Nuclear shape-phase diagrams

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Ground-state energy functions of even-even and odd-A nuclei are derived from simple parameter-dependent Interacting Boson Model (IBM) and Interacting Boson-Fermion Model (IBFM) Hamiltonians. Exact nuclear shape-phase diagrams in the two-parameter $(\eta,\ \chi)$ plane are explicitly described using the energy functions on the basis of the condition of phase equilibrium.

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I. INTRODUCTION

A phase transition can roughly be defined as a qualitative change in a given property of a system. In the past few years, there has sprung up a heated discussion as to shape-phase transitions in finite nuclei [1–13], i.e., at a certain value of the control parameters the ground state flipping from one deformation configuration to another. The Landau theory of continuous phase transition for infinite classical systems [14] is shown to be a useful tool for analyzing shape-phase transitions in even-even nuclei, where the energy function usually is truncated up to the fourth order of the order parameter [5,7,9,10]. In this paper we will employ the condition of shape phase equilibrium to quest for exact nuclear shape-phase diagrams especially in odd-A nuclei without any truncation.

II. OUTLINE OF THE THEORETICAL APPROACH

The study of shape-phase transition in even-even nuclei can be well done from the simple well-known two-parameter IBM Hamiltonian [15]:

$$H_B(N,\eta,\chi)=\eta n_d-\frac{1-\eta}{N}Q(\chi)\cdot Q(\chi),$$

where $n_d=d^\dagger\cdot\widetilde{d}$ represents the d-boson number operator, $Q(\chi)=d^\dagger s+s^\dagger\widetilde{d}+\chi[d^\dagger\times\widetilde{d}]^{(2)}$ is the quadrupole operator and N is the total boson number. Value of the so-called control parameters η ranges from 0 to 1 and χ is located in the interval of $-\sqrt{7}/2$ to $\sqrt{7}/2$. The ground-state energy function can be derived by making use of the coherent state formalism for the IBM [16,17]

$$|N\beta\gamma\rangle=\frac{\left\{s^\dagger+\beta\left[\cos\gamma d_0^\dagger+\sqrt{\tfrac{1}{2}}\sin\gamma(d_2^\dagger+d_{-2}^\dagger)\right]\right\}^N}{\sqrt{N!(1+\beta^2)^N}}|0\rangle. \quad (1)$$

Here intrinsic shape β and γ are used as order parameters in shape-phase transition theory and we set $\gamma=0$ to study only the β dependence. The energy function can therefore take the form

$$\begin{aligned}E(N,\eta,\chi,\beta)&=-5(1-\eta)+\frac{1}{(1+\beta^2)^2}\Big\{[N\eta-(1-\eta)(4N+\chi^2-8)]\beta^2\\&\quad+4(N-1)(1-\eta)\sqrt{\frac{2}{7}}\chi\beta^3\\&\quad+\left[N\eta-(1-\eta)\left(\frac{2N+5}{7}\chi^2-4\right)\right]\beta^4\Big\}.\end{aligned} \quad (2)$$

In order to infer the energy function of the odd-A nuclei within the framework of the IBFM, we resort to a phenomenological method. When an odd fermion is added into the even-even core, we assume a many-body wave function for the system to have the form of product of the wave functions of the single particle and the core [16]

$$\begin{aligned}|N\beta\gamma jm\rangle&=a_{jm}^\dagger|N\beta\gamma\rangle\\&=a_{jm}^\dagger\frac{\left\{s^\dagger+\beta\left[\cos\gamma d_0^\dagger+\sqrt{\tfrac{1}{2}}\sin\gamma(d_2^\dagger+d_{-2}^\dagger)\right]\right\}^N}{\sqrt{N!(1+\beta^2)^N}}|0\rangle\end{aligned} \quad (3)$$

with no fixed value of angular momentum. Here discussion is limited to the case when the odd fermion occupies only one shell model orbital, of angular momentum j and its z component m. The IBFM Hamiltonian [18] is given by

$$H=H_B+H_F+H_{BF}, \quad (4)$$

where H_F is the fermion Hamiltonian and contains only one-body term. Then $H_F=\sum_m\varepsilon_j(a_{jm}^\dagger a_{jm})$ contributes to the ground-state energy function an additive constant depending on quantum number j. H_{BF} is the interaction of the odd fermion and the core usually dominated by three terms, a monopole-monopole, a quadrupole-quadrupole, and an exchange interaction [18]. The quadrupole-quadrupole interaction can be expressed as

$$H_{BF}\propto[Q(\chi)\times(a_j^\dagger\times\widetilde{a}_j)^{(2)}]^{(0)}, \quad (5)$$

where $\widetilde{a}_{j-m}=(-1)^{j+m}a_{jm}$. Then the contribution of H_{BF} to the ground-state energy function for $\gamma=0$ can be obtained [16]

$$\begin{aligned}E_{BF}&=\langle N\beta\gamma jm|H_{BF}|N\beta\gamma jm\rangle\\&=\kappa\langle jm20\mid jm\rangle\left(\frac{2N\beta}{1+\beta^2}-\sqrt{\frac{2}{7}}\chi\frac{N\beta^2}{1+\beta^2}\right).\end{aligned} \quad (6)$$

One can naturally expect the H_{BF} is a perturbing operator in the IBFM Hamiltonian and hence interaction strength κ can be assumed to be a small and positive constant. The energy summation of ε_j and E_{BF}

$$\varepsilon_j+\kappa\langle jm20\mid jm\rangle\left(\frac{2N\beta}{1+\beta^2}-\sqrt{\frac{2}{7}}\chi\frac{N\beta^2}{1+\beta^2}\right) \quad (7)$$

is somewhat similar to the single-particle energy $\varepsilon_{j\Omega}$ of deformed shell model ($\Omega=|m|$) adopted in Ref. [19] due to $\langle jm20|jm\rangle \propto (3m^2 - j(j+1))$, though here we restrict the odd fermion to occupy only one shell model orbital $|jm\rangle$ and ignore the contribution of the levels with the same quantum number m coming from different j-shells. We neglect the remaining monopole and exchange interactions which contribute the energy function a term $\propto \frac{1}{1+\beta^2}$ or $\frac{\beta^2}{1+\beta^2}$ [16] and represent just a renormalization of the core Hamiltonian. So the total energy function is derived

$$\begin{aligned} E(\eta,\chi,\kappa,\beta) &= E(\eta,\chi,\beta) + \varepsilon_j \\ &\quad + \kappa\langle jm20 \mid jm\rangle\left(\frac{2N\beta}{1+\beta^2} - \sqrt{\frac{2}{7}}\chi\frac{N\beta^2}{1+\beta^2}\right) \\ &= \frac{1}{(1+\beta^2)^2}(a_1\beta + a_2\beta^2 + a_3\beta^3 + a_4\beta^4), \quad (8) \end{aligned}$$

where the coefficients a_1, a_2, a_3, and a_4 in the large-N limit read

$$\begin{aligned} a_1 &= 2\kappa\langle jm20 \mid jm\rangle, \\ a_2 &= 5\eta - 4 - \sqrt{\frac{2}{7}}\kappa\langle jm20 \mid jm\rangle\chi, \\ a_3 &= 4(1-\eta)\sqrt{\frac{2}{7}}\chi + 2\kappa\langle jm20 \mid jm\rangle, \\ a_4 &= \eta - \frac{2}{7}\chi^2(1-\eta) - \sqrt{\frac{2}{7}}\kappa\langle jm20 \mid jm\rangle\chi. \end{aligned} \quad (9)$$

With the inverse trigonometric function substitution $\theta = \arctan(\beta)$ $(-\frac{\pi}{4} \leqslant \theta \leqslant \frac{\pi}{4})$ and the use of the trigonometric formulas, we have the energy function and change the variable from β to $2\theta - \frac{\alpha_2}{2}$

$$\begin{aligned} E(\eta,\chi,\kappa,\beta) &= a_1\sin(\theta)\cos^3(\theta) + a_2\sin^2(\theta)\cos^2(\theta) \\ &\quad + a_3\sin^3(\theta)\cos(\theta) + a_4\sin^4(\theta) \\ &= -\frac{a_4}{2}\cos(2\theta) + \frac{a_1+a_3}{4}\sin(2\theta) \\ &\quad + \frac{a_4-a_2}{8}\cos(4\theta) + \frac{a_1-a_3}{8}\sin(4\theta) \\ &\quad + \frac{a_2+3a_4}{8} \\ &= r_1\cos\left(\left(2\theta - \frac{\alpha_2}{2}\right) + \left(\frac{\alpha_2}{2} - \alpha_1\right)\right) \\ &\quad + r_2\cos\left(2\left(2\theta - \frac{\alpha_2}{2}\right)\right) + \frac{a_2+3a_4}{8}, \quad (10) \end{aligned}$$

where the hypotenuses r_1, r_2, angles $\alpha_1 (-\pi \leqslant \alpha_1 < \pi)$ and α_2 $(-\pi/2 \leqslant \alpha_2 < \pi/2)$ have the following relationship with the coefficients a_1, a_2, a_3, and a_4:

$$\begin{aligned} r_1 &= \frac{\sqrt{4a_4^2 + (a_1+a_3)^2}}{4}, \\ \alpha_1 &= \arctan\frac{a_1+a_3}{-2a_4}, \quad a_4 \leqslant 0, \\ \alpha_1 &= \pi + \arctan\frac{a_1+a_3}{-2a_4}, \quad a_4 > 0, \quad a_1+a_3 \geqslant 0; \alpha_1 \\ &= -\pi + \arctan\frac{a_1+a_3}{-2a_4}, \quad a_4 > 0, \quad a_1+a_3 < 0, \\ r_2 &= \frac{\sqrt{(a_4-a_2)^2 + (a_1-a_3)^2}}{8}, \\ \alpha_2 &= \arctan\frac{a_1-a_3}{a_4-a_2}. \end{aligned} \quad (11)$$

III. DISCUSSIONS

Since the the variable $2\theta - \frac{\alpha_2}{2}$ is located within the region of $-\frac{3\pi}{4}$ to $\frac{3\pi}{4}$ and $\cos(2(2\theta - \frac{\alpha_2}{2}))$ has two minima and one maximum as a even function, it can be observed from Eq. (10) that two-phase equilibrium exists in the system only if $\cos((2\theta - \frac{\alpha_2}{2}) + (\frac{\alpha_2}{2} - \alpha_1))$ is also a even function and has one minimum or maximum. So the shape-phase transition curve of the $E(\eta,\chi,\kappa,\beta)$ in (η,χ) plane can then be denoted by a very compact form $\frac{\alpha_2}{2} - \alpha_1 = 0, \pm\pi$

$$\arctan\frac{a_1-a_3}{a_4-a_2} = 2\arctan\frac{a_1+a_3}{-2a_4}. \quad (12)$$

Detailed analysis of the eqnarray leads to identify the phase-transition curve

$$a_1^3 + a_1^2a_3 + 4a_1a_2a_4 - a_1a_3^2 - 8a_1a_4^2 + 4a_2a_3a_4 - a_3^3 = 0. \quad (13)$$

The minima of $E(\eta,\chi,\kappa,\beta)$ as a function of β can be estimated by equating the derivative $\partial E/\partial\beta$ to zero $r_1\sin((2\theta - \frac{\alpha_2}{2}) + \pi) + 2r_2\sin(2(2\theta - \frac{\alpha_2}{2})) = 0$ and we obtain double minima at values

$$\begin{aligned} \beta_\pm &= \tan\left(\frac{\alpha_2}{4} \pm \arccos\left(\frac{r_1}{4r_2}\right)\right) = \tan\left(\frac{\arctan(\frac{a_1-a_3}{a_4-a_2})}{4}\right. \\ &\quad \left. \pm \arccos\left(\frac{\sqrt{4a_4^2 + (a_1+a_3)^2}}{2\sqrt{(a_4-a_2)^2 + (a_1-a_3)^2}}\right)\right). \quad (14) \end{aligned}$$

The solution $\sin(2\theta - \frac{\alpha_2}{2}) = 0$ corresponds to a maximum of $E(\eta,\chi,\kappa,\beta)$, not a minimum. The critical point is determined by $\frac{r_1}{4r_2} = 1$, that is

$$\begin{aligned} &3a_1^2 - 10a_1a_3 + 3a_3^2 - 8a_2a_4 + 4a_2^2 = 0, \\ &\beta_\pm = \tan\left(\frac{\alpha_2}{4}\right) = \tan\left(\frac{\arctan\left(\frac{a_1-a_3}{a_4-a_2}\right)}{4}\right). \end{aligned} \quad (15)$$

When $\kappa = 0$ $(a_1 = 0)$, the shape-phase transition curve $a_3^3 = 4a_2a_3a_4$ [see Eq. (13)] for even-even nuclei is shown in Fig. 1, where the well-known Casten triangle exhibits three phases—spherical, prolate, and oblate deformed—each separated by first-order phase transition. At the triple point where the phases coexist, a second-order phase transition occurs with a well-known critical value $\eta_c = 4/5 (a_2 = 0)$ [5,7,9]. When $\kappa \neq 0$, The exact solution of the cubic eqnarray (13) of η can be obtained for a tentative $\langle jm20 \mid jm\rangle\kappa = -10^{-5}$exhibited in Fig. 2. The section AB in Fig. 2 differs the oblate from the prolate shapes in the (η,χ) plane; the shape-phase transition line BC distinguishes between the oblate and the near-spherical shapes and the equilibrium shape values as a function of the control parameter can be seen in Fig. 3; the prolate and the near-spherical shapes are separated

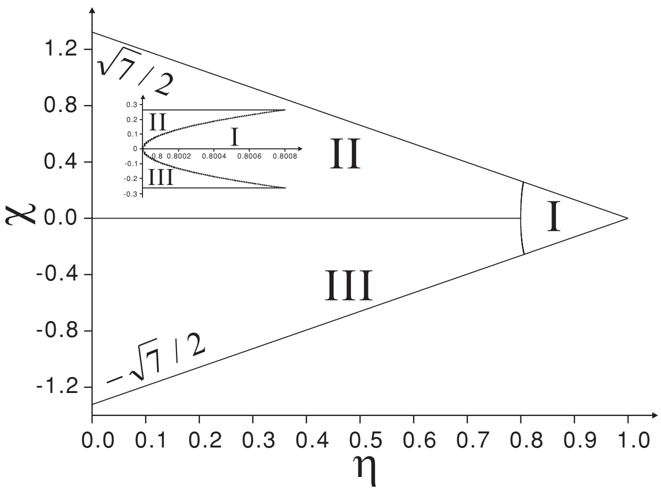

FIG. 1. Phase diagram of even-even nuclei within the framework of the interacting boson model in the large-N limit. I, II, and III stand for spherical, oblate and prolate shapes, respectively.

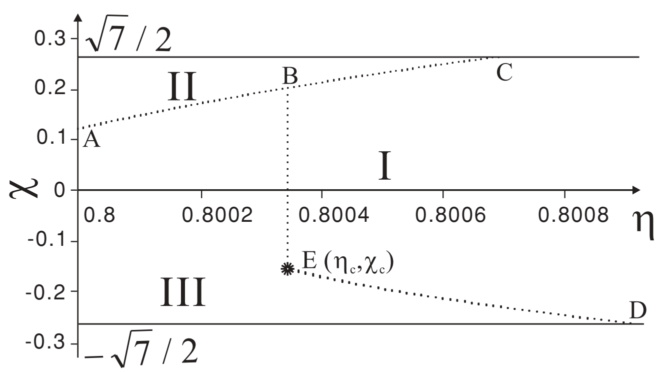

FIG. 2. Phase diagram of odd-A nuclei within the framework of the interacting boson-fermion model in the large-N limit. I, II, and III stand for near-spherical, oblate and prolate shapes, respectively.

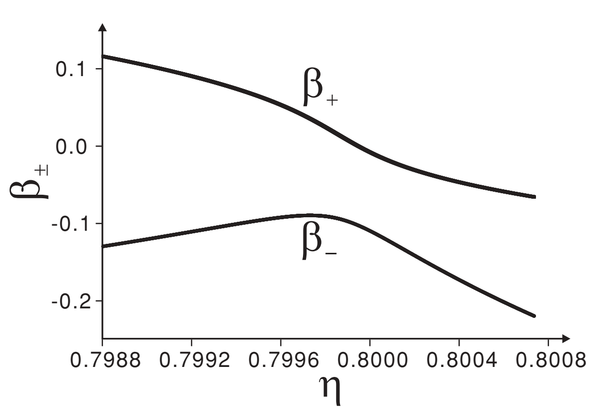

FIG. 3. Values of the respective near-spherical and oblate location $\beta_\pm$ of the double minima of the IBFM energy function against the control parameter η as $\langle jm20 \mid jm\rangle\kappa = -10^{-5}$.

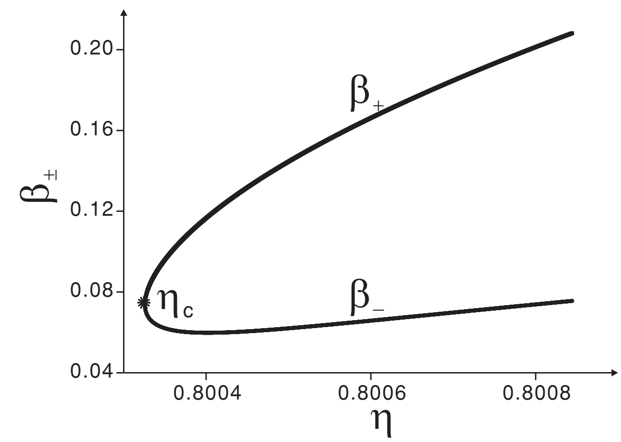

FIG. 4. Values of the respective prolate and near-spherical location $\beta_\pm$ of the double minima of the IBFM energy function against the control parameter η as $\langle jm20 \mid jm\rangle\kappa = -10^{-5}$. The β_+ equals the β_- at the critical point η_c.

by the phase-transition curve ED shown in Fig. 4. The phase equilibrium line ED in the (η, χ) plane terminates at a critical point $E(\eta_c, \chi_c)$. Below η_c, near-spherical shape does not exist. If $\chi_c \leqslant x \leqslant 0$ there is no (η, χ) which satisfies $\frac{r_1}{4r_2} \leqslant 1$ [see Eq. (14)]. Thus no shape-phase transition curve exists in this region. It is obvious that the η_c will be equal to 4/5 if the interaction between the odd fermion and the core vanishes.

In Ref. [20], the interaction strength κ is fixed as 0.032 ± 0.002 MeV to reproduce the data for a wide range of nuclei. For a quantitative investigation of the dependence of the critical point on the interaction strength κ, we resort to solve the nonlinear sets of eqnarrays (13) and (15). The result is shown in Fig. 5. It is obvious that the critical point lies in the Casten

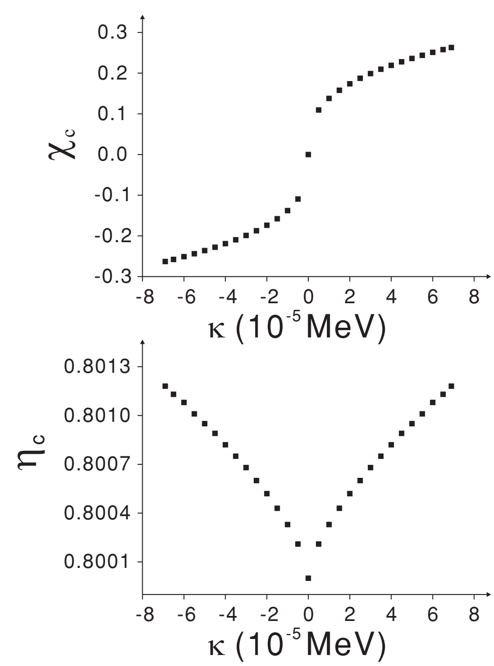

FIG. 5. Dependence of the critical point η_c and χ_c on the interaction strength κ.

triangle when the the interaction strength κ is small, while the critical point is located outside the Casten triangle for the fixed κ value.

IV. CONCLUSIONS

The Landau theory of continuous phase transition is proved to be a useful tool in the study of shape-phase transitions in even-even nuclei. By referring to the shape-phase transitions in even-even nuclei, we employ shape phase equilibrium condition in the framework of IBFM to discuss nuclear shape-phase diagram in odd-A nuclei. Exact nuclear shape-phase diagrams in the two-parameter (η, χ) plane are explicitly described. Three phases—near spherical, prolate, and oblate phases—each separated by first-order phase transitions are found in the boson-fermion mixing system. As expected a first-order phase transition line for odd-A nuclei ends at a critical point. This critical value is equal to the previously known one in the even-even nuclei if the interaction between the odd nucleon and the core vanishes.

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