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High-Spin Anomalies in Yb: Coriolis Antipairing versus Pair Realignment with a Realistic Interaction

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The Hartree-Fock-Bogoliubov cranking equations are solved for ^{168}Yb and ^{170}Yb with an effective interaction obtained from the Reid soft-core nucleon-nucleon potential. Coriolis antipairing in ^{168}Yb and pair realignment in ^{170}Yb explain their anomalous high-spin spectra.

A realistic description of the anomalous high-spin spectra of rare-earth nuclei[1] involves the following program: First, the calculation of an effective interaction based on a realistic nucleon-nucleon potential. Second, a reasonable description of the nuclear ground state, where both deformation and pairing properties are obtained from the same interaction. Third, the application of a unified formalism general enough to encompass the various mechanisms proposed to explain the "backbending" phenomenon. These mechanisms are the Mottelson-Valatin Coriolis antipairing (CAP) effect[2] (a rapid and state-independent reduction of the pairing gap), the Stephens-Simon realignment effect[3] (the decoupling of a neutron pair from the pairing field with subsequent alignment along the rotation axis), and band crossing of shape isomers. Fourth, the adoption of a representation which manifests the precise nature of the backbending mechanism.

We have initiated a program of studies which incorporates all four ingredients. For the effective interaction we have evaluated the Brueckner G matrix (ladder series summation) using the Reid soft-core nucleon-nucleon potential.[4] The Pauli operator preventing scattering into normally occupied states is taken to be isospin independent with a valence space spanning the union of the neutron and proton valence configurations. It is treated exactly in the single-particle basis which is a harmonic oscillator with shell spacing $\hbar\omega = 7.5$ MeV. For simplicity, we employ an average binding energy of 10 MeV for the bound valence single-particle states.

The Hartree-Fock-Bogoliubov (HFB) equations in a rotating frame[5] are

$$\begin{pmatrix} (\mathcal{H} - \omega J_x) & \Delta \\ -\Delta^* & -(\mathcal{H} - \omega J_x)^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}, \qquad (1)$$

where the angular frequency ω is adjusted so that

$$\langle J_x \rangle = [J(J+1)]^{1/2}. \qquad (2)$$

The Hartree-Fock (HF) Hamiltonian $\mathcal{H}$ and the pair potential Δ are both determined by the realistic effective interaction. Matrix elements of the interaction between two particle states $|j_1 j_2 JT\rangle$ of all permissible couplings ($0 \le J \le 13$) are included in $\mathcal{H}$ and Δ. The valence space contains essentially one major shell of each parity for both neutrons and protons and can accommodate 52 protons and 66 neutrons. The spherical single-particle energies (ϵ_c) of the inert core (40 protons and 70 neutrons) are fixed by equating average spherical HF single-particle energies with spherical Nilsson energies. That is,

$$(\epsilon_c)_{jT} + \tfrac{1}{2}[\Gamma_{jT}({}^{154}\mathrm{Gd}, \beta = 0) + \Gamma_{jT}({}^{176}\mathrm{Os}, \beta = 0)] = \epsilon_{jT}(\mathrm{Nilsson}, \beta = 0), \qquad (3)$$

where Γ is the HF potential resulting from a HF calculation. The HFB equations are solved in the σ_x (reflection through the yz plane) representation,[5] which block diagonalizes J_x, $\mathcal{H}$, and Δ. This basis will enhance the interpretation of the high-spin wave functions.

Ground-state properties of ten Er, Yb, and Hf isotopes have been calculated. The systematic experimental dependence of $\epsilon_{\mathrm{spherical}}$, β_2, β_4, Δ_p, and Δ_n on Z and N is reproduced. The magnitude of β_2 is small by 35–40%, presumably because of the "limited" model space, the absence of some core-polarization contributions to the effective interaction, and the relative weakness of G_{nn} (the effective neutron-neutron interaction) caused by choosing $\hbar\Omega_n = \hbar\Omega_p$. The average proton pair gap is underestimated by only 5–20%. However the average neutron gap is 40–50% too small, probably because of the weakness of G_{nn}. Nuclei with $N \ge 98$ have prolate deformations. For $N < 98$, the shapes are oblate.

The excited states of ^{168}Yb and ^{170}Yb have been calculated.[6] The experimental spectra are presented in Fig. 1(a). At high spins the ^{168}Yb curve rises rapidly but remains single valued. The ^{170}Yb curve is multivalued. The latter isotope is especially intriguing, since its even neighbors in the periodic table do not backbend. The calculated spectra are depicted in Fig. 1(b). The essential features are reproduced, i.e., slowly

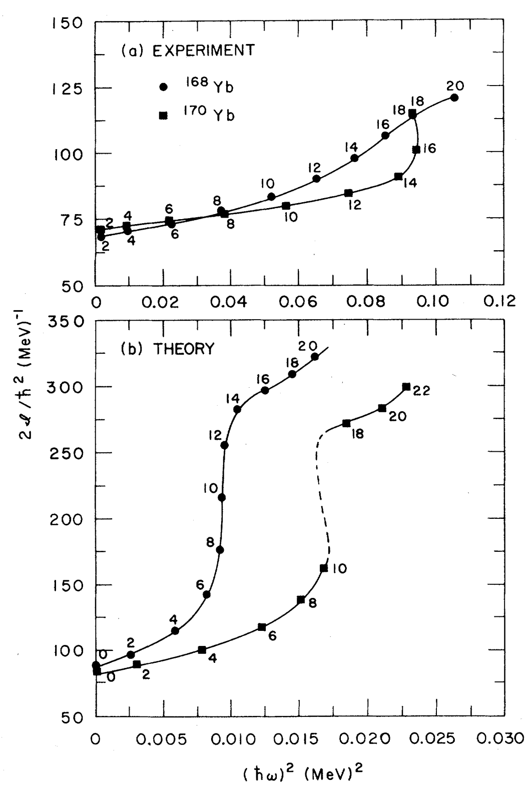

FIG. 1. $\mathcal{I}$ versus ω^2 curves for ^{168}Yb and ^{170}Yb. The dashed line is interpolated, not calculated.

TABLE I. The occupation probabilities v_α^2, the pairing gap $\Delta_{\alpha\hat{\alpha}}$, and the contribution to the angular momentum, $J_\alpha = [(J_x)_{\alpha\alpha} + (J_x)_{\hat{\alpha}\hat{\alpha}}] v_\alpha^2$, are given for four neutron pairs near the Fermi surface for various angular velocities ω. The single-particle basis α diagonalizes the density matrix ρ. At each ω the states α are ordered with increasing v_α^2. The total angular momentum of the nucleus is $\langle J_x \rangle$.

$\hbar\omega$ (MeV)	$\langle J_x \rangle$	α	v_α^2	$\Delta_{\alpha\hat{\alpha}}$ (MeV)	J_α
		^{168}Yb			
0	0	1	0.206	0.520	0
		2	0.731	0.522	0
		3	0.907	0.498	0
		4	0.942	0.483	0
0.095	7.961	1	0.078	0.297	-0.231
		2	0.851	0.301	+1.538
		3	0.964	0.305	+1.771
		4	0.987	0.265	+1.156
0.100	13.819	1	0	0.015	0
		2	1	0.015	-1.225
		3	1	0.019	+3.995
		4	1	0.016	+5.302
		^{170}Yb			
0	0	1	0.438	0.517	0
		2	0.883	0.483	0
		3	0.955	0.450	0
		4	0.969	0.437	0
0.130 lower branch	10.930	1	0.247	0.251	-1.075
		2	0.981	0.278	+0.059
		3	0.987	0.214	+6.118
		4	0.993	0.253	+1.220
0.130 upper branch	17.332	1	0.055	0.225	+0.045
		2	0.984	0.205	-0.622
		3	0.996	0.205	+0.536
		4	1.000	0.045	+11.106

varying moments of inertia ($\mathcal{J}$) at low spins, rapid variation at high spins, with ^{168}Yb single valued and ^{170}Yb multivalued. At low spins $\mathcal{J}_{\text{theor}}$ is only 25% greater than $\mathcal{J}_{\text{exp}}$, but at high spins $\mathcal{J}_{\text{theor}}$ rises twice as much as $\mathcal{J}_{\text{exp}}$. The algorithm employed to solve the HFB equations does not map out the backward-going region of ^{170}Yb. Consequently $J = 12$, 14, 16 have not yet been determined.[7]

To decide which of the proposed mechanisms is operative in each nucleus, a brief analysis of the wave functions is presented in Table I. The properties of four neutron pairs near the Fermi surface are given for various $\hbar\omega$. These neutrons are primarily in the $i_{13/2}$ subshell. In the ground state ($\hbar\omega = 0$), $\alpha = 1$, 2, 3, 4 corresponds to $m_z = \frac{7}{2}$, $\frac{5}{2}$, $\frac{3}{2}$, $\frac{1}{2}$, respectively.

Consider ^{168}Yb. The Fermi surface lies between levels 1 and 2. At $\hbar\omega = 0$ the state-dependent pair gap $\Delta_{\alpha\hat{\alpha}}$ is nearly constant; furthermore the members of each pair are related by time reversal, and hence each pair produces a net $\langle J_x \rangle = 0$. The rapid rise in $\mathcal{J}$ begins at $\hbar\omega = 0.095$ MeV and ends at $\hbar\omega = 0.100$ MeV. It is apparent that $\Delta_{\alpha\hat{\alpha}}$ decreases to zero over this interval very uniformly for all orbits. The angular momentum is spread over several pairs, and no single pair predominates. The maximum for any one pair is 5.3 units whereas a fully aligned $i_{13/2}$ pair would have $\langle J_x \rangle = \frac{13}{2} + \frac{11}{2} = 12$. The nucleus ^{168}Yb therefore presents a clear example of the Mottelson-Valatin CAP effect.

Consider ^{170}Yb. The ground state is similar to that of ^{168}Yb, except that the $m_z = \frac{1}{2}$ pair, where the Coriolis force is strongest, lies even further below the Fermi surface. The lower branch of $\mathcal{J}(\omega^2)$ ends at $\hbar\omega = 0.130$ MeV. The average pairing gap is reduced to 53% of the ground-state value, and $\Delta_{\alpha\hat{\alpha}}$ is not very state dependent. One pair has $\langle J_x \rangle = 6.1$, which is half the aligned value. The upper branch begins at $\hbar\omega = 0.130$ MeV and is drastically altered from the lower branch. A single pair has $\langle J_x \rangle = 11.1$. While the entire nucleus gained 6.4 units of angular momentum, this single pair increased by 5.0 units. (The other three pairs even have reduced contributions to $\langle J_x \rangle$.) Furthermore this pair has decoupled from the pairing field. The average of the state-dependent pairing gap for the first three pairs is 45% of the $\hbar\omega = 0$ strength, while $\Delta_{\alpha\hat{\alpha}}$ is rapidly going to zero for the last pair. Note that this pair is fully occupied.

What is the nature of this decoupled pair in ^{170}Yb? A shell-model assignment is made possible by the σ_x basis. Figure 2 presents $\langle J_x \rangle$ in the critical region for each member of the pair. In the upper branch the orbit $|\alpha\rangle$ has $(J_x)_{\alpha\alpha}$ above 6 and asymptotically approaching $\frac{13}{2}$, which is the maximum possible value for this model space. Similarly $(J_x)_{\hat{\alpha}\hat{\alpha}}$ is approaching $\frac{11}{2}$, which is the next largest allowed value. The identification is completed by the single-particle overlaps depicted in Fig. 2. The HFB orbital $|\alpha\rangle$ and the J_x eigenstate $|i_{13/2} m_x = \frac{13}{2}\rangle$ have a 98% overlap. The overlap of $|\hat{\alpha}\rangle$ and $|i_{13/2} m_x = \frac{11}{2}\rangle$ is 94%. The decoupled pair $|\alpha\hat{\alpha}\rangle$ can therefore be characterized as aligned along the x axis of rotation. Whereas m_z is a good quantum number in the ground state, for high spins m_x is essentially a good quantum

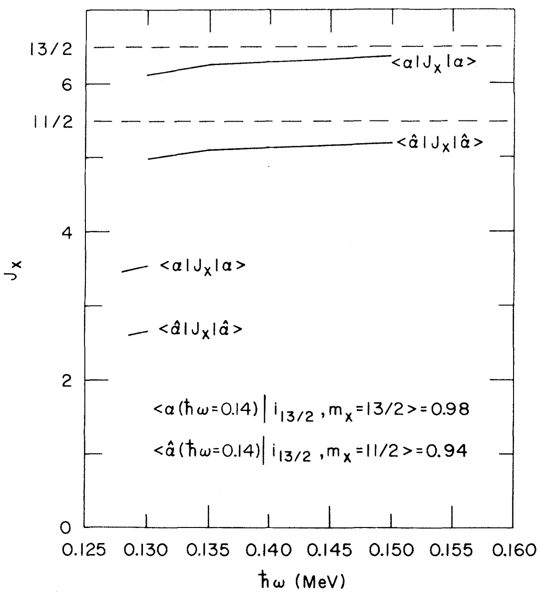

FIG. 2. Matrix elements of J_x for each member of the decoupled pair $|\alpha\hat{\alpha}\rangle$ in ^{170}Yb. Overlaps of $|\alpha\rangle$ and $|\hat{\alpha}\rangle$ with J_x eigenstates.

number for this pair. Calculations performed in the spherical $|jm\rangle$ basis[8] yield only the average of $(J_x)_{\alpha\alpha}$ and $(J_x)_{\hat{\alpha}\hat{\alpha}}$, and therefore do not demonstrate that m_x is a good quantum number for decoupled particles.

It has been proven[5] that even at high spins the HFB wave function $|\Phi\rangle$ has an extremely simple representation. For ^{170}Yb this is

$$|\Phi\rangle = C_\alpha{}^\dagger C_{\hat{\alpha}}{}^\dagger \prod_{\alpha' \neq \alpha} (u_{\alpha'} + v_{\alpha'} C_{\alpha'}{}^\dagger C_{\hat{\alpha}'}{}^\dagger)|0\rangle, \tag{4}$$

where $|\alpha\rangle \cong |i_{13/2} m_x = \frac{13}{2}\rangle$, $|\hat{\alpha}\rangle \cong |i_{13/2} m_x = \frac{11}{2}\rangle$, and $|\hat{\alpha}'\rangle \neq T|\alpha'\rangle$, where T is the time-reversal operator. All single-particle states in $|\Phi\rangle$ are eigenstates of σ_x.

Are the shapes of these nuclei spin dependent? For $J=0$ they are prolate and axially symmetric ($\gamma = 0°$). At high spins β_2 fluctuates by only 4%. The nonaxial deformation parameter γ rises rapidly in the transition region to about 15° for both nuclei. Hence the shapes are very nonaxial at high spins.

The calculation reported in this Letter is the first attempt to explain high-spin anomalies in heavy nuclei with a realistic interaction, where both deformation and pairing properties are derived from the same force. The rapid rise of the moment of inertia in the nonbackbending ^{168}Yb is explained by the Mottelson-Valatin CAP effect. Whereas in the backbending ^{170}Yb it is caused by the decoupling and realignment of an $i_{13/2}$ neutron pair. Nonaxiality also plays a significant role. These conclusions are compatible with the calculations of Banerjee, Mang, and Ring[8] on ^{162}Er and ^{168}Yb with the phenomenological pairing plus quadrupole force and the spherical $|jm\rangle$ basis. The HFB-cranking theory has demonstrated qualitative agreement with experiment, and has exhibited the ability to include and to clearly differentiate between the various mechanisms proposed to explain the high-spin behavior of rare-earth nuclei.

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