Mechanism of shape transition in neutron-rich palladium isotopes

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The high-spin yrast spectra with $J^{\pi}_{\max}=(16^+)$ and the observed gradual shape transition at ^{108}Pd in the nuclei $^{100-114}$Pd are examined by carrying out Hartree-Fock-Bogolubov calculations employing a pairing-plus-quadrupole-quadrupole effective interaction operating in a reasonably large valence space outside an inert ^{80}Zr core. Our calculations reveal that the gradual shape transition at ^{108}Pd is intricately linked with the simultaneous change of relative occupation probabilities of $(g_{7/2})$-neutron and $(g_{9/2})$-proton orbits.

The high-spin spectra in doubly even Pd isotopes has been the subject of a large number of recent experimental studies[1-18] involving inbeam gamma-ray spectroscopy. A striking feature of the observed spectra (see Table I) is that the E_2^+ excitation energy remains almost constant in $^{102-106}$Pd and then suffers a slow decrease around ^{108}Pd. Thereafter it decreases with increasing A, but slowly. For example in $^{102-106}$Pd, the $(E_2^+ - E_0^+)$ separation is almost 0.55 MeV of that in ^{110}Pd where it is 0.37 MeV. From the above observation it appears as if there is a slow shape transition taking place in Pd isotopes at ^{108}Pd. Palladium isotopes with $100 \leq A \leq 106$ seem to be soft vibrational nuclei and those with $A \geq 110$ seem to be quasirotational. ^{108}Pd is thought to be a transitional nucleus forming a zone between soft vibrators on one side and nearly deformed nuclei on the other side. This is also confirmed by a similar trend exhibited by $B(E2,0^+ \rightarrow 2^+)$ and Q_2^+ values. Whereas for ^{104}Pd, the $B(E2,0^+ \rightarrow 2^+)$ value is of the order of (0.51 ± 0.05) e^2b^2, for ^{110}Pd it is $(0.91 \pm 0.06)e^2b^2$. Similarly, the Q_2^+ for ^{104}Pd is (-0.25 ± 0.12) eb, and for ^{110}Pd it is (0.82 ± 0.18) eb. It seems that at least for the isotopes $^{104-110}$Pd there is some correlation between Q_2^+, $B(E2; 0^+ \rightarrow 2^+)$ and the excitation energy of the 2^+ state (ΔE). As ΔE decreases, $B(E2,0^+ \rightarrow 2^+)$ and Q_2^+ increase, all presumably reflecting the occurrence of shape change at ^{108}Pd and increasing susceptibility to deformation for $A > 108$.

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 the Pd region 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 instability 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)→O(6) transition. It has been pointed out that SU(5)→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 also the causes responsible for inducing gradual shape transition at ^{108}Pd in the palladium isotopes.

In this report we carry out a microscopic study of the yrast bands in the nuclei $^{100-114}$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 $^{100-114}$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 $(n\text{-}p)$ components of the quadrupole-quadrupole (qq) interaction were taken as

$$\chi_{nn}(=\chi_{pp}) = -0.0118 \text{ MeV b}^{-4},$$
$$\chi_{np} = -0.02234 \text{ MeV b}^{-4}.$$

TABLE I. The experimental values of excitation energy of E_2^+ state (ΔE), the transition probabilities $B(E2; 0^+ \rightarrow 2^+)$ and quadrupole moment Q_2^+, for some of the Pd isotopes.

Nucleus	E_2^+ in MeV	$B(E2,0^+ \rightarrow 2^+) \times e^2b^2$	$Q_2(e,b)$
^{100}Pd	0.66		
^{102}Pd	0.55	0.46±0.03	−0.2±0.2
^{104}Pd	0.55	0.51±0.05	−0.25±0.12
^{106}Pd	0.51	0.61±0.06	−0.52±0.12
^{108}Pd	0.43		
^{110}Pd	0.37	0.91±0.06	−0.82±0.18
^{112}Pd	0.34		
^{114}Pd	0.33		

Here, $b(=\sqrt{\hbar/m\omega})$ is the oscillator parameter. These values for the strengths of the q·q 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, $\phi_{\text{opt}}(\beta_J)$ has been selected by determining the minimum of the projected energy,

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

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

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

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 $A \sim 100$.

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 work an attempt is made to explain the high-spin yrast spectra and also to quantitatively investigate the causes responsible for inducing the gradual shape transition at ^{108}Pd in the Pd 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 $^{100-114}$Pd. In Figs. 1 and 2 we present a comparison of the calculated low-lying yrast spectra in the isotopes $^{100-114}$Pd with the experimental ones. From the figures, 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 $J^\pi \leq 8^+$ with a maximum discrepancy of only about 500 keV in the case of ^{106}Pd.

In view of the availability of the reliable $B(E2,0^+ \rightarrow 2^+)$ data[17,18] in the $^{102-110}$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 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

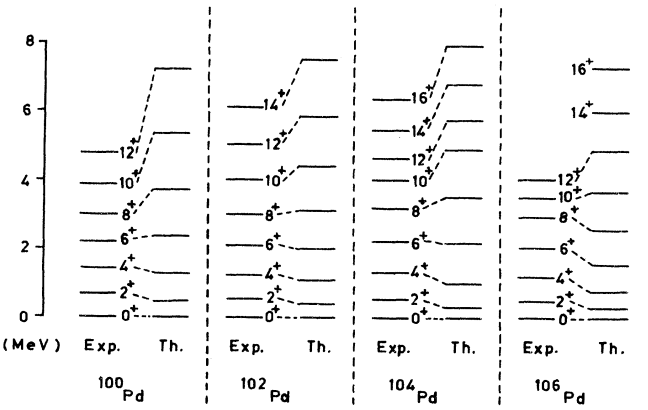

FIG. 1. Comparison of the observed (exp) as well as the calculated (th) yrast spectra in the nuclei $^{100-106}$Pd.

TABLE II. 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	$e_{\text{eff}}=0.30$	$e_{\text{eff}}=0.35$	$e_{\text{eff}}=0.40$	Expt.	$\langle Q_0^2\rangle_\pi$	$\langle Q_0^2\rangle_\nu$
^{100}Pd	0.34	0.39	0.44		23.11	30.90
^{102}Pd	0.35	0.40	0.46	0.46±0.03	23.28	31.88
^{104}Pd	0.50	0.58	0.66	0.51±0.05	26.81	41.06
^{106}Pd	0.61	0.70	0.80	0.61±0.06	29.10	45.19
^{108}Pd	0.65	0.75	0.85	0.70±0.07	29.86	46.52
^{110}Pd	0.67	0.78	0.88	0.82±0.08	30.11	46.96
^{112}Pd	0.64	0.74	0.84		29.40	45.70
^{114}Pd	0.61	0.70	0.80		28.55	44.10

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

In Table II, we present a comparison of the observed $B(E2,0^+\rightarrow 2^+)$ 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 $^{100-114}$Pd given in Table II. It is satisfying to note that the computed $B(E2)$ estimates are almost in agreement with the experiments, provided one chooses $e_{\text{eff}}=0.4$, 0.3, 0.3, 0.3, and 0.35 for ^{102,104,106,108,110}Pd, respectively. These effective charges are no doubt slightly larger but this is not unexpected. The calculated $B(E2)$ values obtained with these effective charges are only expected to provide an upper bound to the experimental $B(E2)$ values, as the formula used for their calculation is strictly valid for perfect rigid rotators. Therefore, our HFB wave function describing the ground-state properties of the Pd isotopes is fairly reliable.

We now focus our attention on the observed shape transition in palladium nuclei. Before trying to investigate the causes for the shape transition, it is important to discuss and highlight some of the well accepted factors responsible for the onset of large deformation in the same mass region but in the nuclei which are isobars of palladium nuclei such as $^{100-106}$Zr and $^{100-106}$Mo. It is generally felt that the neutron-proton (n-p) effective interactions posses a deformation producing tendency, and the neutron-neutron (n-n) or proton-proton (p-p) effective interactions are mostly of the spherifying nature.[35-40] These ideas have played a pivotal role in the development of the stretch scheme[38] of Danos and Gillet, and rotor model[39] of Arima and Gillet, and the recent interacting boson model[40] of Arima *et al.* In this regard, the role of the n-p interaction in the spin orbit partner (SOP) orbits in the context of the general development of collective features was also suggested by Federman and Pittel.[27,35,37,41,42] and by R. F. Casten *et al.*[43] Their calculation provided an evidence suggesting that n-p interaction between the valence nucleons in the SOP orbits—the orbits $(g_{9/2})_\pi$ and $(g_{7/2})_\nu$ in the zirconium and molybde-

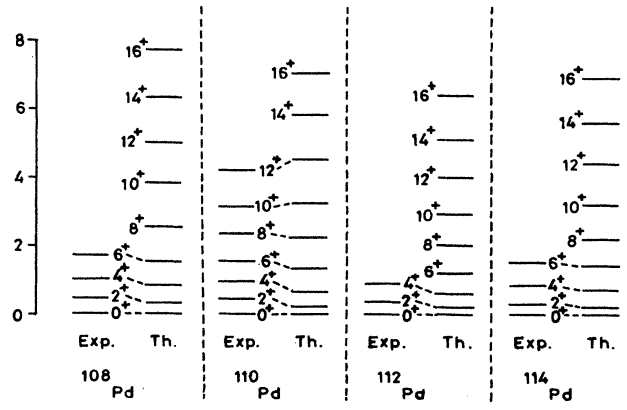

FIG. 2. Comparison of the observed (exp) as well as the calculated (th) yrast spectra in the nuclei $^{108-114}$Pd.

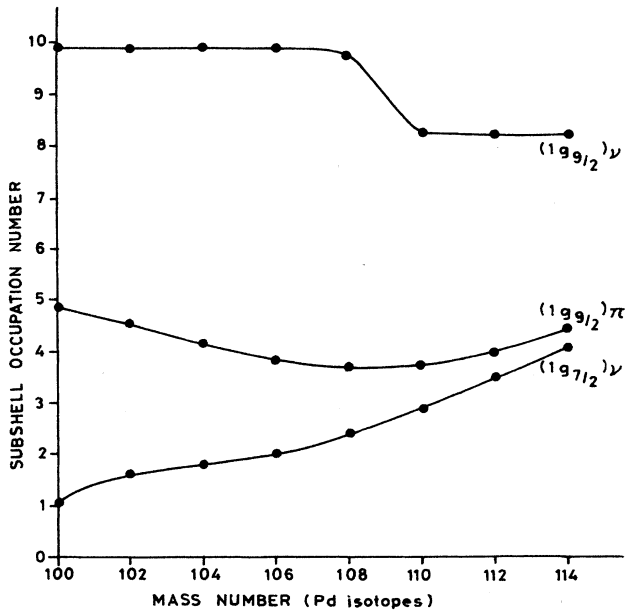

FIG. 3. Subshell occupation numbers for $(1g_{9/2})_\nu$, $(1g_{7/2})_\nu$ and $(1g_{9/2})_\pi$ subshells versus the mass number A for $^{100-114}$Pd isotopes.

num nuclei—may be instrumental *vis-a-vis* the observed onset of deformation in Mo isotopes with $A > 100$. It may also be pointed out that the role of the *np* interaction operating between SOP orbits in producing deformation depends critically on the relative occupation probability of $(g_{9/2})_\pi$ and $(g_{7/2})_\nu$ orbits. Besides this, it has recently been shown by Khosa *et al.*[29] that the sudden polarizability of the $(g_{9/2})_\nu$ shell in neutron rich molybdenum isotopes is responsible for initiating large deformation in molybednum isotopes. From their results one notices that in the case of $^{92-98}$Mo, the $(1g_{9/2})_\nu$ shell is full whereas for the ^{100}Mo the $(1g_{9/2})_\nu$ occupation suddenly falls to about 7.2 and leads to slow shape transition in these isotopes.

In Fig. 3 we display the subshell occupation numbers for $(1g_{9/2})_\nu$, $(1g_{7/2})_\nu$, and $(1g_{9/2})_\pi$ subshells calculated from the HFB wave function generated for $^{100-114}$Pd isotopes. A careful examination of the $(1g_{9/2})_\pi$ and $(1g_{7/2})_\nu$ occupation probabilities reveals that for $^{100-106}$Pd the $(1g_{7/2})_\nu$ occupation increases from 1.03 to 2.0 and that of the $(1g_{9/2})_\pi$ occupation decreases from 4.85 to 3.84. This means that for these isotopes there is no significant simultaneous increase in the occupation probabilities of SOP orbits, thus making the *np* interaction operating between valence particles in SOP orbits ineffective in inducing deformation in these isotopes. Besides this, a quick look at the $(1g_{9/2})_\nu$ occupation probability reveals that in these isotopes this subshell is almost unpolarized. Thus, near constancy of E_2^+ excitation energy in $^{100-106}$Pd isotopes can be understood in terms of a nearly insignificant simultaneous increase in the relative occupation probabilities of $(1g_{9/2})_\pi$ and $(1g_{7/2})_\nu$ orbits and also the nonpolarizability of the $(g_{9/2})_\nu$ subshell. We now discuss the nuclei $^{110-114}$Pd. Note that the $(1g_{9/2})_\pi$ and $(1g_{7/2})_\nu$ occupation probabilities undergo a slow simultaneous increase. This in turn causes an increase in the effectiveness of the *np* interaction operating between the particles in SOP orbits to produce deformation. Thus the E_2^+ energy state gets depressed as we go from ^{106}Pd to ^{110}Pd. Besides this, a study of the $(1g_{9/2})_\nu$ occupation probabilities reveals that in $^{110-114}$Pd this orbit is polarized. Thus, the above two factors act in phase here, and are thus intricately linked with the slow shape transition occurring in Pd isotopes at ^{108}Pd.

Summarizing, the observed shape transition around $A = 108$ in the palladium region can be understood in a microscopic framework in terms of two unrelated factors, namely the polarization of the $(g_{9/2})_\nu$ shell and, secondly, deformation producing tendency of the neutron-proton interaction operating between valence particles in the spin-orbit partner (SOP) orbits—the orbits $(g_{9/2})_\pi$ and $(g_{7/2})_\nu$ in the present context.

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