Interpretation of backbending in ¹⁰⁰Mo in a cranked Nilsson model with pairing

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An interpretation of backbending in the ${}^{100}_{42}Mo_{58}$ nucleus is given in terms of the crossing of the ground-state band with an aligned two-quasiparticle band. Our analysis within the framework of a cranked Nilsson model with pairing shows that this backbend is due to the alignment of two neutrons in $h_{11/2}$ orbitals.

There is an upsurge of interest in high-spin spectroscopy in neutron-rich nuclei far from stability because it exhibits a wide variety of behavior.^{1,2} In a recent systematic nuclear structure investigation of the mass region $A \simeq 100$ by Gelletly *et al.*,³ one finds certain abruptness of changes in behavior with Z, N, and rotational frequency (ω) which makes this region an ideal one for testing our theoretical understanding of nuclear structure. In their $2J/\hbar^2 V_S(\hbar\omega)^2$ plot for ¹⁰⁰Mo, one observes a backbend at $\hbar\omega = 0.4$ MeV. However, their data do not tell us whether this is due to the alignment of two $g_{9/2}$ protons or two $h_{11/2}$ neutrons.

The purpose of this Brief Report is to identify the alignment mechanism and provide an explanation of backbending in terms of crossing of the ground-state band with an aligned two-quasiparticle band. The quantities considered are single-particle energies (Routhian) and alignment. The Routhian is readily recognized as the Hamiltonian in a frame of reference rotating with angular frequency ω about the x axis.

We use the cranked Nilsson model with pairing to calculate the quasiparticle energy as a function of rotational frequency and hence estimate the critical frequency (ω_c) at which backbending occurs. There has been some effort to perform a cranked, deformed, shell-model calculation in a truncated many-particle configuration space,⁴ instead of the usual quasiparticle method, adopted in the present analysis. But these methods depend on alignment properties. It is essential to retain some high-energy stretched configuration to correctly describe the interaction between band crossing. Therefore, it is important to learn the alignment mechanism before performing a thorough calculation for explanation of important physical effects.

A deformed nucleus has a rotational degree of freedom. The nucleus ¹⁰⁰Mo is axially symmetric having a finite positive value for the quadrupole deformation parameter β . Single-particle energies for such a deformed nucleus are obtained by diagonalizing the matrix of the Nilsson Hamiltonian $h_{sp(def)}$ in the $|j\Omega\rangle$ basis. The states thus obtained have degeneracy with respect to Ω .

Since the nucleus is deformed, it can rotate about an axis perpendicular to the symmetry axis. The Hamiltonian for the rotating nucleus is given by⁵

$$h' = h_{\rm sp(def)} - \omega j_x \quad , \tag{1}$$

which is obtained by making a transformation of the coordinates from the laboratory frame to the rotating frame of reference. j_x is the component of angular momentum on the rotating axis (x axis). The frequency of rotation ω is supposed to be constant. The additional term $-\omega j_x$ represents the centrifugal and Coriolis forces acting on the nucleon which move in the rotating potential. The Hamiltonian h' remains invariant with respect to space reflection and rotation about the x axis through 180°. Thus, the eigenvalues e_v^{ω} and the eigenstates $|v^{\omega}\rangle$ of the cranking Hamiltonian can be labeled by the parity of the state π and eigenvalue $r_1(v)$ of the rotation operator:

$$R_1 = \exp(-i\pi j_x) , \qquad (2)$$

where

$$r_1(v) = \exp[-i\pi\alpha(v)] ,$$

i.e.,

$$e^{-i\pi j_x}|v^{\omega}\rangle = e^{-i\pi\alpha(v)}|v^{\omega}\rangle$$
.

 r_1 is called the signature of the state.

There exists a definite relation between the states of good projection quantum number Ω and states of good signature, as $\omega \rightarrow 0$,

$$|K\rangle \equiv |i\pi\alpha = \frac{1}{2}\rangle$$

= $\frac{1}{\sqrt{2}}[(-)^{\Omega_{\nu} - 1/2} |\nu, \Omega_{\nu}\rangle + |\overline{\nu, \Omega_{\nu}}\rangle],$ (3a)

$$|\overline{K}\rangle \equiv |i\pi\alpha = -\frac{1}{2}\rangle$$

= $\frac{1}{\sqrt{2}} [-|\nu, \Omega_{\nu}\rangle + (-)^{\Omega_{\nu} - 1/2} |\overline{\nu, \Omega_{\nu}}\rangle], \qquad (3b)$

where $|\overline{\nu,\Omega_{\nu}}\rangle$ is the time-reversed state with angular momentum projection $-\Omega_{\nu}$. The transformation is known as the Goodman transformation. Thus,

$$(\epsilon - \omega j_x)G = \epsilon^{\omega}G, \ (\epsilon + \omega j_x)H = \overline{\epsilon}^{\omega}H$$
.

The resulting eigenstates can be written as

$$|j\rangle = |\pi, \alpha = \frac{1}{2}\rangle = \sum_{K} G_{K}^{j} |K\rangle , \qquad (4a)$$

$$|\bar{j}\rangle = |\pi, \alpha = -\frac{1}{2}\rangle = \sum_{K} H_{K}^{\bar{i}} |\bar{k}\rangle$$
 (4b)

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To generalize the Hamiltonian h', pairing correlations can be included so that

$$h' = \sum_{\Omega} (\epsilon_{\Omega} - \lambda) C_{\Omega}^{\dagger} C_{\Omega} - \omega \sum_{\Omega, \Omega'} \langle \Omega' | j_{x} | \Omega \rangle C_{\Omega'}^{\dagger} C_{\Omega}$$
$$- \frac{\Delta}{2} \sum_{\Omega} (C_{\Omega}^{\dagger} C_{\overline{\Omega}}^{\dagger} + C_{\overline{\Omega}} C_{\Omega}) . \qquad (5)$$

A transformation can be made from a good Ω basis to a good signature basis. The unitary transformation be-

tween the Nilsson basis (with good signature) and rotating quasiparticle state i is given by

$$b_{i}^{\dagger} = \sum_{\nu} \left(A_{\nu}^{i} C_{\nu}^{\dagger} + B_{\nu}^{i} C_{\nu} \right) , \qquad (6a)$$

$$b_{i} = \sum_{\nu} \left(B_{\nu}^{*i} C_{\nu}^{\dagger} + A_{\nu}^{*i} C_{\nu} \right) \,. \tag{6b}$$

Making these transformations, the quasiparticle equation ${\rm reads}^6$

$$\sum_{\nu} \begin{bmatrix} (\epsilon - \lambda) \delta_{\beta\nu} - \omega(j_x)_{\beta\nu} & \Delta \\ \Delta & -(\epsilon - \lambda) \delta_{\beta\nu} + \omega(j_x)_{\beta\nu} \end{bmatrix} \begin{bmatrix} A_{\nu}^i \\ B_{\nu}^i \end{bmatrix} = \epsilon_i^{\omega} \begin{bmatrix} A_{\beta}^i \\ B_{\beta}^i \end{bmatrix}.$$
(7)

If the classification of states is made in terms of signature quantum number, then this equation splits into two subsets: subset I $(r_1 = -i)$,

$$\sum_{K'>0} \begin{bmatrix} (\epsilon-\lambda)\delta_{KK'} - \omega(j_x)_{KK'} & \Delta_{K\overline{K}}, \\ \Delta_{\overline{K}K'} & -(\epsilon-\lambda)\delta_{KK'} - \omega(j_x)_{\overline{K}\overline{K}}, \end{bmatrix} \begin{bmatrix} A_{K'}^L \\ B_{\overline{K}}^L \end{bmatrix} = \epsilon_L^{\omega} \begin{bmatrix} A_{K'}^L \\ B_{\overline{K}}^L \end{bmatrix} ,$$
(8a)

subset II $(r_1 = i)$,

$$\sum_{K'>0} \begin{bmatrix} (\epsilon-\lambda)\delta_{KK'} + \omega(j_x)_{\overline{K}\,\overline{K}}, & \Delta_{\overline{K}K'} \\ \Delta_{K\overline{K}}, & -(\epsilon-\lambda)\delta_{KK'} + \omega(j_x)_{KK'} \end{bmatrix} \begin{bmatrix} A_{\overline{K}'}^{\overline{L}} \\ B_{K'}^{\overline{L}} \end{bmatrix} = \epsilon_{\overline{L}}^{\omega} \begin{bmatrix} A_{\overline{K}}^{\overline{L}} \\ B_{\overline{K}} \end{bmatrix} .$$
(8b)

K' > 0 implies that K' runs over all states with $r_1 = -i$ while index \overline{K}' runs over all states with $r_1 = i$.

The selection rules for matrix elements are as follows:

 $(\epsilon - \lambda) \delta_{K\bar{K}} = (\epsilon - \lambda) \delta_{\bar{K}K'} = 0$,

FIG. 1. The quasiparticle energies $\epsilon(\hbar\omega_0)$ plotted as a function of rotational frequency (ω/ω_0) . $g_{9/2}$ protons and $h_{11/2}$ neutrons correspond, respectively to the top and bottom part of the figure. The dotted curve represents the $\alpha = -\frac{1}{2}$ levels and the solid curves, the $\alpha = +\frac{1}{2}$ levels.

$$\begin{split} &\Delta_{KK'} = \Delta_{\overline{K} \ \overline{K}} = 0 , \\ &(j_x)_{K\overline{K}} = (j_x)_{\overline{K}K'} = 0 , \\ &(j_x)_{\overline{K} \ \overline{K}} = -(j_x)_{KK'} . \end{split}$$

 ϵ_L^{ω} is the single-quasiparticle energy obtained by diagonalizing the energy matrix at frequency ω . Generally, $\epsilon_L^{\omega} \neq \epsilon_{\overline{L}}^{\omega}$ except at $\omega = 0$.

The choice of parameters are as follows. We assume that the nucleus ¹⁰⁰Mo has axial symmetry, with the z axis being the symmetry axis. The quadrupole deformation parameter $\beta_2=0.253$ and $\beta_4=0$. This is for the



FIG. 2. Experimental $2J/\hbar^2 vs (\hbar\omega)^2$ plot for the yrast bands in the even Mo isotopes (Ref. 1).

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ground state of the nucleus. The gap parameters $\Delta_n = 0.148\hbar\omega_0$ and $\Delta_p = 0.184\hbar\omega_0$, obtained by the oddeven mass difference for the nucleus, and the chemical potential λ are equal to the lowest single-particle energy, i.e., $\lambda_n = 4.853\hbar\omega_0$ and $\lambda_p = 4.292\hbar\omega_0$.

The single-quasiparticle energies as a function of rotational frequency are shown in Fig. 1 for $g_{9/2}$ protons (top) and $h_{11/2}$ neutrons (bottom), respectively. The groundstate band interacts with the two-quasiparticles band at $\hbar\omega_c = 0.55$ MeV for $g_{9/2}$ protons and at $\hbar\omega_c = 0.39$ MeV for $h_{11/2}$ neutrons. The crossing of the two bands is an indication of backbend. The experimental $2J/\hbar^2 vs (\hbar\omega)^2$ curve (Fig. 2) shows a backbend at $\hbar\omega_c = 0.4$ MeV. A comparison of theoretical and experimental critical frequencies indicates that it is the alignment of a pair of neutrons in $h_{11/2}$ orbital which is responsible for the backbending phenomena. It would be highly desirable to identify the alignment mechanism, especially for the yrast bands in other Mo isotopes, because nonbackbending experimental data in this region are in their infancy and proper spectroscopy will allow us to find whether the alignment of a pair of neutrons from $h_{11/2}$ orbitals is consistent with the role of intruder orbitals in other parts of the Periodic Table, particularly Sn nuclei with A = 101-104.

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