Microscopic theory of backbending in some neutron-rich palladium isotopes

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The observed dramatic onset of backbending in ^{104,106}Pd isotopes is examined by carrying out a variational calculation of the high-spin yrast spectra. Our calculation reveals that the observed backbending effect in ^{104,106}Pd isotopes is intimately linked with the occurrence of sharp structural changes in the yrast spectrum of ^{104,106}Pd because of a sudden increase in deformation due to crossing of $h_{11/2}$, $\pm\frac{1}{2}$ and $\pm\frac{3}{2}$ levels at the Fermi surface.

The investigation of the ground-state properties of doubly even palladium isotopes has been the subject of experimental study of a large number of experimental pursuits for quite some time in the past.[1-18] The experimental techniques like Coulomb excitation and inbeam gamma ray spectroscopy have been employed to determine the high-spin spectra and the $B(E2;0^+\rightarrow 2^+)$ transition probabilities of some of these nuclei. Whereas the energy spectra in ^{104,106}Pd have been correctly mapped at least up to 12^+, in ^{108}Pd isotope it is only known correctly up to 6^+ state and in ^{110}Pd up to 12^+ state. The data on $B(E2;0^+\rightarrow 2^+)$ values is, however, available[17,18] only for $^{102-110}$Pd. One of the striking features of the observed yrast spectra is the dramatic onset of backbending in ^{104,106}Pd at $J=10^+$.

In contrast to the large scale effort that has been made on the experimental side, only a few theoretical models[19-24] have been proposed to explain the character of yrast spectra in these nuclei. The earlier phenomenological attempts at understanding the observed levels in Pd have had limited success.[19,20] Apart from the earlier studies in the framework of the variable moment of inertia (VMI) model, an attempt was also made by Smith and Valkov[21] to explain the observed features of the yrast bands in Pd isotopes by invoking unstability towards asymmetric deformations at sufficiently high ($J>8^+$) angular momenta. Recently, Stachel *et al.*[24] have attempted a study of the experimental excitation energies and $E2$ transition probabilities of neutron-rich Pd isotopes in the framework of interacting boson model (IBA-1). Evidence has been presented that Pd isotopes, to a lesser extent, follow the SU(5)$\rightarrow$O(6) transition. It has been pointed out that SU(5)$\rightarrow$O(6) transition calculation should be viewed only as a guideline, and not as the ultimate theoretical calculation. In view of this, a lack of any microscopic calculation has hindered an understanding of the observed spectra in terms of the underlying single-particle states and the causes leading to the backbending effect in ^{104,106}Pd.

In this Brief Report we carry out a microscopic study of the yrast bands in the nuclei $^{104-110}$Pd by employing the variation after projection (VAP) formalism[25] in conjunction with the Hartree-Fock-Bogolubov (HFB) ansatz for the axially symmetric intrinsic wave functions. The choice of the VAP method was dictated by two considerations. Firstly, it is desirable to use a calculational framework which allows for the possibility of having different intrinsic states for each yrast level, in view of the observed large deviations of the yrast levels in these isotopes from the $J(J+1)$ law. Secondly, it is rather easy to compute the intrabands $E2$ transition probabilities in the VAP method.

In the present variational calculation of the yrast levels in the nuclei $^{104-110}$Pd we have employed the usual pairing plus quadrupole-quadrupole effective interaction operating in a valence space spanned by the $3S_{1/2}$, $2d_{3/2}$, $2d_{5/2}$, $1g_{7/2}$, $1g_{9/2}$, and $1h_{11/2}$ orbits for protons as well as neutrons. The nucleus ^{80}Zr has been considered as an inert core. The spherical single-particle energies (SPE's) we have employed are (in MeV): $(1g_{9/2})=0.5$, $(2d_{5/2})=5.4$, $(3S_{1/2})=6.4$, $(2d_{3/2})=7.9$, $(1g_{7/2})=8.4$, and $(1h_{11/2})=8.4$. This set of input SPE's is exactly the same as that employed in a number of successful shell-model calculations in $A\sim 90$ nuclei by Vergados and Kuo[26] as well as by Federman and Pittel[27] except for a slight reduction in the $(1h_{11/2}$-$1g_{9/2})$ separation by 1.1 MeV. The strengths for the like particle (n-n) as well as the neutron proton (n-p) components of the quadrupole-quadrupole (qq) interaction were taken as

$$\chi_{nn}(=\chi_{pp})=-0.0118\ \text{MeV}\,b^{-4}\ ,$$

$$\chi_{np}=-0.02234\ \text{MeV}\,b^{-4}\ .$$

Here b $(=\sqrt{\hbar/m\omega})$ is the oscillator parameter. These values for the strengths of the qq interactions compare favorably with the ones suggested recently by Arima[28] and these values are very near the ones employed in our[29] earlier study of the deformation systematics in the $A\sim 100$ region. The strength of the pairing interaction was fixed (through the approximate relation $G=18-21/A$) at $G=0.22$ MeV. The reduction in the $(1h_{11/2}$-$1g_{9/2})$ separation is intended to mockup, at least partially, the effects due to the neglected, higher-lying single-particle orbits.

The calculation of the energies of the yrast levels has been carried out as follows. We have first generated the self-consistent, axially symmetric HFB solutions $\phi_{K=0}(\beta)$

resulting from the Hamiltonian $(H-\beta Q_0^2)$. The optimum intrinsic state for each J, $\phi_{\rm opt}(\beta_J)$ has been selected by determining the minimum of the projected energy

$$E_J(\beta)=\left[\frac{\langle\phi(\beta)\,|\,HP^J\,|\,\phi(\beta)\rangle}{\langle\phi(\beta)\,|\,P^J\,|\,\phi(\beta)\rangle}\right] \tag{1}$$

as a function of β. In other words, the intrinsic state for each J satisfies the following condition:

$$\delta\left[\frac{\langle\phi(\beta)\,|\,HP^J\,|\,\phi(\beta)\rangle}{\langle\phi(\beta)\,|\,P^J\,|\,\phi(\beta)\rangle}\right]=0\ . \tag{2}$$

Here the operator P^J projects out the eigenstates of J^2 from the intrinsic states $\phi(\beta)$. Our assumption concerning the axial symmetry of the intrinsic states is consistent with the microscopic calculation of potential-energy surfaces in ^{102}Zr by Kumar *et al.*;[30] it is found that the minimum of potential energy $V(\beta,\gamma)$ for the ground-state band occurs at $\beta=0.4$, $\gamma=10°$, and, therefore, the effects, due to nonaxiality, are expected to be small for the yrast levels for nuclei with $A\sim100$.

It may be mentioned that variational methods quite similar to the ones employed here have been used earlier by Fassler, Lin, and Wittman,[31] as well as Nair and Ansari[32] in connection with the study of backbending effects in ^{158}Er. The present calculation, however, employs exact angular momentum projection in contrast with the technique used by Nair and Ansari which used an approximation suggested by Das Gupta and Van Ginneken.[33]

In the present report an attempt is made to quantitatively investigate the causes responsible for the dramatic onset of the backbending effect in ^{104,106}Pd. This feature of the yrast spectra is surprisingly completely absent in the neighboring isotopes. It is important to mention that for a calculation of high-spin levels to be of some reliability, one must get a reasonably good agreement for the available energies as well as the electromagnetic transitions involving the low-lying yrast states in the isotopes $^{104-110}$Pd. In Fig. 1 we present a comparison of the calculated low-lying yrast spectra in the isotopes $^{104-110}$Pd with the experimental ones. From the figure, one observes that the present calculation yields a satisfactory overall agreement with the experimental results, particularly in view of the fact that we have not used any parameter to mockup the contributions of the $N=Z=40$ core towards the moment of inertia. The calculation is seen to reproduce the observed levels with $J^\pi\leq8^+$ within an accuracy of about 300 keV.

In view of the availability of the reliable $B(E2,0^+\rightarrow2^+)$ data[17,18] in the $^{104-110}$Pd we have also subjected the intrinsic states obtained for these isotopes to the following semiquantitative test. It has been shown[34] that if the expectation value of $\hat{J}^2$ is large, the intrinsic electric quadrupole moment is related to the $B(E2;J_i^+\rightarrow J_f^+)$ for $E2$ transitions between the states projected from the intrinsic HFB state, by

$$B(E2);J_i^+\rightarrow J_f^+)=\frac{5\pi}{16}\begin{bmatrix}J_i & 2 & J_f\\ 0 & 0 & 0\end{bmatrix}^2 \times(e_p\langle Q_0^2\rangle_\pi+e_n\langle Q_0^2\rangle_\nu)^2\ . \tag{3}$$

In Table I, we present a comparison of the observed $B(E2;0^+\rightarrow2^+)$ values with the values calculated by substituting, in relation (3), the $\langle Q_0^2\rangle_\pi$ and $\langle Q_0^2\rangle_\nu$ values for $^{104-110}$Pd given in Table I. It is satisfying to note that the computed $B(E2)$ estimates are in excellent agreement with the experiments, provided one chooses $e_{\rm eff}=0.1$, 0.1, 0.1, 0.15 for ^{104,106,108,110}Pd, respectively.

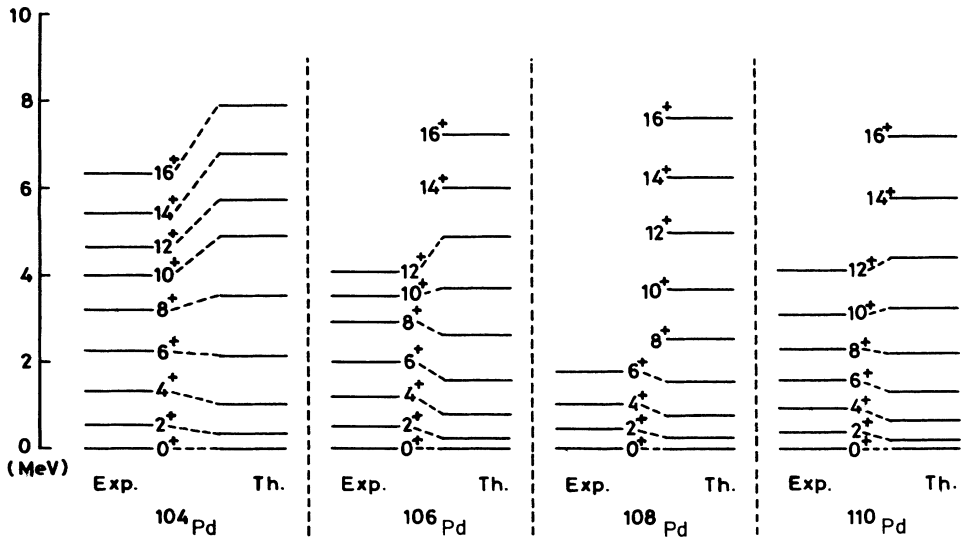

FIG. 1. Comparison of the observed (Exp.) as well as the calculated (Th.) yrast spectra in the nuclei ^{104,106,108,110}Pd.

TABLE I. Comparison of the calculated and the observed $B(E2;0^+\rightarrow 2^+)$ values in some quasirotational Pd isotopes. The effective charges have been used such that for protons the effective charge is $e_p=1+e_{\text{eff}}$ and for neutrons it is $e_n=e_{\text{eff}}$. The values of the oscillator parameter have been calculated from the relation $b=1.01\ A^{1/6}$ fm. Here $\langle Q_0^2\rangle_\pi(\langle Q_0^2\rangle_\nu)$ gives the contribution of the protons (neutrons) to the total intrinsic quadrupole moment.

	$B(E2;0^+\rightarrow 2^+)\times 10^{-48}\ e^2\text{cm}^4$					
	Calculated					
Nucleus	$e_{\text{eff}}=0.1$	$e_{\text{eff}}=0.15$	$e_{\text{eff}}=0.20$	Expt.	$\langle Q_0^2\rangle_\pi$	$\langle Q_0^2\rangle_\nu$
^{104}Pd	0.50	0.61	0.73	0.51±0.05	26.81	41.06
^{106}Pd	0.60	0.73	0.87	0.61±0.06	29.10	45.19
^{108}Pd	0.72	0.78	0.94	0.70±0.07	29.86	46.51
^{110}Pd	0.67	0.81	0.97	0.82±0.08	30.11	46.96

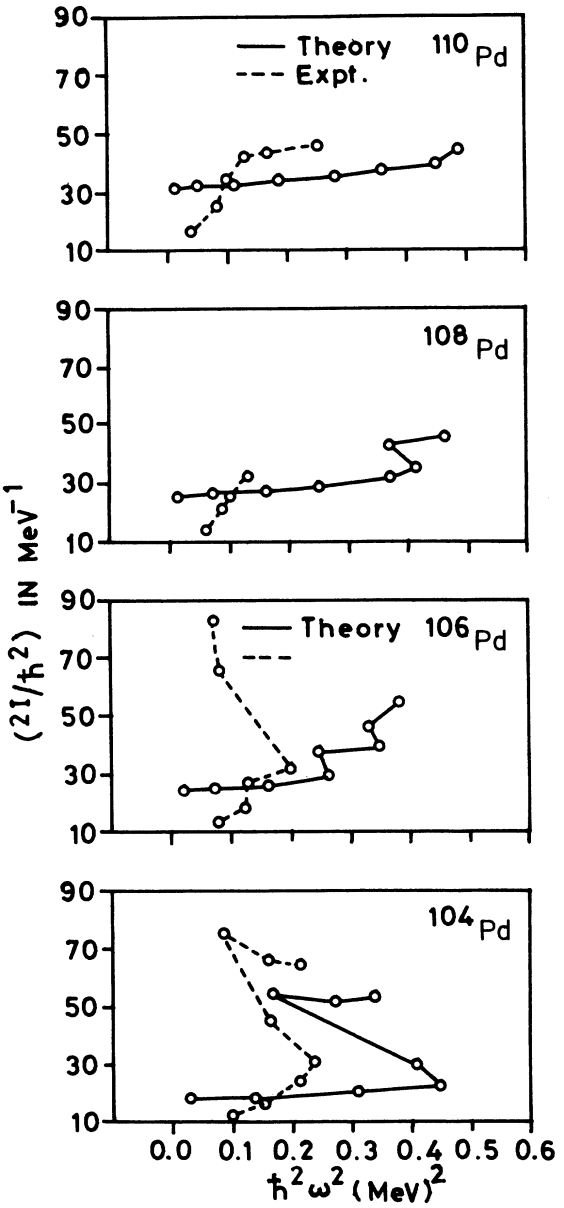

FIG. 2. Moment of inertia vs the square of the angular velocity for the high-spin yrast levels in the nuclei ^{104,106,108,110}Pd.

In Fig. 2 we present the usual I vs ω^2 curves for the nuclei $^{104-110}$Pd. The quantities, moment of inertia (I) and squared angular frequency (ω^2) have been computed in terms of the yrast energies by using the following expressions:

$$2I/\hbar^2=(4J-2)/(E_J-E_{J-2})\ ,$$

$$\hbar^2\omega^2=(J^2-J+1)(E_J-E_{J-2})^2/(2J-1)^2\ .$$

It may be noted that we get a good qualitative agreement between the calculated and observed variation of I as a function of ω^2. The observed backbending effect in ^{104,106}Pd at $J^\pi=10^+$ is also very well reproduced. Whereas our results for ^{104}Pd are in strikingly good agreement with experiments, those for ^{106}Pd correctly predict the onset of backbending at 10^+. Our results also predict the appearance of the backbending effect in ^{108}Pd at $J^\pi=14^+$.

As is evident from the experimental spectra and Fig. 2, the backbending in ^{104,106}Pd appears due to the reduction of (E_J-E_{J-2}) energy gap at $J=10^+$. From the results presented in Table II, we see that the sudden decrease of (E_J-E_{J-2}) at $J^\pi=10^+$ in ^{104,106}Pd is strikingly correlated with the dramatic increase in the quadrupole deformation of the intrinsic states corresponding to the $J=8^+$ and $J=10^+$ states. Whereas, in ^{104}Pd the quadrupole deformation increases from $\langle Q_0^2\rangle=67.87\ b^2$ at $J=8^+$ to $\langle Q_0^2\rangle=87.87\ b^2$ at $J=10^+$ that for ^{106}Pd it increases from $\langle Q_0^2\rangle=74.29\ b^2$ at $J=8^+$ to $\langle Q_0^2\rangle=81.39\ b^2$ at $J=10^+$ along the yrast cascade. An analysis of the subshell occupation numbers (see Table II) further reveals that this increase in the quadrupole deformation of the intrinsic states at $J=10^+$ can be understood in terms of the depletion in the $(1g_{9/2})_\nu$ occupation and sharp enhancement in the occupation numbers of $(1h_{11/2})_\nu$ orbits. It may be pointed out that an increase in the occupation number for the $(1h_{11/2})_\nu$ orbit from 2.57 for $J^\pi=8^+$ to 3.98 for $J^\pi=10^+$ in ^{104}Pd and from 3.99 for $J^\pi=8^+$ to 4.55 for $J^\pi=10^+$ in ^{106}Pd is quite efficacious in enhancing the intrinsic quadrupole deformation since it implies an increased occupation of the $1h_{11/2};\pm\frac{3}{2}$ orbitals which are characterized by large values of the single-particle matrix element of the quadrupole operator.

TABLE II. Quadrupole moments as well as the subshell occupation numbers associated with the optimum intrinsic states for the yrast levels in the nuclei ^{104,106,108,110}Pd.

Nucleus	J^π	$\langle\phi(\beta_J)\mid Q_0^2\mid\phi(\beta_J)\rangle$	Subshell occupation number $(2d_{5/2})_\pi$	$(1g_{9/2})_\pi$	$(2d_{5/2})_\pi$	$(1g_{9/2})_\nu$	$(1h_{11/2})_\nu$
^{104}Pd	0^+-8^+	67.87	1.05	4.19	2.43	9.14	2.57
	10^+-16^+	87.87	1.17	3.06	2.13	7.53	3.98
^{106}Pd	0^+-8^+	74.29	1.10	3.84	2.48	9.35	3.99
	10^+-16^+	81.39	1.13	3.27	2.35	8.77	4.55
^{108}Pd	0^+-10^+	76.38	1.11	3.72	2.79	9.53	5.09
	12^+-16^+	83.20	1.15	3.11	2.58	9.05	5.69
^{110}Pd	0^+-14^+	77.08	1.12	3.70	3.25	9.66	5.89
	16^+	80.31	1.13	3.28	3.19	9.61	6.02

Summarizing, the calculations presented here reveal that the backbending in ^{104,106}Pd can be understood in terms of sudden increase of deformation of the intrinsic states at $J^\pi=10^+$ arising due to the enhanced occupation of $1h_{11/2};\pm\frac{3}{2}$ orbits, which are found to be crossing the respective Fermi surfaces.

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