Identical bands at normal deformation: Necessity of going beyond the mean-field approach

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(Received 22 December 1994)

The validity of BCS theory has been questioned because the appearance of normally deformed identical bands in odd and even nuclei seems to contradict the conventional understanding of the blocking effect. This problem is examined with the projected shell model (PSM), which projects good angular momentum states and includes many-body correlations in both deformation and pairing channels. Satisfactory reproduction of identical band data by the PSM suggests that it may be necessary to go beyond the mean field to obtain a quantitative account of identical bands. [S0556-2813(96)06505-3]

PACS number(s): 21.60.Cs, 21.10.Re

Soon after the BCS theory [1] was developed for superconductivity in metals, Bohr, Mottelson, and many others [2–4] adapted it to explain the spectra of nuclei. For a strongly deformed system, one expects that the pairing correlation tends to reduce the nuclear moment of inertia (MOI) from the rigid-body value. By combining the Inglis cranking formula [5] with the BCS theory and perturbatively calculating the Coriolis term to the lowest order, Belyaev [3] obtained for the MOI

$$\Im = 2 \sum_{k,k'>0} \frac{|\langle k|\hat{J}_x|k'\rangle|^2}{E_k + E_{k'}} (u_k v_{k'} - u_{k'} v_k)^2, \tag{1}$$

where $\langle k|\hat{J}_x|k'\rangle$ is the matrix element of $\hat{J}_x$ in the Nilsson basis, E_k the quasiparticle energy, and u_k and v_k the BCS occupation amplitudes. Practically only four or five single-particle orbitals near the Fermi surface can contribute appreciably to the sum in Eq. (1). Therefore, blocking one of these levels will affect significantly the pairing gap Δ and occupation functions (uv's) [6,7], it is commonly believed that the resulting MOI ($\Im$) will be increased on average by about 15% [8]. Therefore, when Baktash *et al.* recognized [9] that selected rotational bands (mainly those with low j and high Ω) in odd-Z nuclei have nearly identical transition energies for restricted spin intervals when compared with bands in their even-even neighbors, they suggested that this is a serious challenge to the applicability of BCS theory in nuclear structure. This claim has motivated several recent publications [10–13].

However, Eq. (1) uses conventional models that involve a mixture of BCS, cranking, and mean field approximations. Thus, it is not obvious whether the failure of the simple Belyaev formula marks a failure of the BCS approximation considered in isolation. This question can only be addressed by a theory that can go beyond these approximations such as the projected shell model (PSM) [14,15].

The PSM is a spherical shell model truncated in a deformed (Nilsson-type) BCS single-particle basis. More precisely, the truncation is first achieved within the quasiparticle basis with respect to the deformed BCS vacuum $|\phi\rangle$; then rotational symmetry and number conservation are restored for these states by standard projection technique [16] to form a spherical basis in the laboratory frame; finally the shell model Hamiltonian is diagonalized in this basis. The truncation obtained in this way is very efficient. Usually, quite satisfactory results can be obtained by choosing only a few quasiparticle orbitals near the Fermi surface, because the quasiparticle basis already contains most of the pairing and quadrupole correlations.

The PSM and the cranking mean-field theory differ in certain important aspects. In the mean-field approximation, the wave function is a linear combination of the quasiparticle states $|\varphi_\kappa\rangle$ defined in the intrinsic frame:

$$|\omega\rangle = \sum_\kappa f_\kappa(\omega)|\varphi_\kappa\rangle, \tag{2}$$

$|\varphi_\kappa\rangle$ stands for $\{|\phi\rangle,\ \alpha^\dagger_{n_i}\alpha^\dagger_{n_j}|\phi\rangle,\ \alpha^\dagger_{p_k}\alpha^\dagger_{p_l}|\phi\rangle, \ldots\}$ and $\{\alpha^\dagger_{p_l}|\phi\rangle,\ \alpha^\dagger_{n_i}\alpha^\dagger_{n_j}\alpha^\dagger_{p_l}|\phi\rangle,\ \ldots\}$ for even-even and odd-Z systems, respectively, where $\{\alpha, \alpha^\dagger\}$ are the quasiparticle annihilation and creation operators for the vacuum $|\phi\rangle$ and the index n (p) denotes neutrons (protons). In the simplest cranking approach the mixing amplitudes $f_\kappa(\omega)$ are determined by the Coriolis interaction $\omega\hat{J}_x$, but in the PSM the wave function (without number projection) is a linear combination of *projected* quasiparticle states defined in the lab system

$$|IM\rangle = \sum_\kappa f^I_\kappa \hat{P}^I_{MK_\kappa}|\varphi_\kappa\rangle, \tag{3}$$

where $\hat{P}^I_{MK_\kappa}$ is the angular momentum projection operator [16], K_κ is the K quantum number of the states $|\varphi_\kappa\rangle$, and the

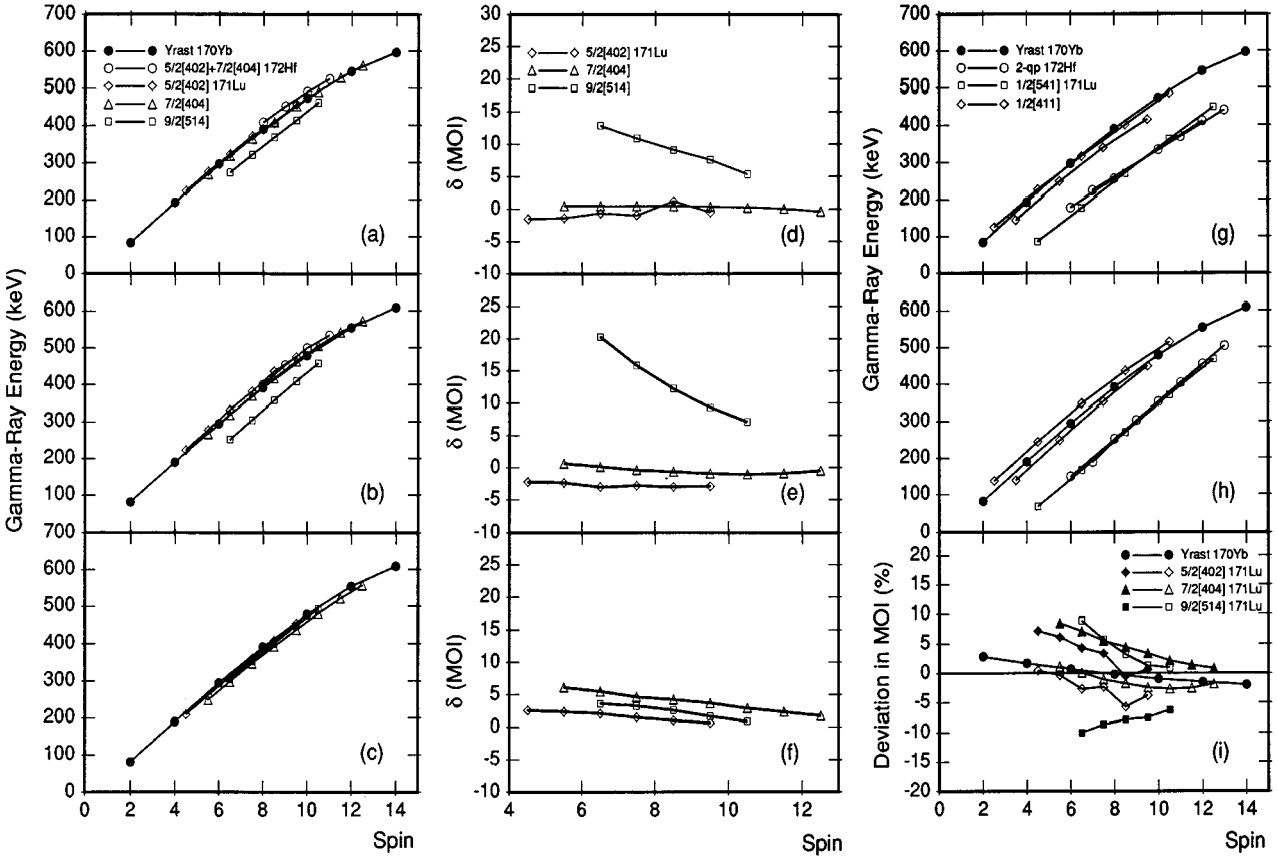

FIG. 1. (a)–(c) are the γ-ray transition energies of the three 1-qp bands in ^{171}Lu and one 2-qp band in ^{172}Hf selected by Ref. [9]; (d)–(f) are the even-odd differences of the MOI for various bands, $\delta(\mathrm{MOI})=\Im(^{171}\mathrm{Lu})-\Im(^{170}\mathrm{Yb})$. (g)–(h) are the γ-ray transition energies for the other 1-qp bands in ^{171}Lu and the 2-qp band in ^{172}Hf that were not presented in Ref. [9]. In (a)–(h), the yrast band of ^{170}Yb is taken as reference . The same symbols for the curves are used in (a)–(c), (d)–(f), and (g)–(h). The data are shown in (a), (d), and (g); (b), (e), and (h) are the PSM calculations with no blocking; (c) and (f) are the PSM calculations with individual blocking; (i) is the deviation $(\Im_{\mathrm{th}}-\Im_{\mathrm{exp}})/\Im_{\mathrm{exp}}$ of the calculated MOI for selected bands. For the three 1-qp bands in ^{171}Lu in (i), dark symbols denote the results with no blocking and open ones with individual blocking. The MOI is defined by $2\Im(I)=(4I-2)/[E(I)-E(I-2)]\ \hbar^2\ \mathrm{MeV}^{-1}$. Data are taken from [21] for ^{170}Yb [22], for ^{171}Lu and [23] for ^{172}Hf.

f^I_κ's are determined by *diagonalizing the entire shell-model Hamiltonian.* Thus, unlike the cranking approximation, many-body correlations and angular momentum conservation are accounted for in the PSM.

In the present calculations, the single-particle space consisted of three major shells: $N=4$, 5, and 6 ($N=3$, 4, and 5) for neutrons (protons), and the size of the basis was determined by imposing quasiparticle energy windows of 1.5 MeV, 2.5 MeV, 3.5 MeV, and 4 MeV for the 1-, 2-, 3-, and 4-qp states, respectively. These windows include the most important configurations and have been demonstrated to be sufficient for the description of low-lying bands [15]. The dimension of the configuration space obtained in this way is typically $\leqslant 50$ and the calculation is very fast.

The Hamiltonian was taken from Refs. [14,15]:

$$\hat{H}=\hat{H}_0-\frac{1}{2}\chi\sum_\mu \hat{Q}^\dagger_\mu\hat{Q}_\mu-G_M\hat{P}^\dagger\hat{P}-G_Q\sum_\mu \hat{P}^\dagger_\mu\hat{P}_\mu, \quad (4)$$

where $\hat{H}_0$ is the spherical single-particle shell model Hamiltonian. The quadrupole interaction strength χ is adjusted so that the quadrupole deformation ε_2 determined from self-consistent Hartree-Fock-Bogoliubov [17] is obtained. The monopole pairing strength is $G_M=[20.92\mp 13.66(N-Z)/A]\times A^{-1}$ with the minus (plus) sign for neutrons (protons). It was shown previously that the quadrupole pairing is crucial to account for the observed anomalous crossing frequency in the odd-Z rare-earth nuclei [18]. The preferred ratio G_Q/G_M is generally found to be about 0.2, and was fixed at 0.18 for the present calculations. The Hamiltonian with these values of the parameters has been demonstrated to be suitable for all deformed nuclei in the rare-earth region [14,15].

Since quadrupole pairing is not included in most standard calculations, it is important to first ascertain the effect of this interaction in the present studies on the MOI. To this end, we have carried out all the calculations with and without the quadrupole pairing term under the same conditions. The results turn out to be nearly identical, except the monopole pairing strength G_M in Eq. (4) was reduced by 10% for the latter case, in order to reproduce the same transition energy $(E_{I=2}-E_{I=0})$ in ^{170}Yb calculated using the quadrupole pairing term. Thus we believe the conclusions of this paper to be independent of whether quadrupole pairing is included.

TABLE I. Comparison of the calculated MOI with experiment as function of angular momentum. The MOI is defined in the caption of Fig. 1. For the yrast band of ^{170}Yb, the first line denotes the experiment and the second the theory. For the three 1-qp bands in ^{171}Lu, the first line denotes the experiment, the second the theory with no blocking and the third the theory with individual blocking.

^{170}Yb	I=2	I=4	I=6	I=8	I=10	I=12	I=14		
yrast	71.21	72.46	74.30	76.90	80.12	84.28	90.44		
	73.17	73.68	74.83	76.73	79.33	83.03	88.67		
	I=9/2	I=11/2	I=13/2	I=15/2	I=17/2	I=19/2			
^{171}Lu	71.42	72.46	74.28	75.25	78.90	78.79			
$5/2^+$ [402]	71.75	72.20	72.29	73.49	74.39	75.79			
	76.56	76.92	77.42	77.78	78.43	79.30			
		I=11/2	I=13/2	I=15/2	I=17/2	I=19/2	I=21/2	I=23/2	I=25/2
^{171}Lu		74.32	75.42	76.71	78.13	79.68	81.40	83.29	85.47
$7/2^+$ [404]		75.19	75.47	75.88	76.74	77.75	79.21	81.18	83.92
		80.65	80.81	80.92	81.63	82.38	83.16	84.45	86.18
			I=13/2	I=15/2	I=17/2	I=19/2	I=21/2		
^{171}Lu			87.78	87.12	86.84	86.89	86.52		
$9/2^-$ [514]			95.62	92.11	89.64	88.02	87.34		
			78.95	79.55	80.00	80.36	81.14		

In this paper, the same examples chosen by Baktash *et al.* [9] are calculated. Standard Nilsson parameters were used [19] and the deformations used to generate the deformed bases for the even-even nuclei ^{170}Yb and ^{172}Hf were taken from Ref. [20]. For odd-Z ^{171}Lu, the deformation was interpolated from its even-even neighbors and is consistent with Ref. [17]. The values (ε_2 and ε_4), respectively, were 0.265 and 0.025 for ^{170}Yb, 0.260 and 0.024 for ^{171}Lu, and 0.254 and 0.023 for ^{172}Hf. Our calculated results are shown in Fig. 1. All bands calculated by the PSM are seen to occur at the right energies: most predicted states deviate from the measured ones by less than 10 keV. Comparing Figs. 1(a) with 1(b), 1(d) with 1(e), and 1(g) with 1(h), it can be seen that the γ-ray energies and the change in the MOI from even-even to neighboring odd nuclei in the data are closely tracked by the calculations.

For the ^{171}Lu calculations presented in Figs. 1(b), 1(e), and 1(h), the blocking effect is taken into account by the usual constraint that the mean value of the proton number equal 71. The calculated value of the proton pairing gap Δ_π in this case is 0.679 MeV, which is very close to Δ_π (0.672 MeV) for the reference ^{170}Yb band. We therefore term this situation *no blocking*.

For comparison, we examined also the effect of *individual level blocking*. The results are presented in Figs. 1(c) and 1(f). When the $5/2$ [402] and $7/2$ [404] orbitals are blocked ($u=0$, $v=1$ for these orbitals), 27% (0.490 MeV) and 52% (0.324 MeV) reductions, respectively, are obtained in Δ_π, but the corresponding transition energies are reduced by only about 6%. The blocking of the $9/2$ [514] orbital is an anomaly and deserves more study: this blocking produces a 30% reduction in Δ_π, but an increase in the transition energy, which implies a decrease in the MOI instead of the commonly expected increase. Investigation of this unexpected result will be reported elsewhere [24].

It is intuitively clear that in a BCS treatment, blocking of a specific orbital in an odd system tends to overestimate the blocking effect because, in the realistic situation, no orbital is 100% blocked. On the other hand, no blocking certainly underestimates the blocking effect due to the number nonconservation. Thus we may expect the correct results from exact particle number projection to lie somewhere between no blocking [Figs. 1(b), 1(e)] and individual blocking [Figs. 1(c), 1(f)]. The difference between Figs. 1(b) and 1(c) [1(e) and 1(f)] may be construed as the error introduced by the failure to exactly conserve particle number in the present calculations. What is relevant here is that the PSM calculations for both limits can already reproduce the data rather well (see Fig. 1 and Table I).

In a recent paper, Zeng *et al.* [12] used a number-conserving cranking approach to account for the observed odd-even differences in these MOI and obtained good agreement with the experimental MOI of the band heads. They diagonalized the pairing interaction in a cranked many-particle configuration basis that did not conserve angular momentum. Their approach is particle-number conserving, and uses configuration mixing to handle effects beyond the mean field in the pairing degrees of freedom. They surmised that for this problem, number conservation is of primary importance.

In the PSM calculations discussed here, angular momentum projection was treated properly, but the particle number is only conserved to first order [25]. The common denominator of the two approaches is the use of configuration mixing to include effects beyond the mean field. The fact that both obtain essentially the correct MOI for the bandheads suggests that the common denominator—*going beyond the mean field*—is the most important factor leading to the improved calculation of the MOI. The lack of many-body correlations in the mean field approach seems to be the primary cause for the difficulty that simple mean-field calculations have in reproducing the data. Exact particle number conservation may have important effects on other aspects, for example, in understanding the BCS phase transition [26], or in the nucleon transfer problem [27].

To go beyond the mean field, the PSM includes many-body pairing and quadrupole correlations, and restores the rotational symmetry by projection techniques. Reference [12], which properly treated the pairing but not the angular momentum, computed only the bandhead MOI. Since angular momentum projection may be important in reproducing the correct angular momentum dependence, it would be interesting to examine the angular momentum dependence of the approach in Ref. [12].

Finally, we wish to emphasize that, unlike the cranking mean field approach, the deformation parameters used as input to the PSM need not correspond exactly to the true nuclear deformation. In particular, one can use the same deformation parameters for the deformed single-particles in both even-even and adjacent odd systems and still reproduce the deformation change due to the even-odd difference (the polarization effects) through the configuration mixing. This is because the deformed single-particle level scheme serves in the PSM merely as an efficient way to select a truncated basis. All observable nuclear properties (including deformation) in the PSM are determined from the many-body wave function obtained by diagonalizing the shell model Hamiltonian in the truncated basis. Of course, the larger the deviation of the true deformation from the input deformation, the larger the configuration space that is required for the diagonalization.

In conclusion, the BCS theory is a simple and efficient treatment of pairing in nuclei, but its validity has been challenged recently because of the existence of normally-deformed identical bands in some odd-Z and neighboring even-even nuclei. Using the projected shell model, which employs the BCS theory to incorporate pairing in the basis but then diagonalizes the shell-model Hamiltonian in the angular momentum projected basis, we were able to reproduce satisfactorily the data that have been cited as evidence against the BCS approximation. Our results suggest that the BCS theory provides a quasiparticle basis, like the Nilsson basis in the deformation degree of freedom, from which one can construct more realistic states. Thus, it is premature to implicate the BCS approximation alone. However, an understanding of the normally deformed identical bands does seem to require correlations beyond the mean field.

ACKNOWLEDGMENTS

Valuable discussions with Peter Ring are acknowledged. Yang Sun is grateful to the Spanish Ministry of Education and Science and the College of Arts and Science of Drexel University for financial support. This work was partially supported by the United States National Science Foundation, by DGICYT, Spain under the project number PB91–0006, and by the National Science Council of the ROC under Contract No. NSC 84–2112–M–033–007. Theoretical nuclear physics research at the University of Tennessee was supported by the U. S. Department of Energy through Contract No. DE–FG05–93ER40770. Oak Ridge National Laboratory is managed by Lockheed Martin Energy Systems, Inc. for the U. S. Department of Energy under Contract No. DE–AC05–84OR21400.

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