Calculation of yrast spectra in the doubly even cadmium isotopes

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(Received 19 June 1990)

The observed systematics of the low-lying states in $^{98-110}$Cd nuclei and the high-spin yrast spectra with $J^{\pi}_{\max} \leq 14^{+}$ are examined by carrying out Hartree-Fock-Bogoliubov 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 systematics of the low-lying yrast states in $^{98-110}$Cd are intricately linked with the deformation producing tendency of the n-p interaction when operating between spin-orbit-partner (SOP) orbits. Our results indicate that such systematics depend crucially on the simultaneous increase of relative occupation probabilities of the $(d_{5/2})$-proton and $(d_{3/2})$-neutron orbits in the $^{98-100}$Cd isotopes.

In this paper we report on the calculations of the yrast spectra of the doubly even nuclei $^{98-110}$Cd. Apart from the energy spectra we shall also discuss here the results of the calculations of the reduced transition probabilities for $E2$ transitions for the yrast states, as well as the subshell occupation numbers for the $3s_{1/2}$, $2d_{3/2}$, $2d_{5/2}$, $1g_{7/2}$, $1g_{9/2}$, and $1h_{11/2}$ orbits in the ground states of these nuclei.

Recent years have witnessed a rapid increase in the experimental activity of measuring the properties of the yrast levels (up to $J^{\pi}=14^{+}$) in the Cd isotopes.[1-11] A striking feature of the observed spectra (see Table I) is that the $E_{2_1^+}$ excitation energy suffers a sharp decrease in its value as one moves from ^{98}Cd to ^{100}Cd. Whereas the $E_{2^+}-E_{0^+}$ $(=\Delta E)$ energy gap in ^{98}Cd is 1.43 MeV, its value in ^{100}Cd is 0.85 MeV. It seems that there is some structural change taking place in the Cd nuclei around ^{98}Cd. After ^{100}Cd a very slow decrease in the value of E_{2^+} with neutron number is observed until ^{106}Cd is reached, whereafter its value in $^{106-110}$Cd remains almost constant. It would therefore be interesting to understand the causes that are responsible for producing such E_{2^+} energy systematics in the Cd isotopes.

In contrast to the large-scale effort that has been made on the experimental side, only a few theoretical models have been proposed to explain the character of yrast spectra in these nuclei. While, in fact, the features of the low-lying states of these nuclei are in qualitative agreement with the predictions of a spherical quadrupole vibrational model, the occurrence of additional $J=0^{+}$ and 2^{+} levels at the energy of the two phonon triplet perturbs this picture. Some time back Sambataro[12] attempted a study of the properties of Cd isotopes in the framework of the interacting boson approximation. The collective features of these nuclei were found to be in satisfactory agreement with the predictions of this model. However, this calculation can only be viewed 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 systematics in terms of the underlying single-particle states.

In this paper we carry out a microscopic study of the yrast bands in the nuclei $^{98-110}$Cd by employing the variation after projection (VAP) formalism[13] in conjunction with the Hartree-Fock-Bogoliubov (HFB) ansatz for the axially symmetric intrinsic wave functions. The choice of the VAP method was dictated by two considerations. First, 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 intraband $E2$ transition probabilities in the VAP method.

In the present variational calculation of the yrast levels in the nuclei $^{98-110}$Cd 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[14] as well as by Federman and Pittel[15] 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 neutron-proton (n-p) components of the quadrupole-quadrupole (qq) interaction were taken as

$$\chi_{nn}(=\chi_{pp})=-0.0118 \text{ MeV } b^{-4},$$
$$\chi_{np}=-0.022\,34 \text{ MeV } b^{-4}.$$

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[16] and these values are very near the ones employed in our[17] earlier study of deformation systematics in the $A\sim 100$ region. The strength of the pairing interaction was fixed (through the approximate relation $G=0.22$ MeV). The

reduction in the $(1h_{11/2}\text{-}1g_{9/2})$ separation is intended to mock up, 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.*[18] 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,[19] as well as Nair and Ansari[20] 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.[21]

We first discuss here the systematics of $E_{2_1^+}$ in $^{98-110}$Cd. As said earlier the energy gap ΔE decreases suddenly as we go from ^{98}Cd to ^{100}Cd; thereafter the decrease in ΔE with A is very slow until ^{106}Cd is reached. For the nuclei $^{106-110}$Cd the value of ΔE remains nearly constant. Phenomenologically it is well known that a nucleus having a smaller energy gap ΔE should have a larger quadrupole moment for the 2_1^+ state. Since Q_{2^+} of a nucleus is directly related to its intrinsic quadrupole moment, one should therefore expect that a smaller energy gap ΔE should manifest itself in terms of a larger intrinsic quadrupole moment and vice versa. In other words the observed systematics of $E_{2_1^+}$ with A should produce a corresponding inverse systematics of the intrinsic quadrupole moment of Cd nuclei with increasing A. Based on the above logic the calculated values of intrinsic quadrupole moments should exhibit a sharp increase in going from ^{98}Cd to ^{100}Cd. For the set of nuclei $^{106-110}$Cd the intrinsic quadrupole moment should be nearly constant and in going from ^{100}Cd to ^{106}Cd they should increase gradually. In Table I the results of HFB calculations are presented. Note that the intrinsic quadrupole moments sharply increase as we move from ^{98}Cd to ^{100}Cd; thereafter the increase in $\langle Q_0^2\rangle$ becomes slower. Whereas the $\langle Q_0^2\rangle$ value for ^{100}Cd is 31.99 units, for ^{102}Cd its value is 36.51 units. Besides this the $\langle Q_0^2\rangle$ values nearly saturate for the $^{106-110}$Cd nuclei, reproducing qualitatively the nearly constant feature of ΔE values for these nuclei. The calculated results, however, show a slightly faster increase in $\langle Q_0^2\rangle$ value in going from ^{102}Cd to ^{104}Cd, which is not consistent with the observed change in ΔE.

We next focus our attention on the factors that are responsible for making the Cd isotopes exhibit such features. In this regard it is important to discuss and highlight some of the well accepted factors responsible for bringing in sizable collectivity in nuclei in the same mass region. It is generally felt that the neutron-proton (n-p) effective interactions possess a deformation producing tendency and the neutron-neutron (n-n) or proton-proton (p-p) effective interactions are mostly of spherical nature.[22–27] These ideas have played a pivotal role in the development of the strech scheme[25] of Danos and Gillet, the rotor model[26] of Arima and Gillet, and the interacting boson model of Arima *et al.*[27] In this regard, the role of the n-p interaction in spin-orbit-partner (SOP) orbits in the context of the general development of collective features was also suggested by Federman and Pittel[15,22,28,29] and by Casten *et al.*[30] Their calculation provided 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 molybdenum nuclei—may be instrumental vis-à-vis the observed onset of deformation in the Mo isotopes with $A>100$. It may also be pointed out that the role of the n-p interaction operating between SOP orbits in producing deformation depends critically on the relative occupation probability of the $(g_{9/2})_\pi$ and $(g_{7/2})_\nu$ orbits.

In Tables II and III we present results for the occupation probabilities of the various proton and neutron subshells. Note that with increasing neutron number the occupation probabilities of the $(g_{9/2})_\pi$ orbit decrease whereas that of the $(d_{5/2})_\pi$ orbit increases. The results indicate that there is a transference of protons from the $(g_{9/2})_\pi$ orbit to the $(d_{5/2})_\pi$ orbit taking place with increasing neutron number. Besides this the occupation probabilities of the $(d_{3/2})_\nu$, $(d_{5/2})_\nu$, and $(g_{7/2})_\nu$ orbits exhibit a systematic increase. Such a transference of protons from the $(g_{9/2})_\pi$ orbit to the $(d_{5/2})_\pi$ orbit causes a simultaneous increase in the occupation probability of SOP orbits—the orbits $(d_{5/2})_\pi$ and $(d_{3/2})_\nu$ in the present context—with increasing neutron number. Since the occupation probability of the $(d_{3/2})_\nu$ orbit in ^{98}Cd is zero, the n-p interaction cannot operate between SOP orbits in this nucleus. Therefore ^{98}Cd exhibits very little collectively. As we move from ^{98}Cd to ^{100}Cd there is a marked increase in the occupation probability of the $(d_{3/2})_\nu$ orbit allowing the n-p interaction between the $(d_{5/2})_\pi$ and the $(d_{3/2})_\nu$ orbits to operate suddenly. As a result of this a sizable collectivity is brought into the nucleus ^{100}Cd which eventually results in a sharp decrease in the value of the excitation energy of $E_{2_1^+}$. Thus the sudden structural change observed in Cd nuclei around ^{98}Cd is intricately linked with the n-p interaction operating be-

TABLE I. The experimental values of excitation energy of the E_{2^+} state (ΔE) and the calculated intrinsic quadrupole moments of the HFB states in some doubly even Cd isotopes. 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. The quadrupole moments have been computed in units of b^2 where b ($=\sqrt{\hbar/m\omega}$) is the harmonic-oscillator parameter.

Nucleus	E_{2^+} (MeV)	$\langle Q_0^2 \rangle_{\text{HFB}}$	$\langle Q_0^2 \rangle_\pi$	$\langle Q_0^2 \rangle_\nu$
^{98}Cd	1.43	14.85	9.79	5.05
^{100}Cd	0.85	31.99	14.99	16.99
^{102}Cd	0.77	36.51	16.05	20.45
^{104}Cd	0.65	53.13	23.65	29.48
^{106}Cd	0.63	68.59	33.13	35.45
^{108}Cd	0.63	71.61	33.53	38.08
^{110}Cd	0.65	73.80	33.78	40.01

TABLE II. The calculated values of the occupation numbers (for protons) of various orbits in the ground states of some Cd isotopes.

Nucleus	$3s_{1/2}$	$2d_{3/2}$	$2d_{5/2}$	$1g_{7/2}$	$1g_{9/2}$	$1h_{11/2}$
^{98}Cd	0.00	0.00	0.13	0.01	7.83	0.00
^{100}Cd	0.01	0.00	0.28	0.01	7.69	0.01
^{102}Cd	0.01	0.00	0.35	0.02	7.50	0.14
^{104}Cd	0.27	0.20	0.83	0.10	6.50	0.07
^{106}Cd	0.60	0.59	1.13	0.24	5.41	0.01
^{108}Cd	0.59	0.62	1.13	0.26	5.37	0.00
^{110}Cd	0.59	0.64	1.14	0.27	5.34	0.00

TABLE III. The calculated values of the occupation numbers (for neutrons) of various orbits in the ground states of some Cd isotopes.

Nucleus	$3s_{1/2}$	$2d_{3/2}$	$2d_{5/2}$	$1g_{7/2}$	$1g_{9/2}$	$1h_{11/2}$
^{98}Cd	0.00	0.00	0.14	0.00	9.84	0.00
^{100}Cd	0.56	0.20	1.30	0.04	9.83	0.04
^{102}Cd	0.61	0.58	2.40	0.41	9.70	0.20
^{104}Cd	0.66	1.23	2.85	1.20	9.70	0.25
^{106}Cd	0.74	1.37	2.81	1.87	9.62	1.56
^{108}Cd	0.79	1.44	3.09	2.32	9.64	2.69
^{110}Cd	0.86	1.53	3.44	2.83	9.68	3.63

TABLE IV. Comparison of the calculated and the observed $B(E2;0^+ \rightarrow 2^+)$ values in some quasirotational Cd 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.

Nucleus	$B(E2;0^+ \rightarrow 2^+) \times 10^{-48}\ e^2\,\text{cm}^4$ Calculated			Expt.
	$e_{\text{eff}}=0.1$	$e_{\text{eff}}=0.15$	$e_{\text{eff}}=0.20$	
^{98}Cd	0.027	0.031	0.035	
^{100}Cd	0.073	0.086	0.101	
^{102}Cd	0.083	0.100	0.117	
^{104}Cd	0.191	0.227	0.267	
^{106}Cd	0.368	0.434	0.50	0.410
^{108}Cd	0.386	0.457	0.629	0.430
^{110}Cd	0.400	0.475	0.557	0.450

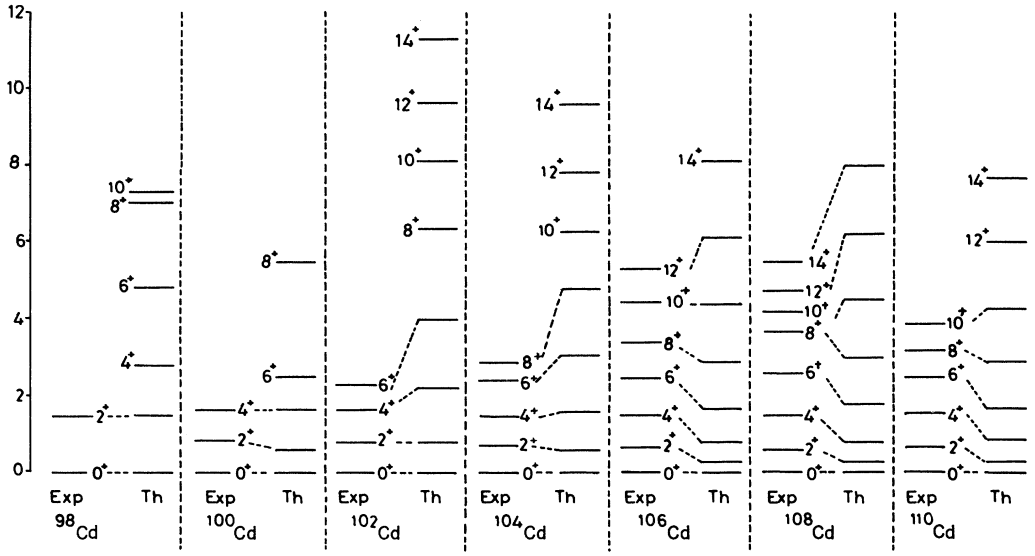

FIG. 1. Comparison of the observed (Exp) and the calculated (Th) yrast spectra in the nuclei ^{98,100,102,104,106,108,110}Cd.

tween SOP orbits suddenly becoming effective. It may further be noted that in $^{100-106}$Cd nuclei there is a simultaneous increase in the relative occupation probabilities of the above-mentioned SOP orbits bringing in more and more collectivity in these nuclei, and this increase could be held responsible for lowering the position of E_{2^+} successively in this set of nuclei. We now discuss the set of nuclei $^{106-110}$Cd. Note that the relative occupation probabilities of the SOP orbits remain nearly constant. Whereas in ^{106}Cd the occupation probabilities of the $(d_{5/2})_\pi$ and the $(d_{3/2})_\nu$ orbits are 1.13 and 1.37, respectively, their values in ^{110}Cd are 1.14 and 1.53. This constant feature exhibited by the calculated results in the nuclei $^{106-110}$Cd on occupation probabilities of SOP orbits, the $(d_{5/2})_\pi$ and $(d_{3/2})_\nu$ in the present context, could be interpreted to imply that no change in the collectivity of the Cd nuclei should be observed with increasing neutron number. This is what is observed experimentally. Thus the systematics of E_{2^+} in $^{98-110}$Cd isotopes can be understood in terms of the important role played by *n-p* interaction operating between SOP orbits.

The validity of the above conclusions, and also of the calculation of high-spin states in $^{98-110}$Cd, depends very much on the reliability of the HFB wave function. We have examined the goodness of the HFB wave function by calculating the low-lying yrast spectra (with $J^\pi < 6^+$) as well as the $B(E2;0^+ \rightarrow 2^+)$ values in the isotopes $^{98-110}$Cd. In Fig. 1 we have compared the calculated yrast spectra with the observed ones. The calculation reproduces the experimental levels with $J^\pi \leq 6^+$ with reasonably acceptable discrepancy. In view of the fact that we have not used any parameter to simulate the contribution of the ^{80}Zr core to the moment of inertia, the overall agreement can be considered fairly satisfactory. As pointed out by Faessler[31] as well as Prahraj[32] the inclusion of $K \neq 0$ bands may provide further quantitative improvements in the calculated yrast spectra.

We next move on to the calculation of the reduced $E2$ transition probabilities. It has been shown[33] 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

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

In Table IV 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 $^{98-110}$Cd given in Table I. It is satisfying to note that the calculated $B(E2)$ estimates are in good agreement with the experiments, provided one chooses $e_{\text{eff}} = 0.15$ for ^{106,108,110}Cd.

Summarizing, the observed structural change around ^{98}Cd can be understood in a microscopic framework in terms of the sudden onset in importance of the *n-p* interaction between the SOP orbits—the $(d_{5/2})_\pi$ and $(d_{3/2})_\nu$ orbits—in the present context. Besides this, the systematics of the low-lying states in $^{98-110}$Cd are intricately linked with the nature of the *n-p* interaction operating between SOP orbits vis-à-vis the bringing in of collectivity in nuclei when the relative occupation probabilities of SOP orbits simultaneously increase.

ACKNOWLEDGMENTS

One of the authors (S.K.K.) would like to thank Prof. H. L. Razdan, Dr. H. S. Rawat, and the staff of the computer center, Nuclear Research Laboratory, Srinagar, for extending the computational facility of the center to us.

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