Importance of the hexadecapole-hexadecapole interaction

E. D. Davis,[1] B. R. Barrett,[2] and A. F. Diallo[3]
[1]*Physics Department, Kuwait University, P.O. Box 5969, Safat, Kuwait*
[2]*Department of Physics, University of Arizona, Tucson, Arizona 85721*
[3]*Universidad tecnológica de Panamá, Centro de Azuero, Apdo 308 Chitré, Republic of Panamá*
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Motivated by the sensitivity of collective $M1$ excitations to the hexadecapole-hexadecapole interaction, we explore the influence of this and other features of sdgIBM on the ground-state band properties of deformed rare-earth nuclei. We adopt microscopically motivated choices of the Hamiltonian parameters and work within the angular-momentum-projected intrinsic state formalism, deriving analytic expressions for observables in which the dependence on wave functions and parameters of the model is explicit. We find that energies of ground-state band excitations are insensitive to the hexadecapole-hexadecapole interaction. On the other hand, its contribution to the deformation energy term in the nuclear binding energy is substantial. Our results indicate that angular momentum projection is important even for well-deformed nuclei and that at least two g bosons should be utilized in the corresponding sdgIBM calculations. [S0556-2813(99)04001-7]

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I. INTRODUCTION

The interacting boson model with s and d degrees of freedom (sdIBM-1) and the generalization in which neutron and proton degrees of freedom are distinguished (sdIBM-2) have provided many insights into the regularities of complex nuclei [1]. Another generalization suggested by microscopic considerations, namely, the inclusion of a g-boson degree of freedom [2], also looks phenomenologically useful. An increasing body of studies have shown that not only is a semiquantitative description of $E4$ data possible within the sdgIBM-1, but also an improved description of rotational bands and $E2$ data is obtained [3–5].

Applications of the sdgIBM-1 and the sdgIBM-2 have been inhibited by their complexity. However, for us, their attraction lies in the hope that sdgIBM parameters may be more amenable to microscopic interpretation than sdIBM parameters. It is, for example, possible within the sdgIBM-2 (but not the sdIBM-2) to reproduce with essentially constant Hamiltonian parameters a spherical-to-deformed shape transition in an isotopic chain [6]. Also, one can accommodate in the sdgIBM-2 the energetics of $M1$ scissors states (while adhering to microscopically motivated values of model parameters) without resorting to the use of the somewhat artificial Majorana interaction invoked in the sdIBM-2 [7].

In the applications of the sdgIBM-1 and -2 to date, there has been no consensus about the overall structure of the Hamiltonian. A Hamiltonian of the form (our notation is defined in Sec. II below)

$$\hat{H}=\sum_{l=2,4}(\epsilon_{lp}\hat{n}_{lp}+\epsilon_{ln}\hat{n}_{ln})-\sum_{k=2,4}\kappa_k\hat{T}_p^{(k)}\cdot\hat{T}_n^{(k)} \tag{1}$$

would be microscopically reasonable, but the hexadecapole-hexadecapole interaction (the $k=4$ term above) has been omitted in several previous phenomenological studies [4,8]. A conclusion of our earlier work on the scissors states is that their excitation energies are as sensitive to the hexadecapole-hexadecapole interaction as they are to the quadrupole-quadrupole interaction (the $k=2$ term above) [7]. This sensitivity has been confirmed independently [9]. The implication would appear to be that use of the hexadecapole-hexadecapole interaction is strongly indicated. But if this is the case, how critical is knowledge of the poorly known parameters in the hexadecapole operator $\hat{T}_\rho^{(4)}$ and how reliable are previous studies in which the hexadecapole-hexadecapole interaction is neglected? More generally, there is the question of the overall compatibility of sdIBM-2 and sdgIBM-2 results for observables. In this paper, we explore these issues in connection with the properties of the ground-state band of deformed nuclei using only *microscopically motivated* parameter estimates.

The structure of this paper is as follows. In Sec. II, we discuss our choice of the sdgIBM-2 Hamiltonian and electric transition (Ek) operators. For the sake of definiteness, we present explicit expressions for our choices of the related model parameters (straight line fits to microscopic estimates). In Secs. III and IV, we review the calculational scheme we employ to obtain the ground-state band expectation values and transition matrix elements of interest. Since we confine our attention to well-deformed nuclei, we calculate ground-state band observables using an angular-momentum-projected intrinsic state. In Sec. III, our choice of intrinsic state is discussed and closed-form expressions for expectation values and matrix elements in terms of overlap integrals arising from angular momentum projection are given. In Sec. IV, we consider the analytic evaluation of these overlap integrals via an asymptotic expansion and establish the order to which it is necessary, in practice, to carry out this expansion. In Sec. V, we pin down an intrinsic wave function of the ground-state band by generalizing the method of Ref. [7] to include, where feasible, the leading corrections arising from angular momentum projection. The effect of these 10% or so corrections on our choice of wave function is substantial and brings it into line with intrinsic state wave functions found in other applications of the sdgIBM. In Sec. VI, we discuss our findings on the systematics of ground-state band observables for deformed rare-earth nuclei. We present several approximate analytical results which make explicit the role of the various ingredients of the sdgIBM-2. Our conclusions are given in Sec. VII. In particular, we find that sdgIBM-2 calculations for deformed nuclei should contain at least two g bosons.

II. MODEL AND ITS PARAMETERS

Our starting point is the sdgIBM-2 model with the Hamiltonian $\hat{H}$ of Eq. (1), in which $\hat{n}_{ln}(\hat{n}_{lp})$ is the number operator for neutron (proton) bosons of spin l and, in terms of the corresponding creation operators $b^\dagger_{ln}(b^\dagger_{lp})$ and their conjugates $\tilde{b}_{ln}(\tilde{b}_{lp})$, the multipole operator ($\rho=n,p$)

$$\hat{T}^{(k)}_\rho=\sum_{l,l'=0,2,4}(t^{(k)}_\rho)_{ll'}[b^\dagger_{l\rho}\times\tilde{b}_{l'\rho}]^{(k)},$$

where $[\cdots]^{(k)}$ denotes coupling to angular momentum k. Below, when the quantum number m for the z component of spin is *not* suppressed, $b^\dagger_{l\rho}\rightarrow b^\dagger_{lm\rho}$ and $\tilde{b}_{l\rho}\rightarrow\tilde{b}_{lm\rho}\equiv(-1)^{l-m}b_{l(-m)\rho}$. By definition, the multipole parameters $(t^{(k)}_\rho)_{ll'}$ are symmetric in l and l' and normalized so that $(t^{(k)}_\rho)_{0k}=1=(t^{(k)}_\rho)_{k0}$.

For simplicity, unless indicated otherwise below, we adopt, for *both* the neutron multipole parameters $(t^{(k)}_n)_{ll'}$ and the proton multipole parameters $(t^{(k)}_p)_{ll'}$, the microscopically motivated estimates of Ref. [7] for the *arithmetic average* $t^{(k)}_{ll'}\equiv\frac{1}{2}[(t^{(k)}_p)_{ll'}+(t^{(k)}_n)_{ll'}]$. (The level of sensitivity to the difference between neutron and proton multipole parameters for the ground-state expectation values we consider does not call for a more careful treatment.) The estimates of the nontrivial independent $t^{(k)}_{ll'}$'s have been expressed as functions of $P\equiv N_nN_p/(N_n+N_p)$, where $N_n(N_p)$ is the number of neutron (proton) bosons. The quadrupole parameters are $t^{(2)}_{22}=-1.1+0.24P$, $t^{(2)}_{24}=0.45$, and $t^{(2)}_{44}=-0.9+0.21P$ and the hexadecapole parameters are $t^{(4)}_{22}=0.6-0.12P$, $t^{(4)}_{24}=-1.1+0.27P$, and $t^{(4)}_{44}=0.95-0.16P$.

For the interaction strengths κ_2 and κ_4, we likewise adopt the microscopically motivated estimates of Ref. [7]: in MeV, $\kappa_2=0.13-0.007P$ and $\kappa_4=0.12+0.006P$. As regards the choice of boson energies $\epsilon_{l\rho}$ (which were not required in Ref. [7]), the most detailed microscopic calculations available [10] yield estimates (denoted below by $\epsilon^0_{l\rho}$) which are far too large. However, the *ratios* $\epsilon^0_{2\rho}/\epsilon^0_{4\rho}$ of these estimates are of the magnitude expected on microscopic grounds (namely, about 0.8 [6]). Also, the variation of the difference in the microscopic d-boson energies $\epsilon^0_{2p}-\epsilon^0_{2n}$ across the $Z=50$–82 and $N=82$–126 shells can account qualitatively for the systematics of F-spin admixtures in the 2^+_1 state [11]. It would thus seem reasonable to suppose that the microscopic estimates can in large part be corrected by a simple adjustment, namely, an additive self-energy renormalization. For simplicity, we take this additive renormalization to be the same for all the bosons. Since g-boson energies are expected on general microscopic grounds to be about twice the corresponding pairing gap energy [6], we set $\epsilon_{l\rho}=\epsilon^0_{l\rho}+[\Delta_p+\Delta_n-\frac{1}{2}(\epsilon^0_{4p}+\epsilon^0_{4n})]$, taking $\Delta_p+\Delta_n\approx2\Delta$, where Δ is the conventional estimate of the pairing gap [$\Delta=(11.8\ \text{MeV})/\sqrt{A}$]. The combinations

$$\epsilon_l=\frac{N_p}{N}\epsilon_{lp}+\frac{N_n}{N}\epsilon_{ln}$$

can be represented approximately over the interval of interest as the linear functions $\epsilon_2=1.92-0.18P$ and $\epsilon_4=2.12-0.10P$ (in MeV).

We assume that the $E2$ transition operator is given in terms of the quadrupole operators $\hat{T}^{(2)}_\rho$ appearing in the Hamiltonian by the one-body ansatz $\hat{T}(E2)=e^{(2)}_p\hat{T}^{(2)}_p+e^{(2)}_n\hat{T}^{(2)}_n$, where $e^{(2)}_p$ and $e^{(2)}_n$ denote the effective $E2$ boson charges. We adopt the analogous one-body ansatz for the $E4$ transition operator $\hat{T}(E4)$ in terms of the hexadecapole operators $\hat{T}^{(4)}_\rho$ in the Hamiltonian and effective $E4$ boson charges $e^{(4)}_\rho$.

In our evaluation of reduced Ek transition matrix elements in Sec. VI, we require the neutron and proton parameters only in the averaged combinations

$$\overline{e^{(k)}}\equiv\frac{N_p}{N}e^{(k)}_p+\frac{N_n}{N}e^{(k)}_n$$

and

$$\overline{t^{(k)}}\equiv\left(\frac{N_p}{N}e^{(k)}_pt^{(k)}_p+\frac{N_n}{N}e^{(k)}_nt^{(k)}_n\right)\Bigg/\left(\frac{N_p}{N}e^{(k)}_p+\frac{N_n}{N}e^{(k)}_n\right).$$

If we use effective $E2$ boson charges $e_\rho=\alpha_{2\rho}e^{\mathrm{F}}_\rho$, where the quadrupole renormalization constants $\alpha_{2\rho}$ are taken from Ref. [10] (on which the estimates of Ref. [7] for multipole parameters are based) and the effective $E2$ fermion charges e^{F}_ρ are standard ($e^{\mathrm{F}}_p=1.7A^{1/3}/100\ e\,\text{b}$, $e^{\mathrm{F}}_n=1.0A^{1/3}/100\ e\,\text{b}$), we find that, to within a few percent or so, $\overline{e^{(2)}}=0.12\ e\,\text{b}$ independent of the value of P (provided $P\gtrsim2$). The combinations $\overline{t^{(2)}}$ of the quadrupole parameters $t^{(2)}_\rho$ also agree to within a few percent with the arithmetic averages $t^{(2)}$ and so we use the latter.

Effective $E4$ fermion charges are less well known than effective $E2$ charges. Nevertheless, we think it is reasonable to assume that the combination $\overline{e^{(4)}}$ of effective $E4$ boson charges is approximately P independent (like the combination $\overline{e^{(2)}}$ of effective $E2$ boson charges) and that, paralleling our findings for $\overline{t^{(2)}}$, the combinations $\overline{t^{(4)}}$ of the hexadecapole parameters $t^{(4)}_\rho$ coincide to a good approximation with the arithmetic averages $t^{(4)}$. In evaluating $E4$ transition matrix elements below, we adopt the arithmetic averages $t^{(4)}$ given earlier and assume $\overline{e^{(4)}}$ is some (unspecified) constant.

Elsewhere, in the reduction of empirical data on the summed $M1$ strength (cf. Sec V), we require differences $g_{pl}-g_{nl}$ in neutron and proton boson g factors. We adopt the spin-independent estimate $g_p-g_n=1.56-0.085P$ based on the microscopic results of Ref. [11].

We believe that the above choices of model parameters are appropriate for the study of systematics and should be useful as starting values in detailed analyses of individual nuclei. In our investigations, we shall base our conclusions on the order of magnitude and the qualitative variation of our choices of model parameters.

III. ANGULAR-MOMENTUM-PROJECTED INTRINSIC STATE FORMALISM

As the intrinsic state of the ground-state band, we adopt the axially symmetric coherent state

$$|\{x_0,x_2,x_4\}\rangle=\frac{1}{\sqrt{N_p!N_n!}}\left[\sum_{l=0,2,4} x_l b^{\dagger}_{l0p}\right]^{N_p}\times\left[\sum_{l=0,2,4} x_l b^{\dagger}_{l0n}\right]^{N_n}|-\rangle, \tag{2}$$

where $|-\rangle$ denotes the vacuum state (containing no bosons) and the spin amplitudes x_l are subject to the normalization condition $\Sigma_l x_l^2=1$. A significant simplification inherent in Eq. (2) is that we take the neutron and proton spin amplitudes to be identical; in technical terms, our intrinsic state is of maximal F spin [12]. This is an idealization but a well-motivated one: admixtures of nonmaximal F spin in ground-state band members of well-deformed nuclei do not seem to occur at more than the few percent level [13], and, in any event, we shall restrict ourselves below to observables (like excitation energies and $E2$ transition strengths), which are insensitive to these small F-spin impurities.

Within the present approximation scheme, individual members $|\Phi^{\rm gsb}_{LM}\rangle$ of a ground-state band are projected out of $|\{x_l\}\rangle$: to within a normalization constant, $|\Phi^{\rm gsb}_{LM}\rangle \propto P^L_{M0}|\{x_l\}\rangle$, where P^L_{MK} denotes the standard angular momentum projection operator [14]. In the calculation of expectation values and transition matrix elements, we can exploit the maximal F spin of our intrinsic state (through the IBM-2 to IBM-1 projection scheme [13]), the spherical tensor character of the $b^{\dagger}_{lm\rho}$'s, and Wick's theorem to derive closed-form expressions involving the overlap integrals

$$\mathcal{I}_{k;j}(\lambda)=\int_0^1 P_k(x)P_j(x)\left[\sum_l x_l^2 P_l(x)\right]^{\lambda}dx,$$

where $P_k(x)$ denotes the Legendre polynomial of order k. (After the IBM-2 to IBM-1 projection, the calculations parallel those described in detail in Refs. [15] and [16].)

For the expectation value H_L of our Hamiltonian in the state $|\Phi^{\rm gsb}_{LM}\rangle$, we find, after some routine angular momentum recoupling algebra,

$$H_L=N\left\{\sum_l \epsilon_l x_l^2\frac{\mathcal{I}_{L;l}(N-1)}{\mathcal{I}_{L;0}(N)}-P\sum_{k,J}\kappa_k A_J^{(k)}\frac{\mathcal{I}_{L;J}(N-2)}{\mathcal{I}_{L;0}(N)}\right\}, \tag{3}$$

where

$$A_J^{(k)}=(2k+1)\sum_{j,j',l,l'}\langle j0j'0|J0\rangle\langle l0l'0|J0\rangle\times\begin{Bmatrix} j & j' & J\\ l' & l & k\end{Bmatrix}(t_p^{(k)})_{jl}(t_n^{(k)})_{j'l'}x_jx_lx_{j'}x_{l'}.$$

Between the states of good angular momentum projected out of $|\{x_l\}\rangle$, the Ek transition operator $\hat{T}(Ek)$ has reduced matrix elements ($L'\geqslant L$)

$$\langle L'\|\hat{T}(Ek)\|L\rangle=\sqrt{(2L'+1)(2L+1)}N\overline{e^{(k)}}\sum_J B_{JL'L}(k)\times\frac{\mathcal{I}_{0;J}(N-1)}{\sqrt{\mathcal{I}_{L';0}(N)\mathcal{I}_{L;0}(N)}}, \tag{4}$$

where

$$B_{JL'L}(k)\equiv\sqrt{2k+1}\sum_{j,l}\langle L'0j0|J0\rangle\langle L0l0|J0\rangle\times\begin{Bmatrix} L' & j & J\\ l & L & k\end{Bmatrix}(\overline{t^{(k)}})_{jl}x_jx_l.$$

After substitution of the overlap integrals above by their asymptotic expansions (see Sec. IV), the summations over J in Eqs. (3) and (4) can be further reduced analytically via the method of Appendix A in Ref. [16]. Observe that Eq. (4) can be written in terms of ratios of the form $\mathcal{I}_{0;J}(N-k)/\mathcal{I}_{0;J'}(N)$.

Results similar to Eqs. (3) and (4) have been obtained earlier within the context of sdgIBM-1 studies [5]. Our results represent a modest generalization inasmuch as the distinction between model parameters for neutrons and protons is, in principle, retained. More significantly, the projection from IBM-2 to IBM-1 is responsible for a different, more physical dependence on N_p and N_n of the expectation value of the interaction terms in the Hamiltonian.

IV. ASYMPTOTIC EXPANSION OF OVERLAP INTEGRALS

The overlap integrals $\mathcal{I}_{k;j}$ can be evaluated analytically as an expansion in *inverse* powers of the average angular momentum squared of the intrinsic state

$$\Lambda\equiv N\sum_l l(l+1)x_l^2,$$

which, for well-deformed nuclei, is a large parameter. These expansions are asymptotic and can be obtained either via Laplace's method for the asymptotic evaluation of integrals [16] or algebraically [17] (although their asymptotic character is then disguised).

For the two ratios of overlap integrals which arise in our work, the asymptotic analysis of Ref. [16] yields

$$\frac{\mathcal{I}_{L;J}(N-k)}{\mathcal{I}_{L;0}(N)}=1-[\overline{J}-km_1]\frac{1}{\Lambda}+\{\tfrac{1}{2}\overline{J}^2-[2(k-1)m_1+m_2/m_1-1-\overline{L}]\overline{J}+km_1[m_2/(2m_1)-1-\overline{L}]\}\frac{1}{\Lambda^2}+\cdots, \tag{5}$$

$$\frac{\mathcal{I}_{0;J}(N-k)}{\mathcal{I}_{0;L}(N)}=1-[\overline{J}-km_1-\overline{L}]\frac{1}{\Lambda}+\{\tfrac{1}{2}\overline{J}^2-[2(k-1)m_1+m_2/m_1-1+\overline{L}]\overline{J}+km_1[m_2/(2m_1)-1]$$
$$+[(k-2)m_1-1+m_2/m_1]\overline{L}+\tfrac{1}{2}\overline{L}^2\}\frac{1}{\Lambda^2}+\cdots, \tag{6}$$

where $\overline{J}\equiv J(J+1)$, m_n is the nth moment of the distribution of spin squared of a deformed intrinsic state boson, i.e.,

$$m_n=\sum_l (\overline{l})^n x_l^2, \tag{7}$$

and it is assumed that $k\ll N$ (in our applications, $k=0,1,2$).

The coefficients in the expansions of Eqs. (5) and (6) do not lend themselves to a simple intuitive interpretation and increase rapidly in complexity with succeeding orders. However, these expansions are useful in gauging the magnitude of the effect of angular momentum projection and in identifying clearly the angular momentum (or state) dependence of ground-state band properties, which would otherwise be difficult, because it is, in general, weak.

With the exception of the moment of inertia I of the ground-state band, we find it sufficient in our calculations to retain only the first two terms in the expansions of Eqs. (5) and (6). With the first term (which survives in the limit $\Lambda\to\infty$), we recover the results of the unprojected intrinsic state formalism; the term of order $1/\Lambda$ thus gives the leading correction arising from angular momentum projection. For $N\gtrsim 10$ (appropriate to the nuclei of interest to us) and reasonable choices of the spin amplitudes x_l (identified in Sec. V below), this leading correction is significant, being typically between 10% and 20% of the unprojected result. As we are dealing with a Poincaré asymptotic expansion, the correction due to all higher orders in $1/\Lambda$ is of the same order of magnitude as the term of order $1/\Lambda^2$, which, using Eqs. (5) and (6), we estimate to be a few percent or so of the unprojected result. We discard the terms of order $1/\Lambda^2$ and higher because they are comparable with the uncertainties already introduced by our neglect of F-spin admixtures.

Up to terms of order $1/\Lambda$, reduced matrix elements of the Ek transition operator between members of the ground-state band are given by the rigid rotor relation

$$\langle L'\|\hat{T}(Ek)\|L\rangle=\sqrt{2L+1}\langle L0k0|L'0\rangle\mathcal{M}_k,$$

in which $\mathcal{M}_k$ is the *state-independent* ground-state-band ''moment'':

$$\mathcal{M}_k=N\overline{e^{(k)}}\overline{\mathcal{O}}^{(k)}(0)\left\{1+[m_1+3-\overline{\mathcal{O}}^{(k)}(1)/\overline{\mathcal{O}}^{(k)}(0)]\frac{1}{\Lambda}\right\}.$$

Above,

$$\overline{\mathcal{O}}^{(k)}(r)\equiv\sum_{j,l}(\overline{j})^r\langle j0l0|k0\rangle(\overline{t^{(k)}})_{jl}x_jx_l.$$

Terms of order $1/\Lambda^2$ introduce a dependence on L and L' in $\mathcal{M}_k$, so that it can no longer be identified (to within a constant of proportionality) as an intrinsic quadrupole-hexadecapole moment of the ground-state band. The behavior for $E2$ transitions of such small state-dependent modifications (which, for the reasons given above, we ignore) has been explored within sdgIBM-1 in Ref. [5].

In the calculation of the moment of inertia I, we have to extract the dependence of the expectation value H_L on the angular momentum quantum number L. In the ratios $\mathcal{I}_{L;j}(N-k)/\mathcal{I}_{L;0}(N)$ in H_L, we keep L-dependent terms of order $1/\Lambda^2$, which is the first order in which L-dependent terms are encountered, and L-dependent terms of order $1/\Lambda^3$ [omitted in Eq. (5) because of their complexity]. To this order, ground-state band excitation energies $E_L\equiv H_L-H_{L=0}$ conform to a rotational spectrum $[=\hbar^2/(2I)L(L+1)]$ with a strictly constant (i.e., state-independent) moment of inertia I. The result for I, which is fairly lengthy, is given in the Appendix.

V. DETERMINATION OF THE WAVE FUNCTION $\{x_l\}$

A conventional variational determination of the wave function $\{x_l\}$ is confronted by the difficulty that reliable microscopic estimates of a crucial ingredient of the variational functional H_L, namely, the combination ϵ_l of boson energies, are *not* available. In Sec. VI B below, we shall see that the average of ϵ_2 and ϵ_4 is constrained by the moment of inertia I: a value of $\epsilon_2+\epsilon_4$ which is some 20% smaller than that obtained with our renormalized estimates of ϵ_2 and ϵ_4 is implied [see Eq. (10) and the related discussion]. Unfortunately, this improved knowledge of the *sum* of ϵ_2 and ϵ_4 is still not sufficient for a definitive variational determination of $\{x_l\}$ because the variational functional depends on ϵ_2 and ϵ_4 separately. (More precisely, the variational solution for x_2 is sensitive to ϵ_2, whereas that for x_4 is sensitive to the difference $\epsilon_4-\epsilon_2$.) Instead, we choose to fix the two independent amplitudes x_2 and x_4 using the empirical data on the summed $M1$ strength $\Sigma_i B(M1,0_1^+\to 1_i^+)$ and its centroid energy

$$E_c=\frac{\sum_i E_iB(M1,0_1^+\to 1_i^+)}{\sum_i B(M1,0_1^+\to 1_i^+)}$$

compiled in [18] and [19], respectively. (Specifically, we use below the data given in these papers for the Nd, Sm, Gd, Dy, and Er isotopes.) Via sum rules, these two observables are related directly to ground-state expectation values and there happen to be fairly reliable microscopic estimates for the model parameters to which these expectation values are sensitive (i.e., the interaction strengths κ_k and the differences in boson g factors g_{pl} and g_{nl}). These observables also have the advantage of being sensitive to the g-boson admixture in the ground state.

The relevant sum rules are the sdgIBM generalization [7,20] of the Ginocchio sum rule [21] for $M1$ strength,

$$\sum_i B(M1,0_1^+\rightarrow 1_i^+)=\frac{3}{4\pi}(g_p-g_n)^2\frac{P}{N-1}\sum_{l=2,4} l(l+1)n_l^{\text{g.s.}},$$

where $n_l^{\text{g.s.}}$ denotes the ground-state occupation number of both neutron and proton bosons of spin l, and the energy-weighted sum rule (a generalization to the present choice of Hamiltonian of the sum rule derived in Ref. [20])

$$\sum_i E_i B(M1,0_1^+\rightarrow 1_i^+)=\frac{3}{8\pi}(g_p-g_n)^2 \times\sum_{k=2,4}\overline{k}\kappa_k\langle 0_1^+,N_p,N_n|\times \hat{T}_p^{(k)}\cdot\hat{T}_n^{(k)}|0_1^+,N_p,N_n\rangle.$$

We find it convenient to work with the spin-weighted sum of ground-state boson occupation number *fractions*

$$O_s\equiv\sum_l l(l+1)n_l^{\text{g.s.}}/N$$

and the $M1$ centroid energy *per boson*, E_c/N [irritating factors of $N-1$ then appear in the combination $(N-1)/N=1-m_1/\Lambda$]. Within our angular-momentum-projected intrinsic state approximation scheme, we find that, to order $1/\Lambda$,

$$O_s=\sum_l \overline{l}x_l^2\frac{\mathcal{I}_{0;l}(N-1)}{\mathcal{I}_{0;0}(N)}=m_1-(m_2-m_1^2)\frac{1}{\Lambda},\qquad (8)$$

$$\frac{E_c}{N}=\frac{1}{2O_s}\frac{(N-1)}{N}\sum_J\left[\sum_k \overline{k}\kappa_k A_J^{(k)}\right]\frac{\mathcal{I}_{0;J}(N-2)}{\mathcal{I}_{0;0}(N)}$$
$$=\frac{1}{2m_1}\sum_{k=2,4}\overline{k}\kappa_k\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(0)\Big\{1+[\tfrac{1}{2}\overline{k}+m_2/m_1 -\mathcal{O}_p^{(k)}(1)/\mathcal{O}_p^{(k)}(0)-\mathcal{O}_n^{(k)}(1)/\mathcal{O}_n^{(k)}(0)]\frac{1}{\Lambda}\Big\},\qquad (9)$$

where, paralleling the definition of $\overline{\mathcal{O}}^{(k)}(r)$, $\mathcal{O}_p^{(k)}(r)\equiv\sum_{j,l}(\overline{j})^r\langle j0l0|k0\rangle(t_p^{(k)})_{jl}x_jx_l$.

Empirical values of O_s and E_c/N vary in a reasonably well-behaved fashion with P, consistent with the fact that the pertinent model parameters and the variational solution for the wave function $\{x_l\}$ prior to angular momentum projection can be characterized as functions of P. For $P>P_{\text{sat}}\simeq 2.5$ (the domain of interest to us), the values of O_s appear to saturate.

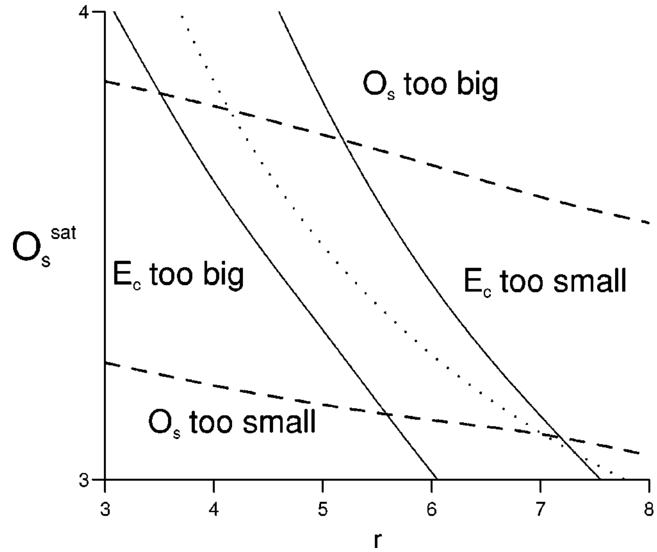

FIG. 1. Admissible ranges of O_s^{sat} and r. The solid (dashed) lines indicate the minimum and maximum values of O_s^{sat} compatible with data on $E_c(O_s)$ for fixed r. For comparison, the locus of points corresponding to $(x_2^{\text{sat}})^2=0.35$ is included (dotted line).

We consequently assume that the spin amplitudes x_l take on approximately constant values x_l^{sat} for $P>P_{\text{sat}}$. We find it convenient to parametrize the spin amplitudes x_l^{sat} in terms of the saturation value O_s^{sat} of O_s and the ratio r of $(x_2^{\text{sat}})^2$ to $(x_4^{\text{sat}})^2$. Neglecting terms of order $1/\Lambda$ in Eq. (8), we have

$$x_4^{\text{sat}}=\sqrt{O_s^{\text{sat}}/(20+6r)},\quad x_2^{\text{sat}}=\sqrt{r}x_4^{\text{sat}},$$

$$x_0^{\text{sat}}=\sqrt{1-(x_2^{\text{sat}})^2-(x_4^{\text{sat}})^2}.$$

We fix r and O_s^{sat} by requiring that, using Eqs. (8) and (9) with the terms of order $1/\Lambda$ included, we reproduce simultaneously the empirical data on O_s and E_c/N for $P>P_{\text{sat}}$. Our scheme for the determination of $\{x_l^{\text{sat}}\}$ (with its neglect of $1/\Lambda$ corrections in the parametrization of $\{x_l^{\text{sat}}\}$ but their inclusion in observables) is akin to the projection-after-variation approximation.

In view of the simplifications we have made, the uncertainties in the empirical values of O_s and E_c/N, and the neglect within the IBM of the fragmentation of $M1$ strength due to coupling to noncollective degrees of freedom, it is appropriate only to delineate reasonable ranges for the values of r and O_s^{sat} (for which eyeball comparisons suffice). Our findings on the range of acceptable values of O_s^{sat} and r are summarized in Fig. 1. Where definite values are required below [Figs. 2–4 and the evaluation of the binomial distribution in Eq. (12)], we shall adopt $O_s^{\text{sat}}=3.5$ and $r=5$ for which $(x_2^{\text{sat}})^2=0.35$ and $(x_4^{\text{sat}})^2=0.07$.

VI. GROUND-STATE BAND SYSTEMATICS

In Figs. 2 and 3, we compare our theoretical estimates for the inverse of the moment of inertia $1/I$ and $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}(=\mathcal{M}_2)$, respectively, with empirical values inferred from good rotors (which we take to mean nuclei for which the ratio of excitation energies $E_{4_1^+}/E_{2_1^+}\geqslant 3.25$).

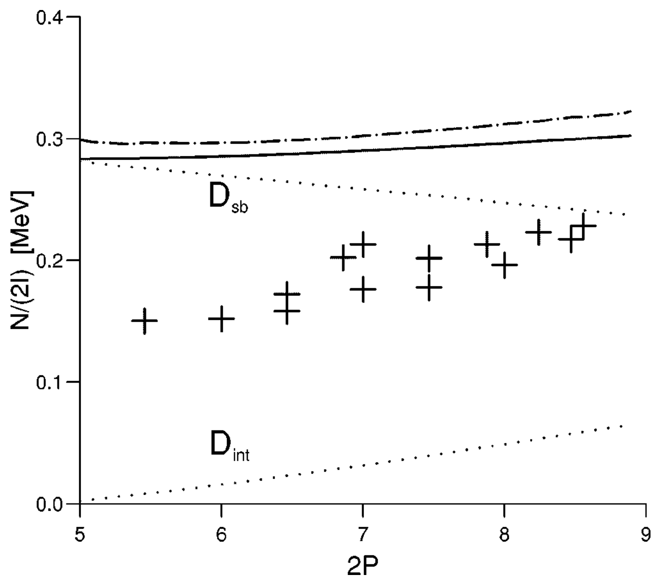

FIG. 2. Comparison with data on the inverse of the moment of inertia I (in units of $\hbar^2$) for the heavy rare-earth nuclei $^{154-158}$Sm, $^{158-162}$Gd, $^{160-166}$Dy, and $^{164-172}$Er (the even-even nuclei in this mass region for which $E_{4_1^+}/E_{2_1^+} \geqslant 3.5$). The unlabeled solid (dot-dashed) line is the theoretical estimate to leading (next-to-leading) order in the $1/\Lambda$ expansion. We identify the empirical value of $\hbar^2/2I$ as the coefficient a of the linear term in a fit of ground-state-band excitation energies $E_{L_1^+}$ (taken from [22]) to the quadratic $a\overline{L}+b\overline{L}^2$ in $\overline{L}\equiv L(L+1)$. (Since we restrict ourselves to good rotors, the values obtained in this way do not differ significantly from those deduced via the simple relation $\hbar^2/I = E_{2_1^+}/3$.)

Our prediction for the systematics of $\sqrt{B(E4;0_1^+\rightarrow 4_1^+)}$ $(=\mathcal{M}_4)$ in units of the combination $\overline{e^{(4)}}$ of effective $E4$ charges is given in Fig. 4. We underestimate the $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}$ data, but there is an encouraging similarity as regards the variation with P. There is an even stronger qualitative resemblance in the P dependence for our estimate of the inverse of the moment of inertia and empirical values (even though they are significantly overestimated). We view this as evidence that use of the P-independent wave function $\{x_l^{\rm sat}\}$ is adequate for the study of the systematics of well-deformed nuclei.

A. Reduced matrix elements

For reasonable choices of the quadrupole parameters $(t_\rho^{(2)})_{jl}$ and wave function $\{x_l\}$, our result for $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}$ is weakly dependent on the quadrupole parameters $(t_\rho^{(2)})_{22}$ (which are the counterparts within sdgIBM of the quadrupole parameters in sdIBM, usually denoted by χ_ρ) and the d-boson amplitude x_2 but almost completely insensitive to the remaining quadrupole parameters (which have no counterpart in sdIBM) and the g-boson amplitude x_4. In fact, to an accuracy of 10% or so, our estimate for

$$\sqrt{B(E2;0_1^+\rightarrow 2_1^+)} \approx N\overline{e^{(2)}}\{2x_0^{\rm sat}x_2^{\rm sat}+(\overline{t^{(2)}})_{22}(x_2^{\rm sat})^2\},$$

where we have dropped the $1/\Lambda$ correction in $\mathcal{M}_2$ and retained in $\overline{\mathcal{O}}^{(2)}(0)$ only the largest two terms. In effect, the expression for $B(E2;0_1^+\rightarrow 2_1^+)$'s reduces to one which would have been obtained within sdIBM-2.

The effective $E2$ boson charges are the model parameters to which $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}$ is most sensitive. Our values for $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}$ can be brought approximately into line with the data for $P \gtrsim 3.5$ by a modest 10% increase in our microscopically motivated choice of the effective $E2$ boson charges.

Our result for $\sqrt{B(E4;0_1^+\rightarrow 4_1^+)}$ displays some sensitivity to the hexadecapole parameters $(t_\rho^{(4)})_{24}$, but the dependence on the remaining hexadecapole parameters is weak. Paralleling our approximation of $\sqrt{B(E2;0_1^+\rightarrow 2_1^+)}$ above, we find that, to an accuracy of 15% or so, our result for $\sqrt{B(E4;0_1^+\rightarrow 4_1^+)}$ may be approximated by

$$\sqrt{B(E4;0_1^+\rightarrow 4_1^+)} \approx N\overline{e^{(4)}}\{2x_0^{\rm sat}x_4^{\rm sat}+2(\overline{t^{(4)}})_{24}x_2^{\rm sat}x_4^{\rm sat}\}.$$

Neither of the above two important contributions to $\sqrt{B(E4;0_1^+\rightarrow 4_1^+)}$ has a counterpart within sdIBM. The implication is that collective $B(E4;0_1^+\rightarrow 4_1^+)$'s cannot be successfully mocked up within sdIBM. Instead, the introduction of a g boson is crucial.

B. Inverse of the moment of inertia 1/*I*

Our estimate of $1/I$ is dominated by the leading term (of order Λ^0) in the noninteracting boson contribution $D_{\rm sb}$ [introduced in Eq. (A1)]. Decomposing ϵ_2 and ϵ_4 into their semisum and semidifference, we find that, for wave functions in the vicinity of our choice $\{x_l^{\rm sat}\}$, this leading term

$$D_{\rm sb}^{(0)} \equiv (e_1-e_0)/m_1 \approx \frac{(\epsilon_2+\epsilon_4)}{2}\frac{(x_0^{\rm sat})^2}{m_1^{\rm sat}} \qquad (10)$$

to an accuracy of 10% or so. We infer that we can easily improve on our estimate of $1/I$ by modifying our choice of single-boson energies. For example, a further decrease of about 10% in all the renormalized energies $\epsilon_{l\rho}$ is enough to achieve agreement with data for $P \gtrsim 3.5$. Given the uncertainties in the additive renormalization of single-boson energies $\epsilon_{l\rho}$, discussed in Sec. II, a change of this magnitude is not unreasonable. Another possibility is to leave our estimates of g-boson energies unchanged and to sharply reduce the d-boson energies by some 40% or so. With this modification, the variational solution for $\{x_l\}$ for $P>3$ is not too dissimilar from our wave function $\{x_l^{\rm sat}\}$. However, the ratio $\epsilon_{2\rho}/\epsilon_{4\rho}$ is then about 0.5, which is difficult to reconcile with the value of about 0.8 anticipated on microscopic grounds [6].

Since angular momentum projection raises the degeneracy of members of the intrinsic state band, we believe that the positive sign of the next-to-leading order contribution (in the $1/\Lambda$ expansion) to our estimate of $1/I$ in Fig. 2 is correct. However, it is apparent that inclusion of this next-to-leading order contribution worsens slightly the agreement with the data. This is presumably a consequence of the fact that, with our present choice of single-boson energies, we overestimate the magnitude of the leading order contribution to $1/I$. With a more felicitous choice of single-boson energies, it would lie below the empirical data.

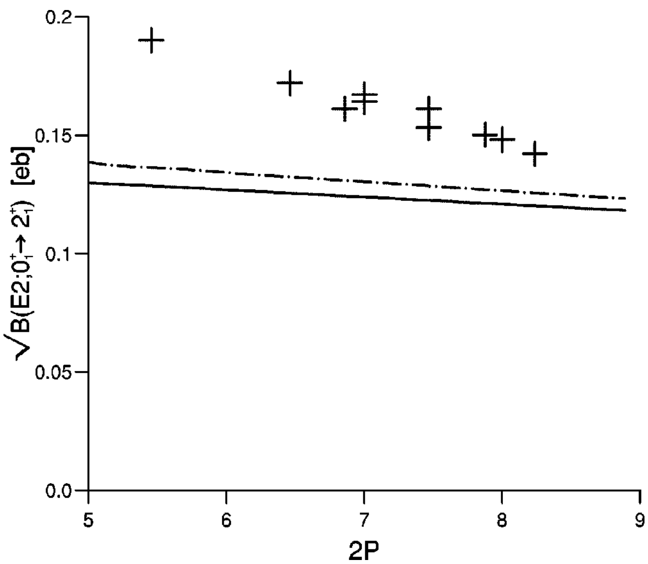

FIG. 3. Comparison with data (from [23]) on $\sqrt{B(E2;0_1^+\to 2_1^+)}$ for the heavy rare-earth nuclei ^{154}Sm, ^{158,160}Gd, $^{160-164}$Dy, and $^{164-170}$Er [the even-even nuclei in this mass region for which $E_{4_1^+}/E_{2_1^+}\geqslant 3.5$ and $B(E2;0_1^+\to 2_1^+)$ is measured]. The solid (dot-dashed) line is the theoretical estimate to leading (next-to-leading) order in the $1/\Lambda$ expansion.

The effect of the hexadecapole-hexadecapole interaction on $1/I$ is small. Near midshell, it is also small in relation to the impact of the quadrupole-quadrupole interaction on $1/I$. To leading order in the $1/\Lambda$ expansion, the contributions $D_{\rm int}(k)$ of the quadrupole-quadrupole interaction $(k=2)$ and the hexadecapole-hexadecapole interaction $(k=4)$ to $N/(2I)$ are given by

$$D_{\rm int}^{(0)}(k)=S_k\,P\,\kappa_k\,\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(0), \qquad (11)$$

where (see the Appendix)

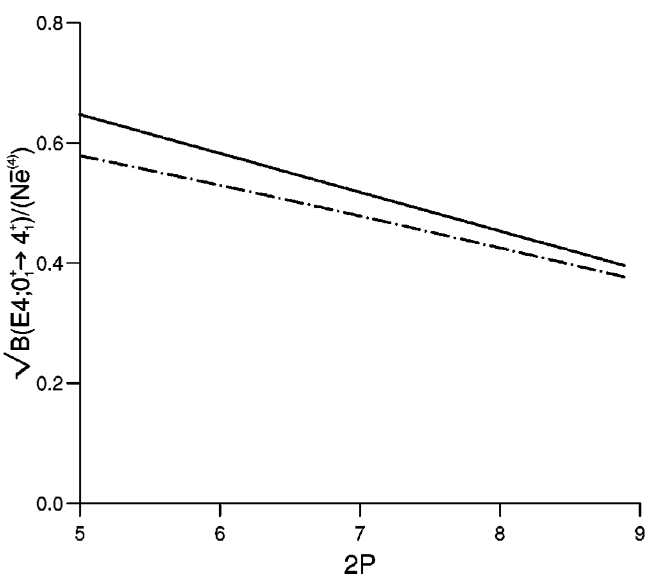

FIG. 4. Systematics of $\sqrt{B(E4;0_1^+\to 4_1^+)}/(\overline{Ne^{(4)}})$. The solid (dot-dashed) line is the theoretical estimate to leading (next-to-leading) order in the $1/\Lambda$ expansion.

$$S_k\equiv\frac{2}{m_1}\left\{1-\frac{1}{2m_1}\left[\frac{\mathcal{O}_p^{(k)}(1)}{\mathcal{O}_p^{(k)}(0)}+\frac{\mathcal{O}_n^{(k)}(1)}{\mathcal{O}_n^{(k)}(0)}-\frac{\overline{k}}{2}\right]\right\}.$$

For the range of P of interest, the S_k's have approximately constant values less than unity. A simple and surprisingly good estimate of the S_k's is obtained by retaining in $\mathcal{O}_\rho^{(k)}(r)$ only the term $(1+\delta_{r0})(\overline{k})^r x_0 x_k$, which is always 50% or more of the full result for $\mathcal{O}_\rho^{(k)}(r)$: then, $S_k=(2/m_1)\{1-\overline{k}/(4m_1)\}$, which, for $m_1\simeq 3.5$, implies that $S_2\simeq+0.3$ and $S_4\simeq-0.2$. When the full expression for $\mathcal{O}_\rho^{(k)}(r)$ is used, we find that, for reasonable wave functions, $S_2(S_4)$ increases from about 0.15 (-0.15) to about 0.2 (-0.1) as P increases from 3 to 4.5. Over the same range of values of P, the ratio $|D_{\rm int}^{(0)}(4)/D_{\rm int}^{(0)}(2)|$ decreases from about 0.4 to about 0.1 and $|D_{\rm int}^{(0)}(4)|$ decreases from about 10% or so of $N/(2I)$ to a few percent or so.

Since the dependence of $\mathcal{O}_\rho^{(2)}(0)$ on x_4 is weak, the effect of the g-boson degree of freedom on $D_{\rm int}^{(0)}(2)$ is negligible. The influence of the g boson on the moment of inertia is confined to the dependence of the noninteracting boson contribution $D_{\rm sb}^{(0)}$ on the g-boson energy ϵ_4 [cf. Eq. (10)]. In the absence of the g-boson degree of freedom, $D_{\rm sb}^{(0)}=\epsilon_2(x_0^{\rm sat})^2/m_1^{\rm sat}$. For our choices of ϵ_2 and ϵ_4, inclusion of the g-boson contribution enhances $D_{\rm sb}^{(0)}$ by about 20% or so.

C. g-boson admixture

The influence of a g-boson admixture on $B(E2)$'s and $B(E4)$'s within a ground-state band has been discussed above in Sec. VI A. In much the same way as the g-boson amplitude is essential to collective $B(E4;0_1^+\to 4_1^+)$'s, the magnitude of the contribution of the hexadecapole-hexadecapole interaction to observables, which, to leading order in the $1/\Lambda$ expansion, is proportional to $\mathcal{O}_n^{(4)}(0)\mathcal{O}_p^{(4)}(0)$ [see, for example, Eqs. (9) and (11)], is crucially determined by the g-boson amplitude: the dominant terms in $\mathcal{O}_n^{(4)}(0)\mathcal{O}_p^{(4)}(0)$ are all proportional to $(x_4^{\rm sat})^2$.

Because of the weighting of the ground-state occupation numbers $n_l^{\rm g.s.}$ by the spin squared $l(l+1)$, the g-boson contribution to the summed $M1$ strength is substantial even with our choice of wave function $\{x_l^{\rm sat}\}$. Within the unprojected intrinsic state formalism $[n_l^{\rm g.s.}=N(x_l^{\rm sat})^2]$, the g-boson contribution is about 40% of the summed $M1$ strength. Including angular momentum projection corrections of order $1/\Lambda$,

$$n_l^{\rm g.s.}=Nx_l^2\left\{1-(\overline{l}-m_1)\frac{1}{\Lambda}+\cdots\right\},$$

which, for $N\simeq 10$, implies a 40% or so reduction in the g-boson ground-state occupation number (corrections of order $1/\Lambda^2$ are a few percent or so). The effect on the g-boson contribution to the summed $M1$ strength is that it is reduced to about 30% or so of the total summed strength.

The truncation to configurations containing no more than one g boson commonly used in numerical diagonalizations of sdgIBM Hamiltonians may be suspect for nuclei near midshell $(N>10)$. In the unprojected intrinsic state approximation, the probability p_k of finding k g bosons in a member of the ground-state band is given by the binomial distribution

$$p_k = \binom{N}{k} (x_4^2)^k (1 - x_4^2)^{N-k}, \tag{12}$$

which, for $(x_4)^2 \simeq 0.07$, implies that the probability for three or more g bosons is negligible (a few percent or so) but that p_2 is substantial: $p_2 \gtrsim 0.1$ (0.2) for $N=10$ (15). Elimination of spurious components of the intrinsic state by angular momentum projection will reduce these estimates of p_2 but, for $N \simeq 15$, not by more than 25% or so (the corresponding reduction in $n_4^{\text{g.s.}}$). Thus, despite the smallness of our g-boson probability amplitude x_4^{sat}, it would seem that the inclusion of configurations with as many as *two g* bosons is necessary to determine ground-state-band wave functions with an accuracy of 10% or so.

D. Hexadecapole-hexadecapole interaction

As discussed above (Sec. VI B), the contribution of the hexadecapole-hexadecapole interaction to the inverse of the moment of inertia $1/I$ is small and negative. Thus, the omission of this interaction in previous sdgIBM studies is justified in as far as the description of the ground-state band spectrum is concerned.

By contrast, the impact of the hexadecapole-hexadecapole interaction on the deformation energy per boson $\mathcal{E}_D$ of the ground state (required for binding energy estimates [1]) is non-negligible. In terms of the expectation values H_L of our Hamiltonian $\hat{H}$ [see Eq. (3)], $\mathcal{E}_D = H_{L=0}/N$. To leading order in the $1/\Lambda$ expansion, this deformation energy per boson is given by

$$\mathcal{E}_D^{(0)} = \sum_l \epsilon_l x_l^2 - P \sum_k \kappa_k \mathcal{O}_p^{(k)}(0) \mathcal{O}_n^{(k)}(0). \tag{13}$$

The two contributions to $\mathcal{E}_D^{(0)}$ from the noninteracting and interacting parts of the Hamiltonian, respectively, are separately about 0.5 MeV or so, but as a result of the cancellation between them, $\mathcal{E}_D^{(0)}$ itself is only of the order of 100 keV or so. This is the same order of magnitude as the contribution of the hexadecapole-hexadecapole interaction to $\mathcal{E}_D^{(0)}$.

In a previous work [7], in which angular momentum projection was omitted, we concluded on the basis of the multipolarity weighting in an expression for the $M1$ centroid energy E_c that the effect of the hexadecapole-hexadecapole interaction on the energetics of orbital $M1$ excitations in deformed nuclei is comparable to that of the quadrupole-quadrupole interaction. This conclusion is not changed by the inclusion of angular momentum projection. The leading angular momentum projection correction [given in Eq. (9)] leaves the magnitude of the hexadecapole-hexadecapole interaction term in E_c essentially unchanged for $N \geqslant 10$. The quadrupole-quadrupole interaction term in E_c is enhanced but only by about 20% at most (when $N \geqslant 10$).

The contribution of the hexadecapole-hexadecapole interaction to the above observables shows the same dependence on the hexadecapole parameters $(t_\rho^{(4)})_{lj}$ as our result for $B(E4;0_1^+ \to 4_1^+)$: there is a little sensitivity only to the parameters $(t_\rho^{(4)})_{24}$.

VII. CONCLUSIONS

We find that angular momentum projection even for rather well-deformed nuclei has a substantial effect. Typically, the correction due to angular momentum projection is between 10% and 20% of the unprojected result, but, in some instances, it is even larger. For example, angular momentum projection can lead to a 40% or so reduction in g-boson occupation numbers for members of the ground-state band.

As conjectured in Ref. [7], we find that use of the intrinsic state formalism without angular momentum projection leads one to overestimate the summed $M1$ strength and underestimate the $M1$ centroid energy: in the case of the summed $M1$ strength, the leading angular momentum projection correction is *always* negative (since it is opposite in sign to the variance $m_2 - m_1^2$ of the spin squared of an intrinsic state boson) and, in the case of E_c, it is positive for all reasonable wave functions. There have been several studies within the unprojected intrinsic state formalism of the influence of F-spin admixtures on the summed $M1$ strength [24,25]. It would seem that the inclusion of the corrections arising from angular momentum projection is at least as important.

Introduction of a g-boson degree of freedom allows one to accommodate collective $B(E4)$'s. Contrary to claims in the literature, we find that differences in sdIBM-2 and sdgIBM-2 results for $B(E2)$'s of the ground-state band of deformed nuclei should be marginal; with a microscopically motivated choice of parameters, the contributions of the additional terms in the sdgIBM-2 $E2$ transition operator are negligible. However, the g-boson degree of freedom does influence the moment of inertia of the ground-state band: it enhances significantly the noninteracting boson contribution. The size of our g-boson amplitude suggests that the truncation to configurations containing at most one g boson commonly used in numerical diagonalizations of sdgIBM Hamiltonians may be inadequate for nuclei near midshell; inclusion of configurations with two g bosons is indicated.

With a microscopically motivated choice of the sdgIBM-2 parameters, the impact of the hexadecapole-hexadecapole interaction on the excitation energies of the ground-state band of deformed nuclei is negligible. This finding is consistent with the intuitively plausible expectation that the hexadecapole-hexadecapole interaction should not be important in determining the structure of the spectrum at excitation energies well below the threshold for the excitation of two g bosons (≈ 3 MeV). On the other hand, we find that the deformation energy of the ground state used in binding energy estimates is very sensitive to the hexadecapole-hexadecapole interaction because of a cancellation between the contributions of the noninteracting and interacting parts of the Hamiltonian.

In a previous study within the IBM-2 of binding energies of astrophysical significance, the deformation energy was, for simplicity, omitted [26]. On the basis of the current work, we estimate that the deformation energy near midshell is somewhere between a few hundred keV and a couple of MeV in magnitude, which is comparable to the rms error of the mass formula of Ref. [26]. Conceivably, an improved mass formula could be obtained by inclusion of the deformation energy, but given the present uncertainties in the single-boson energies ϵ_{l_ρ}, reliable calculation of deformation energies beyond an order of magnitude estimate is not possible. For example, the 10% or so reduction in the choice of all boson energies, which is a reasonable modification suggested by our comparison with moments of inertia for deformed nuclei, is enough to change the sign of the deformation energy. It would also be necessary to take into account the influence of F-spin admixtures on the cancellation between the noninteracting and interacting contributions to the deformation energy.

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APPENDIX: THE MOMENT OF INERTIA I

It is convenient to work with the inverse of the moment of inertia for which our result is of the form (I in units of $\hbar^2$)

$$\frac{1}{I}=\frac{2}{N}(D_{\rm sb}+D_{\rm int}), \tag{A1}$$

where we distinguish between a contribution $D_{\rm sb}$ which arises from the noninteracting or single-boson part of our Hamiltonian $\hat{H}$ and a contribution $D_{\rm int}$ which arises from the interaction part of $\hat{H}$. To the order in $1/\Lambda$ which we work,

$$D_{\rm sb}=\frac{1}{m_1}\left\{e_1-e_0-\left[2\left(1+m_1-\frac{m_2}{m_1}\right)(e_1-e_0)+\frac{m_2}{m_1}(e_2-e_1)\right]\frac{1}{\Lambda}\right\},$$

$$D_{\rm int}=\frac{P}{m_1}\left\{2v_0-v_1+\left[2\left(\frac{m_2}{m_1}-1\right)(2v_0-v_1)-2m_1v_1+\frac{m_2}{m_1}(v_2-v_1)\right]\frac{1}{\Lambda}\right\},$$

where

$$e_j\equiv\frac{1}{m_j}\sum_l (\overline{l})^j\epsilon_l x_l^2, \quad v_j\equiv\frac{1}{m_j}\sum_k \kappa_k\left\{\sum_J (\overline{J})^j A_J^{(k)}\right\}\equiv\sum_k \kappa_k a_j^{(k)}.$$

The summations over J in the $a_j^{(k)}$'s may be evaluated analytically (as in Appendix A of Ref. [16]) to yield

$$a_0^{(k)}=\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(0),$$

$$m_1\,a_1^{(k)}=\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(1)+\mathcal{O}_p^{(k)}(1)\mathcal{O}_n^{(k)}(0)-\frac{\overline{k}}{2}\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(0),$$

$$\begin{aligned}m_2\,a_2^{(k)}=&\frac{\overline{k^2}}{2}\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(0)-2\overline{k}[\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(1)+\mathcal{O}_p^{(k)}(1)\mathcal{O}_n^{(k)}(0)]+\mathcal{O}_p^{(k)}(2)\,\mathcal{O}_n^{(k)}(0)+\mathcal{O}_p^{(k)}(0)\mathcal{O}_n^{(k)}(2)\\&+\frac{6\overline{k}}{\overline{k}+2}\mathcal{O}_p^{(k)}(1)\mathcal{O}_n^{(k)}(1)-\frac{2}{\overline{k}-2}\{\mathcal{O}_p^{(k)}(1)[\mathcal{O}_n^{(k)}(2)-\mathcal{O}_n^{(k)}(1,1)]+\mathcal{O}_n^{(k)}(1)[\mathcal{O}_p^{(k)}(2)-\mathcal{O}_p^{(k)}(1,1)]\}\\&+\frac{2}{\overline{k}(\overline{k}-2)}[\mathcal{O}_p^{(k)}(2)-\mathcal{O}_p^{(k)}(1,1)][\mathcal{O}_n^{(k)}(2)-\mathcal{O}_n^{(k)}(1,1)],\end{aligned}$$

where

$$\mathcal{O}_\rho^{(k)}(s,t)\equiv\sum_{j,l} (\overline{j})^s(\overline{l})^t\langle j0l0|k0\rangle(t_\rho^{(k)})_{jl}x_jx_l$$

and $\mathcal{O}_\rho^{(k)}(s)\equiv\mathcal{O}_\rho^{(k)}(s,0)[=\mathcal{O}_\rho^{(k)}(0,s)]$. Higher orders in the $1/\Lambda$ expansion introduce a $\overline{L}$ dependence into $D_{\rm sb}$ and $D_{\rm int}$.

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