Approach to Vibrational to Axially Rotational Shape Phase Transition Along the Yrast Line

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Abstract

With the energy surface of the nucleus in U(5) symmetry being analyzed in the framework of thermodynamics, the vibration and rotation phase diagram in terms of the angular momentum and deformation parameter is given. Together with examining the energy spectrum, we propose a theoretical approach to describe the vibrational to axially rotational phase transition along the yrast line. By analyzing the available experimental data we show that the vibrational to rotational shape phase transition along the yrast line takes place in many nuclei.

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It has been well known that shape phase transition is one of the most significant topics in nuclear structure research. Many evidences of nuclear shape phase transition have been observed. For instance, in several isotopes, there exists shape phase transition from vibration to axial rotation or $\gamma$-unstable rotation with respect to the variation of neutron number$^{[1]}$, and a triple point may appear$^{[2, 3]}$. Even in one mode of collective motion there may involve different characteristics, for example, along the yrast line there exists transition between rotations holding different relations between angular momentum and rotational frequency (referred to as band crossing and exhibiting a backbending)$^{[4]}$. Very recently it was found that there involves evolution from vibration to rotation along the yrast line of a nucleus$^{[5]}$. On the theoretical side, the interacting boson model (IBM) has been shown to be successful in describing the shape phase transition along a series of isotopes$^{[1, 6]}$. And analytic solutions for the critical points of the phase transitions have been found$^{[7, 8, 9]}$. The cranked shell model (CSM)$^{[10]}$ has been known to be able to describe the band crossing very well. However, a theoretical approach to describe the shape phase transition from vibration to rotation along the yrast line in a nucleus has not yet been established. Especially the phase diagram in terms of the angular momentum and the deformation parameter has not yet been obtained. Even so, the energy level statistics analysis has shown that the states in the U(5) symmetry with $A < 0$ involve the coexistence of vibrational and axially rotational shapes$^{[11]}$. By analyzing the energy surface and the energy spectrum of the U(5) symmetry, we will show that the U(5) symmetry with a special choice of parameters can be an approach to describe the shape phase transition along the yrast line and such kind phase transition takes place in many nuclei.

In the original version of the IBM (IBM1), the collective states of nuclei are described by the coherent states of $s$- and $d$-bosons. The corresponding dynamical group is U(6), and involves three dynamical symmetry limits U(5), O(6) and SU(3). Taking into account one- and two-body interactions among the bosons, one has the Hamiltonian of the nucleus in U(5) symmetry as$^{[11]}
\begin{equation}
H_{U(5)} = E_0 + \varepsilon_d C_{1U(5)} + AC_{2U(5)} + BC_{2O(5)} + CC_{2O(3)} ,
\end{equation}
where $C_{kG}$ is the $k$-rank Casimir operator of the group $G$ and the parameters hold relation $C \ll |B| \ll |A| \ll \epsilon_d$. Making use of the coherent state formalism\cite{12, 13, 14} of the IBM, one can express the energy functional for the U(5) Hamiltonian as

\[
E(N, \epsilon, A; \beta) = E_0 + \epsilon N \frac{\beta^2}{1 + \beta^2} + AN(N-1) \frac{\beta^4}{(1 + \beta^2)^2},
\]

(2)

where $\beta$ is a monotonous function of the usual deformation parameter (for example, for the rare earth nuclei, the usual quadrupole deformation parameter $\beta_2$ and the $\beta$ hold relation $\beta_2 \approx 0.16 \beta_1$) and the $\epsilon$ can be expressed in terms of the parameters in Eq. (1) as $\epsilon = \epsilon_d + 5A + 4B + 6C$. If $\beta^2$ is small (less than one), Eq. (2) can be rewritten as

\[
E(N, \epsilon, A; \beta) = E_0 + \epsilon N \beta^2 + [AN(N-1) - \epsilon N] \beta^4 + [\epsilon N - 2AN(N-1)] \beta^6 + \cdots \cdots.
\]

(3)

On the basis that the “deformation parameter” $\beta$ is a quantity to characterize the shape of a nucleus, one can take the $\beta$ as the order parameter to identify the nuclear shape phase transition.

In the general framework of Landau’s phase transition theory\cite{15}, it has been pointed out that, if the Landau free energy $F(T, \xi)$ can be expressed as

\[
F(T, \xi) = F_0 + \frac{1}{2} \alpha(T - T_0) \xi^2 + \frac{1}{4} g_4 \xi^4 + \frac{1}{6} g_6 \xi^6 + \cdots \cdots
\]

(4)

where $T$ is the control quantity, $\xi$ is the order parameter, $\alpha$ is a constant. It has been known that, if the other coefficients which depend also on the control quantity $T$ hold relation $g_4 < 0$, $g_6 > 0$, the system may involve a first order phase transition\cite{16}.

For a nucleus involving vibration to rotation phase transition along the yrast line, the control quantity is the angular momentum $L$. Comparing Eq. (3) with Eq. (4), we propose that the Eq. (3) can be rewritten as

\[
E(N, \epsilon, A; \beta) = E_0 + \frac{1}{2} \alpha(L - L_0) \beta^2 - \frac{1}{2} \alpha(L - L_0) - AN(N-1)) \beta^4
\]

\[
+ [\frac{1}{2} \alpha(L - L_0) - 2AN(N-1)] \beta^6 + \cdots \cdots
\]

(5)

where $AN(N-1)$ relies also on the control quantity $L$. It is evident that, if $\alpha < 0$ (i.e., $\alpha(L - L_0) > 0$ for $L < L_0$) and $A < 0$, Eq. (5) stands for the free energy of a
nucleus just the same as Eq. (4) with $g_4 < 0$, $g_6 > 0$. Even if $A > 0$, we may have 
\[ \frac{1}{2} \alpha (L - L_0) - 2AN(N - 1) > 0, \]
Eq. (5) corresponds also to Eq. (4) with $g_4 < 0$ and $g_6 > 0$. Analyzing the free energy in Eq. (5) more cautiously, one can recognize that there 
exists an angular momentum $L_0$ with which the $\frac{\partial^2 E(N,\varepsilon,A;\beta)}{\partial \beta^2} = 0$. And $\alpha (L - L_0) > 0$, $\frac{\partial^2 E(N,\varepsilon,A;\beta)}{\partial \beta^2} > 0$, if $L < L_0$; $\alpha (L - L_0) < 0$, $\frac{\partial^2 E(N,\varepsilon,A;\beta)}{\partial \beta^2} < 0$, if $L > L_0$. Meanwhile, there 
exists an angular momentum $L_c = L_0 - (\sqrt{3} - 2) \frac{AN(N - 1)}{\alpha}$ (if $A < 0$) with which the 
free energy involves one maximum and two equal minima, one of which is generated at 
$\beta = 0$, another corresponds to $\beta \neq 0$. There exists also a maximal angular momentum 
$L_{max} = L_0 + (\sqrt{6} + 2) \frac{AN(N - 1)}{\alpha}$ (if $A < 0$). If $L \geq L_{max}$, the energy surface has only 
one maximum at $\beta = 0$ but no minimum. The $\beta$ dependence of the free energy at 
some typical angular momenta is illustrated in Fig. 1. The figure shows apparently that, 
as the angular momentum $L < L_c$ the nucleus has a stable vibrational phase (the free 
energy takes the smaller minimum at $\beta = 0$). If the angular momentum $L_c \leq L < L_0$, 
the nucleus has a stable rotational phase (the free energy takes the smaller minimum at 
$\beta \neq 0$). Meanwhile there may involve coexistence of rotation and vibration, since the 
energy surface holds two minima at $\beta = 0$, $\beta \neq 0$, respectively. If the angular momentum 
$L_0 < L < L_{max}$, the nucleus has only a rotational phase. The angular momentum $L_c$ 
is definitely the critical angular momentum for the phase transition from vibration to 
rotation to happen. In addition, if $L \geq L_{max}$, the nucleus will collapse. We obtain then 
explicitly how the stable phase of a nucleus is determined by the angular momentum and 
the “deformation parameter”. The phase diagram in terms of the angular momentum 
$L$ and the “deformation parameter” $\beta$ can thus be displayed in Fig. 2. We reach thus 
a conclusion that the U(5) symmetry with $A < 0$ can describe well the vibrational to 
rotational nuclear shape phase transition along the yrast line. And the transition is a 
first order phase transition. Even if $A > 0$, the first order phase transition may also 
happen in the system if the interaction strengths satisfy the constraint mentioned above. 
It manifests that, the vibrational to rotational phase transition along the yrast line can 
take place in the nucleus holding the U(5) symmetry in IBM1.

On the phenomenological side, the energy spectrum of a nucleus in U(5) symmetry
can be given as
\[ E_{U(5)} = E_0 + \varepsilon_d n_d + A n_d(n_d + 4) + B \tau(n + 3) + C L(L + 1). \]  
(6)

where \( n_d, \tau, \) and \( L \) are the irreducible representations (IRREPs) of the group U(5), O(5) and O(3), respectively.

From the spectrum generating process one can recognize that, if \( A > 0 \) and \( B > 0 \), the states with \( \tau = n_d, L = 2n_d \) form the ground state band and the yrast band, and appear as the anharmonic vibrational ones with increasing frequency \( \hbar \omega = \varepsilon_d + (n_d + 4)A \).

If \( A < 0 \), the \( E_{gsb}(n_d) \) \( (E_{gsb}(L)) \) is an upper-convex parabola against the \( n_d \) \( (L) \), and can describe the collective backbending of high spin states[17]. In the case with \( A < 0, B < 0 \), the freedom of \( \tau \) in Eq. (6) can be washed out. It turns out then the state with \( \tau = n_d \) may still be the yrast one and there exists a d-boson number \( n_d^{(c)} \) and an angular momentum

\[ L_c = 2n_d^{(c)} = -\frac{2(\varepsilon_d + 4A + 3B)}{A + B} - 2N_0, \]  
(7)

where \( N_0 = N \) with \( N \) being the total boson number. As the angular momentum \( L \geq L_c \), the yrast states are no longer the anharmonic vibrational ones mentioned above, but the quasi-rotational ones with \( \tau = n_d = N_0 \). It indicates that the U(5) symmetry with parameters \( A < 0 \) and \( B < 0 \) may describe the vibrational to rotational phase transition along the yrast line. The \( L_c \) given in Eq. (7) is the critical angular momentum. For each yrast state with angular momentum \( L \leq L_c \), its energy can be given as

\[ E(L \leq L_c) = E_0 + \frac{A + B + 4C}{4} L^2 + \frac{\varepsilon_d + 4A + 3B + 2C}{2} L. \]  
(8)

and can be illustrated as a part of an upper-convex parabola. Whereas for the one with angular momentum \( L > L_c \), its energy should be expressed as

\[ E(L > L_c) = E'_0 + CL(L + 1), \]  
(9)

and can be displayed as a part of an upper-concave parabola. For instance, for a system with \( N = 15 \) and parameters \( \varepsilon_d = 0.80 \) MeV, \( A = -0.025 \) MeV, \( B = -0.01 \) MeV and \( C = 0.004 \) MeV, with Eq. (7) we can fix the critical angular momentum \( L_c = 8\hbar \). The energy of the yrast states against the angular momentum \( L \) can be illustrated in the left
panel of Fig. 3. It has been known that the energy of E2 transition \( \gamma \)-ray over spin (E-GOS) \( R = \frac{E_{\gamma}(L\rightarrow L-2)}{L} \) can be taken as a quite good signature to manifest the vibrational to axially rotational phase transition along the yrast line\(^5\). As an auxiliary evidence, we show also the E-GOS of the yrast states with these parameters in the right panel of Fig. 3. The figure indicates apparently that the yrast states involve a vibrational to axially rotational phase transition and the angular momentum \( L_c \) is definitely the critical point for the phase transition to take place. Such a transition is quite similar to that between the states with \( n_p = 0 \) and \( n_p = N \) in the vibron model\(^{10, 20} \) with random interactions.

In the case \( A < 0, B > 0 \) or \( A > 0, B < 0 \), there may exist a critical angular momentum \( L_c \) with \( \frac{L_c^2}{2} \leq N_0 < N \), too. For the states with \( L \leq L_c \), if \( \varepsilon_d + A(N_0 + 4) + B(N_0 + 3) > 0 \), their energies behave like an anharmonic vibrator’s. For the ones with \( L > L_c \), their energies behave as the quasi-rotational states with \( N_0 \) bosons. It is also possible that the \( N_0 \) takes several values less than the \( N \). Then the second and more higher backbending may emerge.

We have analyzed the available experimental data of the yrast states of the nuclei with \( 30 \leq Z \leq 100 \) and simulated the data with least-square fitting in our present approach. Both the experimental data\(^{21-24, 26-28, 29} \) and the best fitted energy spectra of the yrast states in some even-even nuclei are illustrated in Fig. 4 (the other data are available if required). It shows obviously that, besides the ones identified in the \( A \sim 110 \) mass region\(^5\), there exist vibrational to axially rotational phase transition along the yrast line in other nuclei. For example, \(^{72}\text{Se}, {^{90}}\text{Zr}, {^{92}}\text{Zr}, {^{98}}\text{Pd}, {^{108}}\text{Sn}, {^{116}}\text{Sn}, {^{136}}\text{Te}, {^{146}}\text{Gd}, {^{148}}\text{Gd}, {^{148}}\text{Dy}, {^{150}}\text{Dy}, {^{186}}\text{Hg}, {^{194}}\text{Pb}, {^{196}}\text{Pb}, {^{198}}\text{Pb}, {^{200}}\text{Po}, {^{202}}\text{Po}, {^{206}}\text{Po}, {^{214}}\text{Rn} \) and others are the ones whose anharmonic vibrational frequency in the corresponding phase decreases against the increasing of angular momentum. While \(^{66}\text{Zn}, {^{66}}\text{Ge}, {^{68}}\text{Se}, {^{82}}\text{Sr}, {^{84}}\text{Sr}, {^{86}}\text{Mo}, {^{114}}\text{Pd}, {^{116}}\text{Pd}, {^{116}}\text{Cd}, {^{118}}\text{Cd}, {^{120}}\text{Cd}, {^{112}}\text{Te}, {^{114}}\text{Te}, {^{116}}\text{Te}, {^{116}}\text{Xe}, {^{118}}\text{Xe}, {^{124}}\text{Xe}, {^{128}}\text{Xe}, {^{130}}\text{Xe}, {^{124}}\text{Ba}, {^{130}}\text{Ba}, {^{148}}\text{Sm}, {^{142}}\text{Gd}, {^{144}}\text{Dy}, {^{156}}\text{Er}, {^{158}}\text{Yb}, {^{160}}\text{Yb}, {^{160}}\text{Hf}, {^{162}}\text{Hf}, {^{164}}\text{W}, {^{170}}\text{Os}, {^{188}}\text{Pt}, {^{192}}\text{Pt}, {^{194}}\text{Pt}, {^{184}}\text{Hg} \) and so on are the ones whose vibrational frequency increases against the increasing of angular momentum.
In summary, by analyzing the energy surface of the nucleus in U(5) symmetry in the framework of thermodynamics, we give a phase diagram of the vibration and the rotation in terms of the angular momentum and the deformation parameter in this letter. We have then proposed an approach to describe the vibrational to axially rotational phase transition along the yrast line. With the energy spectrum being examined, we show that our presently proposed approach can describe very well the vibrational to axially rotational phase transition along the yrast line. We have also analyzed the energy spectra of the even-even nuclei with $30 \leq Z \leq 100$. It shows that, besides the ones in $A \sim 110$ mass region identified by Regan and collaborators$^5$, there exist many other nuclei involving vibrational to axially rotational phase transition along the yrast line.

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Figure 1: The energy surface (Landau free energy) of a nucleus against the “deformation parameter” $\beta$ at some typical angular momentum $L$ (with the parameters in Eq. (5) being taken as $E_0 = 0$, $L_0 = 20$, $\alpha = -10.0000$, $AN(N-1) = -64.6667$, (in arbitrary unit)).
Figure 2: The vibration and rotation phase diagram of a nucleus in terms of the angular momentum $L$ and the “deformation parameter” $\beta$ (with the same parameters for Fig. 1).
Figure 3: An example of the energy against spin (left panel) and the E-GOS (right panel) along the yrast line (filled diamonds and triangles, respectively) in the approach of U(5) symmetry with $A < 0$ (with parameters $\varepsilon_d = 0.80$ MeV, $A = -0.025$ MeV, $B = -0.01$ MeV, $C = 0.004$ MeV. The solid and dashed lines are implemented to guide the eye.)
Figure 4: The experimental data of the energy against spin (filled squares) of some even-even nuclei and the simulated results in the present approach (solid, dashed curves for vibrational, rotational mode, respectively).