3) &= \sum_{\{i\}} R_{\{i\}} \\
 & \times \frac{(\Omega_1 - m_1)(\Omega_2 - m_2 - \delta_{12})(\Omega_3 - m_3 - \delta_{13} - \delta_{23})}{\Omega_1(\Omega_2 - \delta_{12})(\Omega_3 - \delta_{13} - \delta_{23})},
 \end{aligned} \quad (14)$$

$$\begin{aligned}
 S_{32}(j_1, j_2, j_3) &= \sum_{\{i\}} R_{\{i\}} \frac{(\Omega_1 - m_1)(\Omega_2 - m_2 - \delta_{12})m_3}{\Omega_1(\Omega_2 - \delta_{12})(\Omega_3 - \delta_{13} - \delta_{23})}, \quad (15)
 \end{aligned}$$

$$R_{\{i\}} = [(N-1)!]^2 \prod_{i=1}^k \alpha_i^{2m_i} \binom{\Omega_i}{m_i}. \quad (16)$$

In these equations, $\{i\}$ represents a given decomposition of the $2(N-1)$ particles in S pairs over the k active orbits, i.e. $\{i\} = (m_1, \dots, m_k)$ such that $\sum_{i=1}^k m_i = N-1$. These expressions should be compared with eqs. (A.3-9) in ref. [5]. By recognizing terms in this fashion, we have been able to derive the necessary formulae for $v=3$ matrix elements, which will be presented in a future article.

We have carried out calculations of the parameters of the neutron quadrupole operator in the 50-82 major shell. Necessary input to the calculations are the structure coefficients α_j and $\beta_{j_1 j_2}$ of the S and D correlated fermion pair creation operators. In this investigation, we assume for simplicity that for all neutron numbers the α_j coefficients have the following relative values:

$$\alpha_{g_{7/2}} = 0.9, \quad \alpha_{d_{5/2}} = 0.8, \quad \alpha_{h_{11/2}} = 0.3,$$

$$\alpha_{d_{3/2}} = 0.1, \quad \alpha_{s_{1/2}} = 0.05.$$

Furthermore, we assume that the D pair creation operator can be obtained from the S pair creation operator by requiring that

$$D^+ (S^+)^N | \tilde{0} \rangle_F \propto Q_F^{(2)} (S^+)^{N+1} | \tilde{0} \rangle_F. \quad (17)$$

Finally, in evaluating the reduced matrix elements of

Table 2

Multi-orbit predictions for the parameters $\Lambda_{j_1 j_2 j_3}$ of the IBFA model neutron quadrupole operator for 13 valence neutrons outside an $N = 50$ core. The two sets of results presented are explained in the text.

j_1	j_2	Exact										Approx.									
		$j_3 = j_1 - 2$	$j_1 - 1$	j_1	$j_1 + 1$	$j_1 + 2$	$j_1 - 2$	$j_1 - 1$	j_1	$j_1 + 1$	$j_1 + 2$	$j_1 - 2$	$j_1 - 1$	j_1	$j_1 + 1$	$j_1 + 2$	$j_1 - 2$	$j_1 - 1$	j_1	$j_1 + 1$	$j_1 + 2$
7/2	7/2	0.3014	-0.0108	0.0933	-0.0297	-0.0146	0.2877	0.0216	0.1271	0	0	0.2877	0.0216	0.1271	0	0	0.2877	0.0216	0.1271	0	0
	5/2	0.2751	-0.1090	0.0923	0.0011	0	0.2284	-0.1080	0.0905	0	0	0.2284	-0.1080	0.0905	0	0	0.2284	-0.1080	0.0905	0	0
	11/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	3/2	-0.1534	-0.0518	-0.3205	0	0	-0.1176	-0.0509	-0.2688	0	0	-0.1176	-0.0509	-0.2688	0	0	-0.1176	-0.0509	-0.2688	0	0
5/2	7/2	-0.1160	0.1077	0	0	0	-0.0889	0.0912	0	0	0	-0.0889	0.0912	0	0	0	-0.0889	0.0912	0	0	0
	5/2	0	0.2605	-0.1135	0.0853	-0.0166	0	0.2311	-0.1087	0.0909	0	0	0.2311	-0.1087	0.0909	0	0	0.2311	-0.1087	0.0909	0
	11/2	0.3089	0.0199	0.1077	-0.0123	-0.0124	0.2932	0.0459	0.1361	0.0162	0	0.2932	0.0459	0.1361	0.0162	0	0.2932	0.0459	0.1361	0.0162	0
	3/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11/2	7/2	0.1766	-0.0716	0.1624	-0.1251	0	0.1273	-0.0472	0.1282	-0.0961	0	0.1273	-0.0472	0.1282	-0.0961	0	0.1273	-0.0472	0.1282	-0.0961	0
	5/2	0	-0.0356	-0.2710	0	0	0	-0.0357	-0.2298	0	0	0	-0.0357	-0.2298	0	0	0	-0.0357	-0.2298	0	0
	11/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	3/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3/2	7/2	-0.0088	-0.0132	0.1045	-0.0049	-0.0086	0	0	0.1075	0	0	0	0	0.1075	0	0	0	0	0.1075	0	0
	5/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	11/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	3/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1/2	7/2	0	0	-0.1664	-0.0625	-0.2994	0	0	-0.1331	-0.0518	-0.2723	0	0	-0.1331	-0.0518	-0.2723	0	0	-0.1331	-0.0518	-0.2723
	5/2	0	0.1645	-0.0603	0.1465	-0.1096	0	0.1433	-0.0528	0.1298	-0.0968	0	0.1433	-0.0528	0.1298	-0.0968	0	0.1433	-0.0528	0.1298	-0.0968
	11/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	3/2	0	0.0149	0.0127	0.0285	0.1561	0	0.0156	0.0136	0.0306	0.1439	0	0.0156	0.0136	0.0306	0.1439	0	0.0156	0.0136	0.0306	0.1439
1/2	7/2	0	0	0.0229	-0.1190	0	0	0	0.0206	-0.1097	0	0	0	0.0206	-0.1097	0	0	0	0.0206	-0.1097	0
	5/2	0	0	0	-0.1095	0.1005	0	-0.1095	0.1005	0.0924	0.0924	0	0	0.1005	-0.1007	0.0924	0	0	0.1005	-0.1007	0.0924
	11/2	0	0	0	-0.0605	-0.2490	0	-0.0605	-0.2490	-0.2314	-0.2314	0	0	-0.2490	-0.0400	-0.2314	0	0	-0.2490	-0.0400	-0.2314
	3/2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1/2	7/2	0	0	0	0.0229	-0.1205	0	0.0229	-0.1205	0.0206	0.0206	0	0	0.0206	0.0206	0.0206	0	0	0.0206	0.0206	0.0206
	3/2	0	0	0	0.0061	0.1018	0	0.0061	0.1018	0.0977	0.0977	0	0	0.1018	0.0078	0.0977	0	0	0.1018	0.0078	0.0977

$r^2Y^{(2)}$ required in (9) and (17), we assume harmonic oscillator radial wave functions.

We report here the results of our calculations for 13 valence neutrons ($N = 6$). Our results for the parameters $\Gamma_{j_1j_2}$ and $\Lambda_{j_1j_2j_3}$ are given in the columns labelled "exact" in tables 1 and 2, respectively. We also include in the columns labelled "approx." the approximate results that emerge from the NOA formalism discussed in ref. [3]. The formulae we use are

$$\Gamma_{j_1j_2} = q_{j_1j_2}(u_{j_1}u_{j_2} - v_{j_1}v_{j_2}), \quad (18)$$

$$\Lambda_{j_1j_2j_3} = -(10/N)^{1/2} q_{j_3j_2}(u_{j_3}v_{j_2} + v_{j_3}u_{j_2}) \times \frac{\bar{\beta}_{j_1j_3}}{\sqrt{2j_3+1}} \frac{1}{1+\delta_{j_1j_2}} \quad (19)$$

where

$$\bar{\beta}_{jj'} = A\beta_{jj'}\sqrt{1+\delta_{jj'}} u_j u_{j'}, \quad (20)$$

$$v_j^2 = {}_F\langle \tilde{0} | (S^y)^{n/2} | \hat{N}_j | (S^+)^{n/2} | \tilde{0} \rangle_F / (2j+1), \quad (21)$$

$$u_j^2 = 1 - v_j^2. \quad (22)$$

The normalization constant A appearing in (20) is obtained by requiring that

$$\sum_{j,j'} \bar{\beta}_{jj'}^2 = 1. \quad (23)$$

The expression (19) for $\Lambda_{j_1j_2j_3}$ differs from that in ref. [3] by a factor $(1+\delta_{j_1j_2})^{-1}$. This factor improves the agreement between the exact and approximate results (for $j_1 = j_2$) and its origin is currently under investigation.

From the tables, it is clear that the approximate formalism reproduces the exact results quite well, typically within 10%. Thus, it is reasonable to use the very simple expressions (18)–(22) to estimate the parameters of the model. A similar conclusion was reached independently by van Egmond and Allaart

[9], who carried out microscopic calculations in the framework of the Broken Pair Approximation.

We have also compared our exact results for the pure boson quadrupole operator $Q_B^{(2)}$ with those of the approximate theory and there too the numerical agreement is very good.

Finally, we have considered alternative prescriptions for choosing the D pair creation operator that enhance subshell effects relative to the prescription (17). Again reasonable agreement with approximate NOA calculations is achieved.

In summary, we have presented the results of microscopic calculations for the parameters of the quadrupole operator of the Interacting Bose–Fermi Approximation. We have shown that these parameters can be evaluated exactly including subshell effects that arise from the nondegeneracy of the valence orbits and also that an earlier treatment in which subshell effects were treated approximately gives a reasonably accurate reproduction of the exact results.

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