Analytic Description of Critical Point Nuclei in a Spherical-Axially Deformed Shape Phase Transition

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An approximate solution at the critical point of the spherical to axially deformed shape phase transition in nuclei is presented. The eigenvalues of the Hamiltonian are expressed in terms of zeros of Bessel functions of irrational order.

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Many physical systems (nuclei, molecules, atomic clusters, etc.) are characterized in their equilibrium configuration by a shape. These shapes are in many cases rigid. However, there are several situations in which the system is rather floppy and undergoes a phase transition between two different shapes. A challenging problem is how to describe properties of the system in the phase transition region and in particular at the phase transition point.

One way to achieve this description is within the framework of algebraic models [1,2]. In this approach, the different shapes (phases) correspond to dynamic symmetries of some algebraic structure $\mathcal{G}$ and the phase transition corresponds to the breaking of the dynamical symmetries. This approach has been used extensively in nuclei, and it is beginning to be used in molecules. In nuclei, where the algebraic structure is U(6) it has been found that there are three dynamical symmetries characterized by the first algebra in the chain originating from $\mathcal{G}$, that is, U(5), SU(3), SO(6), with spherical, axially deformed, and (so-called) γ-unstable shapes. It has been found [3] that the phase transition between spherical, U(5), and γ-unstable, SO(6), shapes is second order, while that between spherical, U(5), and axially deformed shapes, SU(3), is first order. No phase transition occurs between axially deformed and γ-unstable shapes. Properties of the system in the transition region and, in particular, at the critical point can be found by solving numerically the eigenvalue problem for the Hamiltonian, H. However, it is of interest to find explicit solutions in terms of quantum numbers which contain the essential features of the critical point. Such analytic solutions describe well-defined structural standards that can serve as benchmarks for experimental studies.

Recently, it has been suggested [4] that by replacing the potential at the critical point by a five-dimensional square well potential, one can find an analytic solution which describes (approximately) the situation at the critical point of the U(5) $-$ SO(6) shape phase transition in nuclei. The solution was obtained by analyzing the differential equation $H\Psi = E\Psi$. The eigenfunctions were $\Psi(\beta, \gamma, \theta_i) = c\beta^{-3/2} J_{\tau+3/2}(k_{s,\tau}\beta)\Phi_{\tau,\nu_\Delta,L,M}(\gamma, \theta_i)$. These functions are eigenfunctions of the invariant operators of the chain of algebras E(5) $\supset$ SO(5) $\supset$ SO(3) $\supset$ SO(2). The differential equation with a square well potential has therefore a dynamical symmetry in the same sense in which the five-dimensional harmonic oscillator has a dynamical symmetry U(5) $\supset$ SO(5) $\supset$ SO(3) $\supset$ SO(2). The symmetry of the square well differs from that of the harmonic oscillator in that a nonsemisimple Lie algebra, E(5), replaces the semisimple algebra U(5). Experimental examples of this "critical symmetry" have been found [5]. The symmetry associated with the Euclidean algebra, E(5), can be generalized to describe shape phase transitions of the type U(n) $-$ SO($n + 1$), $n \geq 2$, with dynamic symmetry E(n), and thus used for applications to other areas of physics where shape phase transitions occur. The fact that the eigenfunctions are representations of the Euclidean algebra in n dimensions gives also the possibility to cast the problem in group theoretical language and connect it with the underlying algebraic description, without resorting to the differential equation.

However, as mentioned above, in nuclei one has another type of shape phase transition, between U(5) and SU(3), that is, between spherical and axially deformed shapes. A numerical description of nuclei exhibiting such behavior in terms of the interacting boson model has been given in [6]. It is the purpose of this Letter to show that one can obtain an approximate analytic solution at the critical point by exploiting the special character of the potential at this point. Compared to E(5), the situation here is by far more complex. The differential Bohr equation with [7]

$$H = -\frac{\hbar^2}{2B}\left[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} + \frac{1}{\beta^2\sin3\gamma}\frac{\partial}{\partial\gamma}\sin3\gamma\frac{\partial}{\partial\gamma} - \frac{1}{4\beta^2}\sum_\kappa\frac{Q_\kappa^2}{\sin^2(\gamma - \frac{2}{3}\pi\kappa)}\right] + V(\beta,\gamma) \quad (1)$$

does not support any other exact solution of the type discussed in [4]. While the algebras of E(5) and SO(5) can be easily constructed from the variables in the Bohr Hamiltonian [E(5) is composed of the five dimensional momenta, π_μ, and five dimensional angular momenta, $L_{\mu\nu}$, and SO(5) by $L_{\mu\nu}$], other algebras, for example, that of SU(3), cannot. In order to find exact dynamic symmetries associated with the transition U(5) $-$ SU(3) one must resort to other differential equations, or to an algebraic construction [1]. Nonetheless, it turns out that there is an approximate solution of the Bohr Hamiltonian, which describes many of the properties of this phase transition. It is the purpose of this Letter to present this solution. A comparison with experiment will be presented separately [8].

Returning to Eq. (1), consider the case in which the potential has a minimum at $\gamma = 0°$ and seek solutions of the type $\Psi(\beta, \gamma, \theta_i) = \varphi_K^L(\beta, \gamma)\mathcal{D}_{M,K}^L(\theta_i)$, where $\mathcal{D}$ is a Wigner function of the Euler angles $\theta_i (i = 1, 2, 3)$. By noting that around $\gamma = 0°$ the last term in Eq. (1) can be written as

$$\sum_{\kappa=1,2,3} \frac{Q_\kappa^2}{\sin^2(\gamma - \frac{2\pi}{3}\kappa)} \simeq \frac{4}{3}(Q_1^2 + Q_2^2 + Q_3^2) + Q_3^2\left(\frac{1}{\sin^2\gamma} - \frac{4}{3}\right), \quad (2)$$

and introducing reduced energies and potentials $\varepsilon = \frac{2B}{\hbar^2}E$, $u = \frac{2B}{\hbar^2}V$, one can rewrite the equation as

$$\left\{-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} - \frac{1}{\beta^2\sin3\gamma}\frac{\partial}{\partial\gamma}\sin3\gamma\frac{\partial}{\partial\gamma} + \frac{1}{4\beta^2}\left[\frac{4}{3}L(L+1) + K^2\left(\frac{1}{\sin^2\gamma} - \frac{4}{3}\right)\right] + u(\beta,\gamma)\right\}\varphi_K^L(\beta,\gamma) = \varepsilon\varphi_K^L(\beta,\gamma). \quad (3)$$

Consider now the case in which $u(\beta, \gamma) = u(\beta) + v(\gamma)$. Then the equation can be approximately separated into

$$\left[-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} + \frac{1}{4\beta^2}\frac{4}{3}L(L+1) + u(\beta)\right]\xi_L(\beta) = \varepsilon_\beta\xi_L(\beta),$$
$$\left[-\frac{1}{\langle\beta^2\rangle\sin3\gamma}\frac{\partial}{\partial\gamma}\sin3\gamma\frac{\partial}{\partial\gamma} + \frac{1}{4\langle\beta^2\rangle}K^2\left(\frac{1}{\sin^2\gamma} - \frac{4}{3}\right) + v(\gamma)\right]\eta_K(\gamma) = \varepsilon_\gamma\eta_K(\gamma), \quad (4)$$

with $\varepsilon = \varepsilon_\beta + \varepsilon_\gamma$ and where $\langle\beta^2\rangle$ is the average of β^2 over $\xi(\beta)$. Suppose now that the potential is a square well in the variable β and harmonic oscillator in γ. This is an approximation to the "true" potential. It is possible to express the potential as a function of β and γ, by using the method of intrinsic states [3,9,10] as applied to the interacting boson model. One obtains the following potential for the U(5) − SU(3) transition

$$V(\beta,\gamma) = \frac{N\beta^2}{1+\beta^2}\left[1 + \frac{5}{4}\zeta\right] - \frac{N(N-1)}{(1+\beta^2)^2} \times \zeta\left[4\beta^2 + 2\sqrt{2}\beta^3\cos3\gamma + \frac{1}{2}\beta^4\right]. \quad (5)$$

Here N is the number of bosons and $0 \leq \zeta \leq 1$ the control parameter. As ζ varies from 0 to 1 one spans the transition region. The potential at the critical point of the phase transition is shown in Fig. 1, for $N = 10$. The harmonic approximation in γ is obtained by expanding $\cos3\gamma$ and the square well potential is obtained by approximating the β dependence. If this assumption is made, then both equations for $\xi_L(\beta)$ and $\eta_K(\gamma)$ can be solved. For a square well potential, $u(\beta) = 0$ for $\beta \leq \beta_W$ and $u(\beta) = \infty$ for $\beta > \beta_W$, by setting $\tilde{\xi}(\beta) = \beta^{3/2}\xi(\beta)$, $\varepsilon_\beta = k_\beta^2$, $z = \beta k_\beta$, and

$$\nu = \left(\frac{L(L+1)}{3} + \frac{9}{4}\right)^{1/2}, \quad (6)$$

one obtains a Bessel equation

$$\tilde{\xi}'' + \frac{\tilde{\xi}'}{z} + \left[1 - \frac{\nu^2}{z^2}\right]\tilde{\xi} = 0; \qquad \tilde{\xi}(\beta_W) = 0. \quad (7)$$

The boundary condition determines the eigenvalues and eigenfunctions to be

$$\varepsilon_{\beta;s,L} = (k_{s,L})^2; \qquad \xi_{s,L}(\beta) = c_{s,L}\beta^{-3/2}J_\nu(k_{s,L}\beta); \qquad k_{s,L} = \frac{x_{s,L}}{\beta_W}, \quad (8)$$

where $x_{s,L}$ is the sth zero of $J_\nu(z)$. The normalization constants are obtained by imposing the condition $\int_0^\infty \beta^4\xi_{s,L}^2(\beta)\,d\beta = 1$.

The energy levels obtained from Eq. (8) are shown in Fig. 2 in units of $E_{1,2} - E_{1,0}$, where the notation is $E_{s,L}$. Note that the levels are assigned to different families labeled by the quantum number s. The different families are characterized by the energy ratio $R_s = \frac{E_{s,4}-E_{s,0}}{E_{s,2}-E_{s,0}}$. This ratio is 2.91, for $s = 1$, and decreases steadily for higher lying families ($s = 2, 3, \ldots$). The location of the various families is also fixed by symmetry. In particular, the location of the $s = 2$ family is given by the ratio $\frac{E_{2,0}-E_{1,0}}{E_{1,2}-E_{1,0}} = 5.67$.

When the expansion in powers of γ is made, the equation in the γ variable becomes the radial equation of a two

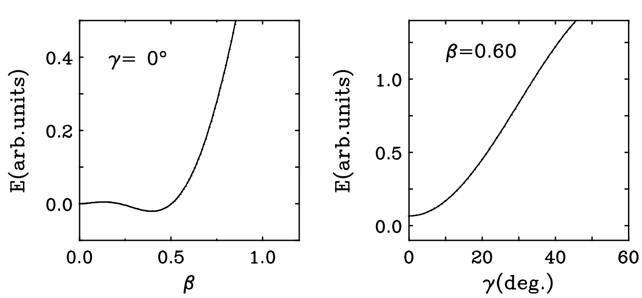

FIG. 1. Potential energy surfaces at the critical point of the U(5) − SU(3) shape phase transition obtained from the interacting boson model Hamiltonian by the method of coherent states. Left panel: $V(\beta, \gamma = 0^0)$. Right panel: $V(\beta = 0.6, \gamma)$.

dimensional oscillator

$$\left[-\frac{1}{\langle\beta^2\rangle}\frac{1}{\gamma}\frac{\partial}{\partial\gamma}\gamma\frac{\partial}{\partial\gamma} + \frac{(K/2)^2}{\langle\beta^2\rangle}\frac{1}{\gamma^2} + (3a)^2\frac{\gamma^2}{2}\right]\eta_K(\gamma) = \tilde{\varepsilon}_\gamma\eta_K(\gamma), \qquad \tilde{\varepsilon}_\gamma = \varepsilon_\gamma + \frac{(K/2)^2}{\langle\beta^2\rangle}\frac{4}{3}, \tag{9}$$

with solution

$$\tilde{\varepsilon}_\gamma = \frac{3a}{\sqrt{\langle\beta^2\rangle}}(n_\gamma + 1); \qquad n_\gamma = 0,1,2,\ldots,$$
$$n_\gamma = 0, \quad K = 0; \quad n_\gamma = 1; \quad K = \pm 2;$$
$$n_\gamma = 2; \quad K = 0, \pm 4; \ldots \tag{10}$$
$$\eta_{n_\gamma,K}(\gamma) = c_{n,K}\gamma^{|K/2|}e^{-(3a)\gamma^2/2}L_n^{|K|}(3a\gamma^2);$$
$$n = \left(\frac{n_\gamma - |K|}{2}\right),$$

where $L_n^{|K|}$ is a Laguerre polynomial. Combining all variables, β, γ, θ_i, one obtains the most general expression

$$E(s,L,n_\gamma,K,M) = E_0 + B(x_{s,L})^2 + An_\gamma + CK^2,$$
$$\Psi(\beta,\gamma,\theta_i) = c_{s,L}\beta^{-3/2}J_\nu(k_{s,L}\beta) \tag{11}$$
$$\times\ \eta_{n_\gamma,K}(\gamma)\mathcal{D}^L_{MK}(\theta_i),$$

where E_0, B, A, C are arbitrary parameters. The values of L in a sequence s, n_γ are determined by K. For $K = 0$, $L = 0,2,4,\ldots$, and for $K \neq 0$, $L = K, K+1, K+2, \ldots$ [7]. In Fig. 2 only sequences with $n_\gamma = 0$ are shown. Also the wave functions $\Psi(\beta,\gamma,\theta_i)$ must be properly symmetrized, $\Psi(\beta,\gamma,\theta_i) = (1/\sqrt{2})[\varphi_{L,K}(\beta,\gamma)\mathcal{D}^L_{MK}(\theta_i) + (-)^{I+K}\varphi_{L,-K}(\beta,\gamma)\mathcal{D}^L_{M,-K}(\theta_i)]$, to obtain the full solution.

Transition rates can be calculated by taking matrix elements of the quadrupole operator

$$T^{(E2)} = t\beta\left[\mathcal{D}^{(2)}_{\mu,0}\cos\gamma + \frac{1}{\sqrt{2}}(\mathcal{D}^{(2)}_{\mu,2} + \mathcal{D}^{(2)}_{\mu,-2})\sin\gamma\right], \tag{12}$$

where t is a scale factor. The evaluation of the matrix elements here is more complicated than in [4]. In the same approximation used for the Hamiltonian, $\gamma \simeq 0°$, only the $\mathcal{D}^{(2)}_{\mu,0}$ term survives. The integral over the Euler angles θ_i can be done using the properties of the Wigner $\mathcal{D}$ functions. One is left with the β part $\int \beta\xi_{s,L}(\beta)\xi_{s',L'}(\beta) \times \beta^4\,d\beta = \int_0^1 c_{s,L}c_{s',L'}J_\nu(k_{sL}\beta)J_{\nu'}(k_{s'L'}\beta)\beta^2\,d\beta = I_{s,L;s',L'}$. Evaluation of these integrals gives the results of Fig. 2 for BE(2) values in units of $B(E2; 2_1 \rightarrow 0_1) = 100$.

The solution described here can be used to study phase transitions between spherical and axially deformed shapes [8]. It is interesting to compare the properties of this solution with those of the E(5) symmetry that describes the U(5) − SO(6) transition. In Table I, some key properties are confronted. In particular, the order ν of the Bessel functions whose zeros provide the energy eigenvalues is different. For E(5) it is a half-integer number related to the quantum number τ of the common SO(5) subalgebra of U(5) and SO(6). For the solution described here, denoted by X(5) in the table, it is an *irrational* number related to the common SO(3) subalgebra of U(5) and SU(3). This order is crucial for applications, since it determines all properties (energy eigenvalues, transition rates, ...) of the system and is the arresting feature of the analysis presented in this Letter.

An important question is whether or not the solution presented here is a dynamical symmetry. The wave functions are written in Eq. (11). The Wigner $\mathcal{D}$ functions, solutions of the quantum mechanical problem of a symmetric top, can be written in terms of the totally symmetric representations of SO(4) ~ SO(3) ⊗ SO(3), and the two-dimensional Laguerre polynomials are related to representations of the two dimensional harmonic oscillator, SU(2). However, the Bessel functions with *irrational* order cannot be written in terms of (tensor or spinor) representations of E(n), obtained by contraction of those of SO($n+1$). The eigenfunctions of the invariant operators of E(n) are Bessel functions with integer (for $n = even$) or half-integer (for $n = odd$) order ν [11]. Thus the situation described here is not a dynamical symmetry in the usual sense.

However, there exists another class of representations of Lie groups, called *projective* representations. These are proper representations of the algebra, but multivalued representations of the group. These representations have been only marginally investigated, except for SO(3) ~ SU(2) and its complex extensions SO(2,1) ~ SU(1,1) [12]. The eigenfunctions of the invariant operators of these groups are Legendre polynomials $P^m_\ell(\theta)$. In the projective

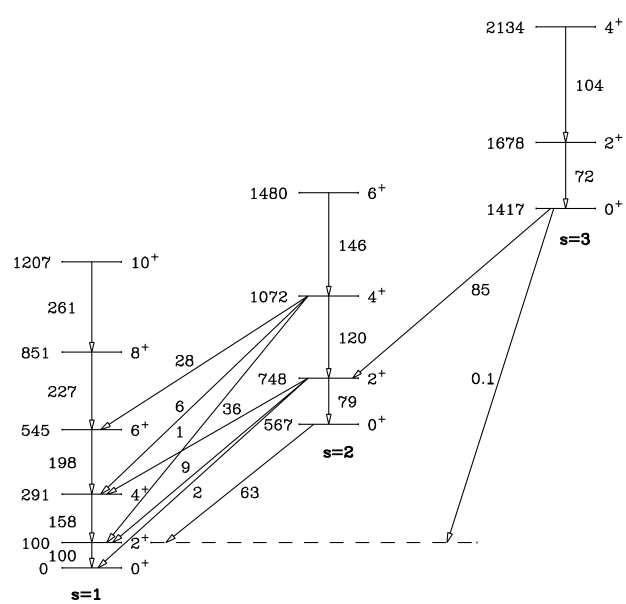

FIG. 2. Schematic representation of the lowest portion of the spectrum of X(5) symmetry. Only states with $n_\gamma = 0$ are shown. Energies are in units of the energy of the first excited state, $E_{2_1} - E_{0_1} = 100$. B(E2) values are in units of $B(E2; 2_{1_1} \rightarrow 0_{1_1}) = 100$.

TABLE I. Some properties of critical symmetries and usual dynamic symmetries. (a) Vibrational energies in these symmetries depend on additional parameters in the Hamiltonian.

Property	E(5)	X(5)	U(5)	O(6)	SU(3)
"Critical" order ν	$\tau + \frac{3}{2}$	$(\frac{L(L+1)}{3} + \frac{9}{4})^{1/2}$			
"Rotational" excitations $R = \frac{E_{4_1} - E_{0_1}}{E_{2_1} - E_{0_1}}$	2.20	2.91	2.00	2.50	3.33
"Vibrational" excitations $R' = \frac{E_{0_2} - E_{0_1}}{E_{2_1} - E_{0_1}}$	3.03	5.67	a	a	a

representations, m is not necessarily an integer. In the case discussed here, the Bessel functions with irrational order can be associated with projective representations of E(n), and consequently the solution presented here is a dynamic symmetry, albeit of unusual nature. When these representations are included, the corresponding algebra is often denoted by placing a tilde over it, $\tilde{\mathrm{E}}(5)$. The notation X(5) (which is not intended as a group label) has been used in Table I in order to distinguish it from the E(5) symmetry discussed in [4]. A full discussion of these group theoretical aspects will be given elsewhere.

Finally, the solution presented here is only an approximate solution in which the β and γ degrees of freedom are decoupled and only the β term is retained in the transition operator. To obtain a solution that includes $\beta - \gamma$ couplings and β^2 terms in the transition operator, one must resort to a more general equation than the Bohr equation (see p. 123 of [1]) or return to the algebraic description. Again, a full account will be presented in a longer publication.

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