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Phase transitions in configuration mixed models

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The phase diagram of models with configuration mixing is investigated in mean-field approximation. The configurations correspond to different limits of a dynamical algebra U(n), such as U($n-1$) and SO(n), and are allowed to mix. It is shown that this diagram has unusual properties not present in models with a single configuration. Applications to nuclear and molecular physics are discussed.

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Qualitative changes in the properties of physical systems are called phase transitions. The properties of a system are characterized by order parameters, the expectation values of some suitable chosen operators in the ground state, $\langle \hat{P} \rangle$. Phase transitions occur as some of the parameters, called control parameters, that constrain the system, are varied. Phase transitions in which the control parameter is the temperature T (so-called thermodynamic phase transitions) have been known for many years. In the late 1970's, Gilmore *et al.* [1] introduced phase transitions in which the control parameter, ξ, is a parameter appearing in the quantum Hamiltonian describing the system, $\hat{H} = (1-\xi)\hat{H}_1 + \xi \hat{H}_2$. They called these "ground-state-energy phase transitions," and pointed out the analogy with the thermodynamic phase transitions. In recent years, they have been renamed "quantum phase transitions" and have become very popular in connection with condensed-matter systems. Particularly well-suited systems for studying quantum phase transitions are those described by algebraic Hamiltonians with a dynamical group U(n), for instance in atomic nuclei with U(6) [2], and in molecules with U(4), U(3), and U(2) [3]. An important aspect of the study of phase transitions is the construction of the phase diagram. For algebraic models, this can be achieved with the theory of coherent states. An algorithm has been devised, wherein the order of the phase transition according to Ehrenfest's classification can be determined [4]. The expectation value of the Hamiltonian in the ground coherent state is called its classical limit [5,6].

Quantum phase transitions in algebraic models were studied early on [6–8] and have been the subject of many recent investigations [9–11], including the study of finite-particle-number effects [12]. We briefly recapitulate, for purposes of later comparison, the results for the phase transition U($n-1$)–SO(n), investigated in general in Ref. [8], and in particular the phase transition U(5)–SO(6) which occurs in the interacting boson model [6,7]. Consider the Hamiltonian describing a system of interacting s and d bosons undergoing a phase transition between so-called spherical and γ-unstable phases [2, p. 113],

$$\hat{H} = (1-\xi)\frac{\hat{n}_d}{N} + \xi \frac{\hat{P}_6}{N(N-1)}, \tag{1}$$

where N is the number of bosons (a constant), $\hat{n}_d$ the number operator for d bosons, $\hat{P}_6$ the pairing operator associated with SO(6) and ξ the control parameter with $0 \leqslant \xi \leqslant 1$. The expectation value of this Hamiltonian in the group coherent state [8, p. 37] is

$$\langle \hat{H} \rangle \equiv E(\beta;\xi) = (1-\xi)\frac{\beta^2}{1+\beta^2} + \xi \frac{1}{4}\left(\frac{1-\beta^2}{1+\beta^2}\right)^2, \tag{2}$$

where β is the deformation. (The value of β at equilibrium, β_0, is the order parameter. The energy $E(\beta;\xi)$ is often called the Landau potential.) The nature of the phase transition as a function of the control parameter ξ can be studied analytically. There is a second-order phase transition at the critical value $\xi = \xi_c = \frac{1}{2}$, as one can see by evaluating the minimum energy and its derivatives with respect to the control parameter ξ and noting that the second derivative is discontinuous at ξ_c (Ehrenfest classification). The same result is obtained in the Landau approach, where the critical value is obtained by requiring that the coefficient of β^2 in $E(\beta;\xi) \approx \frac{1}{4}\xi + (1-2\xi)\beta^2 - (1-3\xi)\beta^4 + \dots$ vanishes. The order parameter is $\beta_0 = 0$ for $\xi \leqslant \frac{1}{2}$ and $\beta_0 = \sqrt{2\xi - 1}$ for $\xi \geqslant \frac{1}{2}$.

Both in nuclei and molecules it has been found that, in some cases, two different intrinsic configurations occur, either nucleonic (in nuclei) or electronic (in molecules). These coexisting configurations cannot be accounted for by a single Hamiltonian but rather by two coupled Hamiltonians. Their properties have been investigated by quantum calculations, e.g., within the framework of the interacting boson model with configuration mixing, the so-called IBM-CM [13]. Since the two configurations may have different ground-state properties, it is of interest to investigate quantum phase transitions in configuration-mixed situations. In this Rapid Communication, we present results for the case in which the first configuration has U($n-1$) symmetry, while the second has SO(n) symmetry, and compare the results with those obtained for the single configuration, summarized above. In particular, we investigate the U(5)–SO(6) transition within the framework of IBM-CM.

In models with configuration mixing the quantum Hamiltonian has the matrix form

$$\begin{bmatrix} (1-\xi)\hat{H}_1 & \hat{W} \\ \hat{W} & \xi\hat{H}_2+\Delta \end{bmatrix}, \tag{3}$$

where $\hat{H}_1$ acts on a first and $\hat{H}_2$ on a second configuration space, $\hat{W}$ mixes both spaces and Δ represents an energy off-set. In nuclei, the first space typically corresponds to valence excitations, while the second involves core-excited configurations. Phase transitions associated with this kind of Hamiltonian shall be called of type II.

Ground-state phase transitions for configuration-mixed systems can be studied by introducing the concept of eigenpotential [14]. The expectation value between appropriate group coherent states yields the classical limit of each element of the matrix (3), the lowest eigenstate of which describes the ground state of the configuration-mixed system. (Eigenpotentials had been introduced in molecular physics earlier [15, p. 296], although not with the same name.) As an example, we consider the case in which the Landau potential matrix has the form

$$\begin{bmatrix} (1-\xi)\dfrac{\beta^2}{1+\beta^2} & \omega \\ \omega & \xi\dfrac{1}{4}\left(\dfrac{1-\beta^2}{1+\beta^2}\right)^2+\Delta \end{bmatrix}. \tag{4}$$

This form can be obtained from Eq. (3) by taking the expectation values of $\hat{H}_1=\hat{n}_d$, $\hat{H}_2=\hat{P}_6$, and $\hat{W}=s^\dagger s^\dagger+d^\dagger\cdot d^\dagger+\mathrm{hc}$ (scaled with the appropriate values of N_1 and N_2) between group coherent states. This potential matrix has three control parameters, ξ,ω, and Δ. For $\Delta=0$ the two configurations are degenerate. The range of the control parameters is $0\leqslant\xi\leqslant 1$, $0\leqslant\omega<+\infty$, and $-\infty\leqslant\Delta\leqslant+\infty$. We restrict our attention to $\Delta\geqslant 0$.

The phase diagram of the eigenpotential (4) can be obtained by studying the properties of its lowest eigenvalue $E_-(\beta;\xi,\omega,\Delta)$. This represents a challenge, as $E_-(\beta;\xi,\omega,\Delta)$ is not a polynomial in the variable β, and thus not considered in the usual Landau treatment of phase transitions. It is the purpose of this Rapid Communication to determine the phase diagram of the eigenpotential (4) as a function of the control parameters ξ,ω, and Δ.

We first expand $E_-(\beta;\xi,\omega,\Delta)$ about $\beta=0$,

$$\begin{aligned} &E_-(\beta;\xi,\omega,\Delta) \\ &\approx \frac{1}{8}\left(4\Delta+\xi-\sqrt{(4\Delta+\xi)^2+64\omega^2}\right) \\ &\quad+\frac{1}{2}\left(1-2\xi+\frac{4\Delta+\xi}{\sqrt{(4\Delta+\xi)^2+64\omega^2}}\right)\beta^2-\frac{1}{2}\left(1-3\xi\right. \\ &\quad\left.+\frac{(4\Delta+\xi)^3(1+\xi)+64\omega^2[2+(1+\xi)(4\Delta+\xi)]}{[(4\Delta+\xi)^2+64\omega^2]^{3/2}}\right)\beta^4. \end{aligned}$$

This expansion shows that there is always an extremum at $\beta=0$; it is a minimum if the coefficient of β^2 is positive and a maximum if this coefficient is negative. (The minimum at $\beta=0$ will henceforth be called spherical and a minimum at $\beta\neq 0$ deformed.) A first critical line (called the anti-spinodal curve, defined as the locus of points at which the minimum at $\beta=0$ disappears) can be found analytically by requiring that the coefficient of β^2 vanishes. This gives the following equation:

$$\omega=\frac{(4\Delta+\xi)\sqrt{(1-\xi)\xi}}{4(2\xi-1)}, \tag{5}$$

defined for $\frac{1}{2}<\xi\leqslant 1$. To the right of the curve (5) in the (ξ,ω) plane, the potential has a maximum at $\beta=0$; to the left it has a minimum. The curve tends to $\omega\to\infty$ as $\xi\to\frac{1}{2}$. There are two special points on (5) for which the coefficient of β^4 vanishes as well. This happens for $(\xi,\omega)=(1,0)$ and $(\xi,\omega)=\frac{1}{7}(4(1+\Delta),\sqrt{4(1+\Delta)(3-4\Delta)})$. In the first point, the lowest eigenvalue of Eq. (4) is zero for all β. In the second, the potential behaves as β^6 around $\beta=0$. These points meet for $\Delta=\frac{3}{4}$. The curve (5) is shown in the phase diagram of Fig. 1 for various values of Δ. (Anti-spinodal values of ξ will be denoted by ξ^{**}.)

The anti-spinodal curve satisfies the equations

$$\left.\frac{\partial E_-}{\partial\beta}\right|_{\beta=\beta_0}=0,\qquad \left.\frac{\partial^2 E_-}{\partial\beta^2}\right|_{\beta=\beta_0}=0, \tag{6}$$

with $\beta_0=0$. One obtains a second critical line (henceforth called the spinodal curve, defined as the locus of points where a deformed minimum appears) satisfying the same equations but with $\beta_0\neq 0$. These equations also define points where the character of the potential changes. For each Δ and for a given choice of β_0, they can be solved numerically in the two control parameters ξ and ω, and this procedure leads to a parametric curve in the (ξ,ω) plane, where β_0 plays the role of the parameter. The range of values available to β_0 depends on Δ. The spinodal curve is also shown in Fig. 1. (Spinodal values

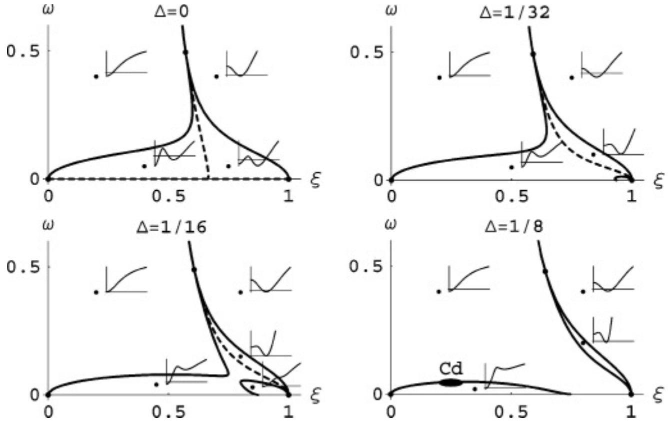

FIG. 1. Phase diagram for the eigenpotential (4) for several values of $\Delta\geqslant 0$. The figure shows the physical region of the parameter space with $0\leqslant\xi\leqslant 1$ and $0\leqslant\omega$. The locus of spinodal points ξ^* and anti-spinodal points ξ^{**} is indicated by full lines and that of critical or Maxwell points ξc by dashed lines. The inset plots illustrate the potentials in the different regions. The region corresponding to the cadmium isotopes ^{110,112,114}Cd is indicated in grey.

of ξ will be denoted by ξ^* .) Its structure is more complex than that of the anti-spinodal curve since it cannot be obtained from an expansion around $\beta = 0$.

In the region where the potential has two minima, the so-called coexistence region, it is of interest to know which of the two lies lowest. This (Maxwell or critical) set of (ξ, ω) points where the potential has two degenerate minima can be found by solving the equations

$$\left.\frac{\partial E_-}{\partial \beta}\right|_{\beta=\beta_0} = 0, \quad E_-(\beta_0; \xi, \omega, \Delta) = E_-(0; \xi, \omega, \Delta), \quad (7)$$

which again gives a parametric curve (depending on Δ) in the (ξ, ω) plane in terms of β_0, henceforth called the critical curve. On the left of this curve the spherical minimum is lowest whereas on the right of it the deformed minimum is. The critical curve is also shown in Fig. 1. (Critical values of ξ will be denoted by ξ_c.)

The phase diagrams of Fig. 1 have some interesting features worth commenting. We begin with $\Delta = 0$. For $\omega = 0$ the potential has two degenerate minima at $\beta_0 = 0$ and $\beta_0 = 1$ for any value of ξ. The entire line $0 \leqslant \xi \leqslant 1$ is critical. For $\omega \neq 0$ the critical curve has the following limiting values: $\omega \to 0, \xi_c \to \frac{2}{3}$ and $\omega \to \infty, \xi_c \to \frac{1}{2}$. The spinodal and anti-spinodal curves have the following limiting values: $\omega \to 0, \xi^* \to 0, \xi^{**} \to 1$ and $\omega \to \infty, \xi^* \to \frac{1}{2}, \xi^{**} \to \frac{1}{2}$. For fixed, small $\omega \neq 0$ the system undergoes a first-order transition, as one can see by plotting the order parameter β_0 as a function of control parameter ξ, Fig. 2. As ω increases from zero, the region of coexistence between the spinodal and antispinodal curves shrinks, the phase transition becomes of second order, and tends to the phase transition for a single configuration summarized above. For increasing values of $\Delta > 0$ the region between the spinodal and antispinodal lines shrinks and a region develops around the point $(\xi, \omega) = (1, 0)$ with a single spherical minimum. The latter region grows until the two spherical regions become connected and the region of coexistence splits in two regions that become smaller as Δ increases and disappear completely for $\Delta = \frac{3}{4}$. Above this value of Δ, the lowest energy surface of the matrix (4) must necessarily have either a spherical minimum or a deformed one. Already at $\Delta \approx 0.1$, the situation is clear as only a very small coexistence region remains for a limited range of ω values and the critical, spinodal and anti-spinodal curves essentially coincide for all ω.

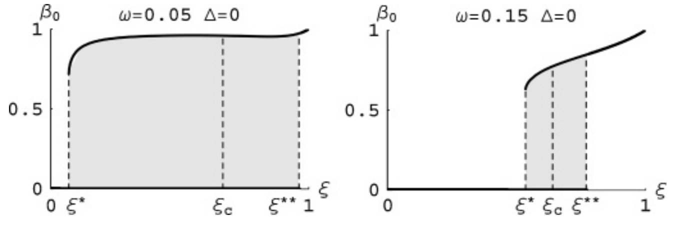

FIG. 2. Behavior of the order parameter β_0 as a function of the control parameter ξ for the eigenpotential (4) for two sets of values of Δ and ω. The region of coexistence (grey) is bordered by the spinodal and anti-spinodal points ξ^* and ξ^{**} , and contains the critical point ξ_c.

Experimental evidence for type-II phase transitions should be searched for in nuclei where configuration mixing is known to occur. The main feature of type-II phase transitions is the occurrence of *first*-order transitions with a *large* coexistence region. The order of the phase transition can be determined experimentally from ground-state energies. If the phase transition is first order, there should be a discontinuity in the first derivative of $E_{\min}$, i.e., in the separation energies. For second-order transitions the discontinuity is in the second derivative.

Configuration mixing is known to occur in many nuclei, most notably in the Pb–Hg–Pt, Sn–Cd–Pd, Sr–Zr–Mo and Ge–Se regions [16]. One of the main results of this Rapid Communication is that the order of the phase transition is greatly influenced by the strength of the coupling ω and by the energy off-set Δ. A small value of ω is necessary for the transition to be of first order; as ω increases the transition becomes similar to that in the single configuration (second order). Furthermore, the region of coexistence disappears for large Δ (i.e., if $\Delta \gtrsim 0.1$).

The strength of the coupling ω is essentially proportional to the number of active pairs, which in the Pb–Hg–Pt (and in the Sn–Cd–Pd) region is the number of proton hole pairs. This should be contrasted with Δ which is independent of boson number. Our results thus indicate that phase transitions between the two configurations, if they occur at all, are expected to be sharp first-order transitions in Pb (Sn) and to become progressively less sharp in Hg (Cd) and Pt (Pd). This qualitative finding appears to be confirmed by quantum calculations. In Pt (strong coupling), data can be fitted either with [17] or without [18,19] configuration mixing.

We illustrate these qualitative arguments with the example of the Cd nuclei. The isotopes ^{110,112,114}Cd have been extensively studied by Lehmann and Jolie [20] in the context of U(5)–SO(6) coexistence in the IBM-CM. The Landau potential matrix of the Hamiltonian is

$$\begin{bmatrix} (1-\xi)\dfrac{\beta^2}{1+\beta^2} & \omega \\ \omega & \xi\dfrac{1}{4}\left(\dfrac{1-\beta^2}{1+\beta^2}\right)^2 + \zeta\dfrac{\beta^2}{1+\beta^2} + \Delta \end{bmatrix}, \quad (8)$$

and can be analyzed in the same way as above. The effect of the additional term in ζ is to shrink the regions of deformation and coexistence of the phase diagram. All parameters can be obtained from Ref. [20] except the strength of the pairing $\hat{P}_6$ (unknown for the core-excited configuration in the Cd nuclei) which, from *I*-spin arguments [21], is determined from ^{106,108,110}Ru. In this way one obtains $\xi \approx 0.2$ to 0.3, $\omega \approx 0.03$ to 0.06, and $\Delta \approx 0.1$ to 0.2. This allows to locate the Cd isotopes in the region indicated in Fig. 1. The transition is at best of second order or, more likely, there is no transition at all because of the additional term in ζ. This is consistent with measured neutron separation energies (see Fig. 3).

The situation is different in the Zr–Mo [22] and Ge–Se [23] regions, where Δ approaches zero and even becomes negative. Experimental evidence for type-II phase transitions should be looked for in these nuclei. The separation energies in the Sr–Zr–Mo region suggest that a first-order phase transition occurs

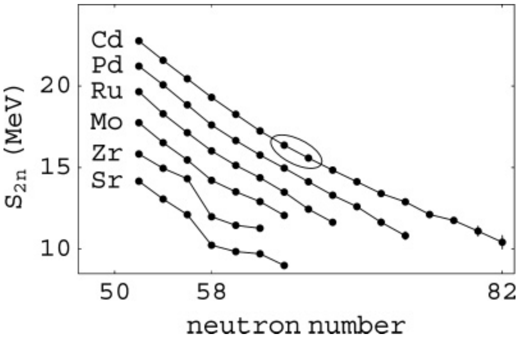

FIG. 3. Two-neutron separation energies S_{2n} as a function of neutron number N in the Sr–Zr–Mo–Ru–Pd–Cd isotopes. The points involving binding-energy differences between the cadmium isotopes ^{110,112,114}Cd are indicated.

in Sr and Zr at neutron number $N = 58$ and a second-order phase transition in Mo at the same N (see Fig. 3). Other nuclear regions, for example associated with the coexistence of axially deformed and spherical shapes or of more than two configurations, can be investigated likewise. The formalism proposed in this paper offers the possibility to undertake a systematic study of nuclear coexistence in the framework of IBM-CM [24], with the aim to locate nuclei on the type-II phase diagram.

In molecules, configuration mixing has been known for years, although one potential usually has a minimun whereas the other does not. However, configuration mixing plays an important role in the phenomenon of predissociation, as in the case of the molecules AlH and BH [15]. To treat this problem, the scheme presented here should be modified to include situations in which $\beta_0 \to \infty$. The case in which the eigenpotential has a second minimum at finite β_0 may be of importance in van der Waals molecules. This is where evidence for Type-II phase transitions should be looked for.

In conclusion, we presented an analysis of quantum phase transitions in coexistence models and developed a geometric framework that opens up a wide area of research to test phase-transitional/coexistence behavior of quantum systems. The structure of the phase diagram is rather complex and it has some unusual features not present in the single configuration because the eigenpotential is no longer a polynomial in β.

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