Phase Transitions in Angle Variables

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Phase transitions in angle variables are studied. An example of angular phase transition, an axially to triaxially deformed "shape" transition in nuclei, is discussed. Spectroscopic signatures for the occurrence of these transitions are suggested. Preliminary experimental evidence is presented.

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The purpose of this Letter is twofold: (i) to introduce quantum phase transitions for systems in which the order parameter is an angle and present the corresponding results; (ii) to suggest a system where these phase transitions can occur and indicate how they can be detected (signatures) by analyzing the solutions at the critical point. Preliminary experimental evidence for their occurrence is presented.

The simplest way to study quantum phase transitions is to expand the "effective potential" as a function of the coordinate (Landau approach). In the case in which the coordinate is an angle α, a convenient expansion is in terms of trigonometric functions. I begin therefore by considering the potential

$$V(\alpha) = -\cos\alpha + \xi\cos^2\alpha, \qquad 0 \leq \alpha \leq \pi. \tag{1}$$

This potential appears in the problem to be discussed below and is the angle equivalent of the Landau potential (up to quartic terms). As a function of the control parameter ξ, the system described by the potential (1) undergoes a quantum phase transition at $\xi = \xi_c = \frac{1}{2}$. For $\xi < \frac{1}{2}$, the potential has a minimum at $\alpha_e = 0$, while for $\xi > \frac{1}{2}$ the potential has a minimum at $\alpha_e = \arccos(\frac{1}{2\xi})$. The values at the minimum and its derivatives are

$$V_{\min} = \begin{Bmatrix} -1 + \xi \\ -\frac{1}{4\xi} \end{Bmatrix}, \qquad \begin{matrix} \xi < \frac{1}{2} \\ \xi > \frac{1}{2}, \end{matrix}$$

$$\frac{\partial V_{\min}}{\partial \xi} = \begin{Bmatrix} 1 \\ \frac{1}{4\xi^2} \end{Bmatrix}, \qquad \frac{\partial^2 V_{\min}}{\partial \xi^2} = \begin{Bmatrix} 0 \\ -\frac{1}{8\xi^3} \end{Bmatrix}, \qquad \begin{matrix} \xi < \frac{1}{2} \\ \xi > \frac{1}{2}. \end{matrix} \tag{2}$$

Since the function and its first derivative are continuous at $\xi = \xi_c$ while the second derivative is not, the transition is *second* order. The critical exponent μ is $\frac{1}{2}$, as one can see by expanding α_e around the critical point $\xi_c = \frac{1}{2}$ using

$$\arccos(1 - z) = (2z)^{1/2}\left[1 + \sum_{k=1}^{\infty} \frac{1 \times 3 \times 5 \times \cdots \times (2k-1)}{2^{2k}(2k+1)k!} z^k\right]. \tag{3}$$

An example of "angular" quantum phase transition is provided by shape phase transitions in atomic nuclei. Ellipsoidal shapes of nuclei are described in terms of two intrinsic Bohr variables β, γ. If $\beta = 0$, one has a sphere. If $\beta \neq 0$ and $\gamma = 0°$, one has an ellipsoid with axial symmetry while, if $\beta \neq 0$ and $\gamma \neq 0°$, the ellipsoid has an axially asymmetric shape. Potentials for this situation can be obtained from the interacting boson model by making use of the method of coherent states [1]. With only two-body boson interactions, the potential is of the type

$$V(\beta, \gamma) = f(\beta) - g(\beta)\cos 3\gamma; \qquad \beta \geq 0; \\ 60° \geq \gamma \geq 0°, \tag{4}$$

where $f(\beta)$ and $g(\beta)$ are functions of β given in [1] and $g(\beta) \geq 0$ for $\beta \geq 0$. This potential has a minimum at $\gamma_e = 0°$. Most known nuclei are in this situation. However, if three-body terms are added, the potential takes the form [2]

$$V(\beta, \gamma) = f(\beta) - g(\beta)\cos 3\gamma + h(\beta)\cos^2 3\gamma, \tag{5}$$

with $h(\beta) \geq 0$ for $\beta \geq 0$. This is precisely the situation described above, with $\alpha = 3\gamma$. Thus, one may have the possibility of rigid triaxial shapes ($\gamma_e \neq 0°$) and phase transitions from rigid axial to rigid triaxial. If this phase transition occurs, one must find signatures for it. It has been suggested recently that spectroscopic signatures for phase transitions can be found by analyzing the situation at the critical point [3]. At this point $\xi = \frac{1}{2}$, the potential is flat, as shown in Fig. 1. The spectrum at the critical point of the axial to triaxial shape phase transition in nuclei can be studied by considering the Bohr equation with [4]

$$H = -\frac{\hbar^2}{2B}\left[\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} + \frac{1}{\beta^2\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma} - \frac{1}{4\beta^2}\sum_{\kappa}\frac{Q_\kappa^2}{\sin^2(\gamma - \frac{2}{3}\pi\kappa)}\right] + V(\beta, \gamma). \tag{6}$$

If the potential is separable, $u(\beta, \gamma) = (\frac{2B}{\hbar^2})V(\beta, \gamma) = u(\beta) + v(\gamma)$, the equation can be approximately separated

$$\left[-\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta}+\frac{1}{4\beta^4}\frac{4}{3}L(L+1)+u(\beta)\right]\xi_L(\beta)=\varepsilon_\beta\xi_L(\beta),$$
$$\left[-\frac{1}{\langle\beta^2\rangle\sin 3\gamma}\frac{\partial}{\partial\gamma}\sin 3\gamma\frac{\partial}{\partial\gamma}+\frac{1}{4\langle\beta^2\rangle}K^2\left(\frac{1}{\sin^2\gamma}-\frac{4}{3}\right)+v(\gamma)\right]\eta_K(\gamma)=\varepsilon_\gamma\eta_K(\gamma), \quad (7)$$

where $\langle\beta^2\rangle$ is the average of β^2 over $\xi(\beta)$ [5]. Consider now the situation in which the potential is a harmonic oscillator in the variable β, $u(\beta)=\frac{1}{2}u_0(\beta-\beta_0)^2$ and a square well in the variable γ, $v(\gamma)=0$ for $\gamma<\gamma_W$ and $v(\gamma)=\infty$ for $\gamma\geq\gamma_W$. This potential is a special case of the generic potential of Eq. (5), when $f(\beta)=u(\beta)$, the functions $g(\beta)$ and $h(\beta)$ are approximated by $g(\beta_0)$ and $h(\beta_0)$ (valid if u_0 is sufficiently large, corresponding to rigid deformations with equilibrium value β_0) and the combination $-g(\beta_0)cos3\gamma+h(\beta_0)cos^2 3\gamma$ is approximated by a square well in γ [valid at the critical point, $\xi=h(\beta_0)/g(\beta_0)=1/2$, where the potential is very flat, Fig. 1]. It describes (approximately) the situation at the critical point of the rigid axial to rigid triaxial shape phase transition in nuclei.

In understanding the spectrum at this point, one is interested in solving the equation in the variable γ. (The equation in the variable β was solved by Bohr.) If $\gamma_W\ll 60°$, one can make the further simplification $\sin\gamma\sim\gamma$ and reduce the equation to that of a particle in a two-dimensional square well,

$$\left[-\frac{1}{\gamma}\frac{\partial}{\partial\gamma}\gamma\frac{\partial}{\partial\gamma}+M'^2\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)\right]\eta(\gamma)=\bar{\varepsilon}_\gamma\eta(\gamma), \quad (8)$$

with $M'=(\frac{K}{2})=0,\pm1,\pm2,\ldots$ and with boundary condition $\eta(\gamma_W)=0$. The solutions of this equation are well known and given in terms of Bessel functions

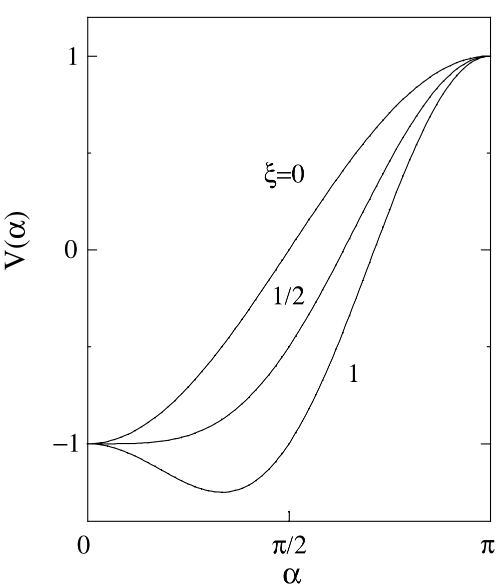

FIG. 1. The Landau potential $V(\alpha)$ for three values of the control parameter, $\xi=0<\xi_c$, $\xi=\xi_c=1/2$, and $\xi=1>\xi_c$.

$$\eta_{s',M'}(\gamma)=c_{s',M'}J_{M'}(k_{s',M'}\gamma),$$
$$\bar{\varepsilon}_{\gamma,s',M'}=k^2_{s',M'}-\frac{4}{3}M'^2; \qquad k_{s',M'}=\frac{x_{s',M'}}{\gamma_W}, \quad (9)$$

where $x_{s',M'}$ is the s'th zero of $J_{M'}(z)$. Since the spectrum in this approximation is doubly degenerate, except for $M'=0$, M' here denotes $|\frac{K}{2}|$. For γ_W small, the correction due to the second term is negligible and will be omitted. The main properties of this spectrum are indicated in Table I. Here the ratio of the energies of the states to that of the fundamental vibration, $E_{s',M'}=\bar{\varepsilon}_{\gamma,s',M'}/\bar{\varepsilon}_{\gamma,1,1}$, is shown. One can see that the γ vibrations are anharmonic with *positive* anharmonicities (the harmonic limit is 2). The anharmonicities have specific values that do not depend on the parameters in the Hamiltonian.

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

$$T^{(E2)}=t\beta\left[\mathcal{D}^{(2)}_{\mu,0}\cos\gamma+\frac{1}{\sqrt{2}}(\mathcal{D}^{(2)}_{\mu,2}+\mathcal{D}^{(2)}_{\mu,-2})\sin\gamma\right]. \quad (10)$$

With the approximation $\sin\gamma\sim\gamma$, only the second term survives when computing transitions between states of Table I. In the evaluation, one needs the integrals $I_{s',M';s''M''}=\int_0^1\gamma^2 c_{s',M'}c_{s'',M''}J_{M'}(k_{s',M'}\gamma)J_{M''}(k_{s'',M''}\gamma)\,d\gamma$.

Evaluation of these integrals gives the results of Table I. Here the integrals are normalized to $I_{1,1;1,0}$. Again one can see deviations from the harmonic approximation, where the integral is $\sqrt{2}\cong 1.41$, and that the $\gamma\gamma,0\rightarrow\gamma$ transition is smaller than the $\gamma\gamma,4\rightarrow\gamma$ transition, due to the fact that the states $g,\gamma,(\gamma\gamma,4)$ are all in the same sequence ($s'=1$) of two-dimensional square-well states, while $(\gamma\gamma,0)$ is not ($s'=2$).

In order to obtain the full solution, one of course must add the β part. The full solution can be written as

TABLE I. Energies and intrinsic matrix elements of the Y(5) solution.

Spectroscopic notation	Bessel notation s',M'	$E_{s',M'}$
g	1,0	0
γ	1,1	1
$\gamma\gamma$,4	1,2	2.3139
$\gamma\gamma$,0	2,0	2.7742
	$s',M'\rightarrow s'',M''$	$I_{s',M';s'',M''}$
$\gamma\rightarrow g$	$1,1\rightarrow 1,0$	1
$\gamma\gamma,4\rightarrow\gamma$	$1,2\rightarrow 1,1$	1.2370
$\gamma\gamma,0\rightarrow\gamma$	$2,0\rightarrow 1,1$	−0.7291

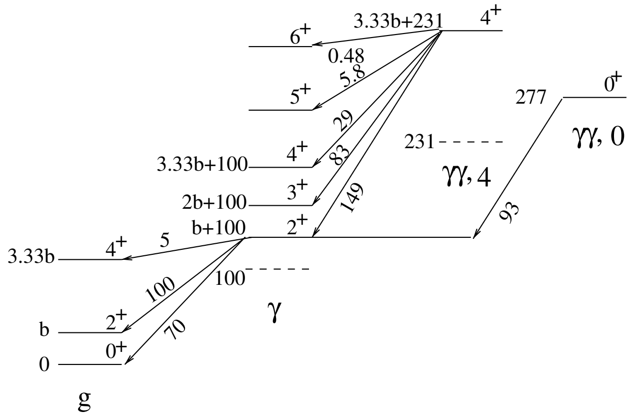

FIG. 2. Schematic representation of the spectrum of a nucleus at a critical point of the axially to triaxially deformed shape phase transition. The scale of energy is set to the energy of the intrinsic γ vibration, $A[x_{1,1}^2 - x_{1,0}^2] = 100$. The rotational energies are in units of $b = 6B$. The intrinsic states are shown by a dashed line. The scale of $B(E2)$ values is set by $B(E2; 2_\gamma^+ \rightarrow 2_g^+) = 100$.

$$\Psi(\beta, \gamma, \theta_i) = c_{s',M'} J_{M'}(k_{s',M'}\gamma)\xi_{n_\beta,L}(\beta)\mathcal{D}_{MK}^L(\theta_i),$$
$$E(n_\beta, L, s', K, M) = E_0 + B' n_\beta + BL(L+1) + A(x_{s',M'})^2, \quad (11)$$

with $M' = | K/2 |$. Here B', B, and A are parameters that are related to frequency of β vibrations, moments of inertia, and frequency of γ vibrations. [An additional contribution, CK^2 with $C > 0$ (prolate) or $C < 0$ (oblate) has been omitted from Eq. (11). As mentioned above, this contribution is small for $\gamma_W \ll 60°$.] This solution will be called, for simplicity of notation, Y(5). The portion of the spectrum with $n_\beta = 0$ is shown in Fig. 2.

Equipped with the full solution, one can also evaluate the $B(E2; L_i, K_i \rightarrow L_f, K_f)$ values between states. These are also shown in Fig. 2. In the approximation of Eq. (11), bands are rotational, all with the same moment of inertia, and ratios of $B(E2)$ values originating from the same state are given by the rotational (Alaga) rules. Noteworthy is instead the ratio of energies of $(\gamma\gamma, 4)$ and $(\gamma\gamma, 0)$ states to γ, $E_{\gamma\gamma,4}/E_\gamma$, and $E_{\gamma\gamma,0}/E_\gamma$ and the ratio of $B(E2; \gamma\gamma, 4 \rightarrow \gamma)$ and $B(E2; \gamma\gamma, 0 \rightarrow \gamma)$ to $B(E2; \gamma \rightarrow g)$.

It is interesting to compare properties of Y(5) with other situations, in particular, with the symmetry SU(3) of the interacting boson model. The comparison is shown in Table II. In SU(3), vibrations in the γ direction are nearly harmonic (they become exactly harmonic in the $N \rightarrow \infty$ limit). The anharmonicities are negative. In the table, a comparison is also made with the symmetry SU(3)* of the interacting boson model, corresponding to rigid triaxial deformations. In this symmetry, the γ and $\gamma\gamma, 4$ states become part of the ground band, since they belong to the SU(3)* representation $(2N_\pi, 2N_\nu)$ (zero energy mode) [1], while the $\gamma\gamma, 0$ belongs to another SU(3)* representation, lying at higher energy. The ratio $E_{\gamma\gamma,0}/E_\gamma \rightarrow \infty$.

TABLE II. Some properties of Y(5) compared with those of the usual dynamical symmetries.

Property	Y(5)	SU(3)	SU*(3)
E_γ	1	1	0
$E_{\gamma\gamma,4}/E_\gamma$	2.32	$\frac{4N-6}{2N-1} \sim 1.8$	0
$E_{\gamma\gamma,0}/E_\gamma$	2.77	$\frac{4N-5}{2N-1} \sim 1.8$	∞

In conclusion, instability towards *rigid* gamma deformations is revealed by properties of the gamma vibrations. It is characterized by vibrations with *positive* anharmonicities. The ratio of the energy of double vibration with $K = 4$ to the energy of single vibration $K = 2$ is expected to be, at the critical point, ~2.32. This signature may be used in identifying nuclei that are at the critical point of the axially deformed to triaxially deformed phase transition. The situation here is not as rich as that of nuclei at the critical point of spherical to γ-unstable shapes, E(5) [6], or spherical to axially deformed shapes, X(5) [7]. A preliminary scan of the periodic table appears to indicate that a small cluster of nuclei around mass 168 are in this situation [8]. This is summarized in Table III. It appears that ^{166}Er, ^{168}Er are the most likely candidates. Indeed, studies of ^{166}Er and ^{168}Er within the framework of the interacting boson model with three-body interactions indicate this to be the case [9]. It would be of utmost importance from the point of view presented here to (i) determine the ensemble of nuclei with positive $\gamma\gamma$ anharmonicities and (ii) attempt measurements of other signatures for instability towards rigid stable γ deformations.

It should be noted that the solution presented here is not the SU(3) to SO(6) transition of the interacting boson model with two-body interactions (axially deformed to γ-unstable transition), found to be a crossover point and not a phase transition [10,11]. In the classification in terms of symmetries of the interacting boson model [1], it is the transition from the symmetry SU(3) to SU(3)* induced either by higher order terms in the boson Hamiltonian or by the elimination of the proton-neutron degree of freedom. The phase diagram of the system is now a tetrahedron instead of a triangle (see p. 178 of [1]) (Fig. 3). The present Letter concludes the classification of shape phase transitions within the framework of the Bohr Hamiltonian.

TABLE III. Experimental values of $E_{\gamma\gamma,4}$ in some nuclei.

Nucleus	$E(2_\gamma^+)$ (keV)	$E(4_{\gamma\gamma}^+)$ (keV)	$E_{\gamma\gamma,4}/E_\gamma$ (Exp)
^{168}Er	821	2056	2.42
^{166}Er	786	2028	2.50
^{164}Dy	762	2173	2.80

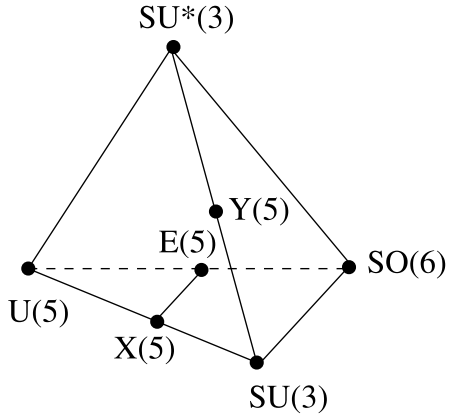

FIG. 3. Phase diagram including the γ degree of freedom. The ^{166}Er and ^{168}Er nuclei may lie on the edge of the tetrahedron towards the Y(5) point.

Phase transitions in angle variables, discussed here for applications to nuclei, are also important in other areas of physics and chemistry, for example, molecular physics, where the angle is that between bonds in the molecule. The potentials in the bending angle between a linear and a nonlinear configuration are written as in Eq. (1) [12]. Example of molecules at the critical point of this (second order) phase transition have been found (fulminic acid, HCNO) [13].

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[1] For a review, see F. Iachello and A. Arima, *The Interacting Boson Model* (Cambridge University Press, Cambridge, England, 1987).
[2] P. Van Isacker and J. Q. Chen, Phys. Rev. C **24**, 684 (1981).
[3] F. Iachello, Phys. Rev. Lett. **85**, 3580 (2000).
[4] A. Bohr, Mat. Fys. Medd. K. Dan. Vidensk. Selsk. **26**, 14 (1952).
[5] F. Iachello, Phys. Rev. Lett. **87**, 052502 (2001).
[6] R. F. Casten and N. V. Zamfir, Phys. Rev. Lett. **85**, 3584 (2000).
[7] R. F. Casten and N. V. Zamfir, Phys. Rev. Lett. **87**, 052503 (2001).
[8] X. Wu, A. Aprahamian, S. M. Fischer, W. Reviol, G. Liu, and J. X. Saladin, Phys. Rev. C **49**, 1837 (1994).
[9] J. E. Garcia-Ramos, C. E. Alonso, J. M. Arias, and P. Van Isacker, Phys. Rev. C **61**, 047305 (2000).
[10] A. E. L. Dieperink, O. Scholten, and F. Iachello, Phys. Rev. Lett. **44**, 1747 (1980).
[11] D. H. Feng, R. Gilmore, and S. R. Deans, Phys. Rev. C **23**, 1254 (1981).
[12] For a review, see F. Iachello and R. D. Levine, *Algebraic Theory of Molecules* (Oxford University Press, Oxford, England, 1995).
[13] F. Iachello, F. Perez-Bernal, and P. H. Vaccaro, Chem. Phys. Lett. **375**, 309 (2003).