Quantum Phase Transitions in Mesoscopic Systems

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Quantum phase transitions in mesoscopic systems are studied. It is shown that the main features of phase transitions, defined for infinite number of particles, $N \to \infty$, persist even for moderate $N \sim 10$. A Landau analysis of first order transitions is done and a "critical" exponent at the spinodal point is defined. Two order parameters are introduced to distinguish first from second order transitions. Applications to atomic nuclei, molecules, atomic clusters, and finite polymers are mentioned. Experimental evidence in atomic nuclei is presented.

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In recent years, quantum phase transitions (that is phase transitions that occur at zero temperature as a function of a coupling constant) have become very important in connection with condensed matter systems. The simplest example is that occurring in the Ising model in a transverse field, where as a function of the applied magnetic field one observes a second order phase transition at some critical value. The phase transition is observed by measuring an order parameter as a function of the control parameter. Quite often, the order parameter cannot be directly measured, in which case a function of the order parameter, the susceptibility or such, is measured. The concept of quantum phase transition can also be used in mesoscopic systems, that is, systems with a finite number of particles N, where in fact it was introduced years ago [1,2]. Recently, the advance of experimental techniques has opened the way for a deeper understanding of quantum phase transitions in a variety of mesoscopic systems, atomic nuclei, molecules, atomic clusters, and finite polymers. The transitions in these systems are between different shapes or geometric configurations and can thus be also termed "shape transitions." It is of great interest to understand the modifications (if any) brought in by the finiteness of these systems. It is the purpose of this Letter to address this question, show results, and suggest experiments. Although we treat explicitly the case of atomic nuclei, described by the interacting boson model [3], similar results can be obtained for other cases, such as molecules, described by the vibron model [4], and polymers, described by the algebraic anharmonic model [5].

There are two ways of addressing quantum phase transitions: (i) the potential approach, due to Landau, and (ii) the direct quantum computation of order parameters. As a generic example of the situations encountered within the framework of boson models, we consider the "Landau" potential,

$$V(\beta) = \beta^2 + \xi[(2 - \beta^2)^2 - \eta\beta^3], \quad \beta \geq 0. \qquad (1)$$

This potential depends on two control parameters, $\xi \geq 0$ and $\eta \geq 0$, and encompasses all situations encountered so far within the framework of algebraic models. When $\eta = 0$, the potential reduces to a quartic function, extensively studied by Landau [6]. As a function of ξ, the system has a second order phase transition at $\xi = \xi_c = \frac{1}{4}$. We concentrate rather on first order transitions, since these have not been much investigated. For a fixed value of $\eta \neq 0$, the system experiences a first order transition as a function of ξ, as one can see by evaluating $V_{\min}$, $\frac{\partial V_{\min}}{\partial \xi}$, and $\frac{\partial V^2_{\min}}{\partial \xi^2}$ and observing that $\frac{\partial V_{\min}}{\partial \xi}$ is discontinuous. One can also evaluate the three important points of a first order transition, the so-called spinodal point ξ^*, that is the value of ξ at which the second minimum appears, the critical point at which the two minima are equivalent ξ^c, and the antispinodal point ξ^{**} at which the first minimum disappears. The spinodal and antispinodal points can be easily obtained analytically: $\xi^* = \frac{32}{128+9\eta^2}$ and $\xi^{**} = \frac{1}{4}$. The expression for the critical point is complex but one can obtain a good estimate, $\xi^c \simeq \frac{32}{128+8\eta^2}$.

In Fig. 1 (top), we give a plot of the potentials, and in Fig. 1 (bottom) the classical order parameter, $\beta_{e\text{equilib}} = \beta_e$, as a function of the control parameter ξ for $\eta = 1$. For $\xi \geq \xi^*$, the upper branch of the order parameter is given by

$$\beta_e = \frac{3}{8}\eta + \frac{1}{2}\sqrt{\frac{9}{16}\eta^2 + 8\left(1 - \frac{1}{4\xi}\right)}. \qquad (2)$$

One can define a critical or "spinodal" exponent by expanding around the spinodal point ξ^* as $[\beta_e - \beta_e(\xi^*)] \propto (\xi - \xi^*)^\mu$.

As mentioned above, at $\eta = 0$, the transition becomes second order, the spinodal, critical, and antispinodal points all converge to the same point, and one obtains the usual expression for $\beta_e = \sqrt{2[1 - (1/4\xi)]}$, with critical exponent $\mu = \frac{1}{2}$. The classical Landau analysis provides an understanding of the class of problems discussed above. In order to study the effects of the finiteness of the system, we must resort to specific models. We consider here the class of quantum models described by the

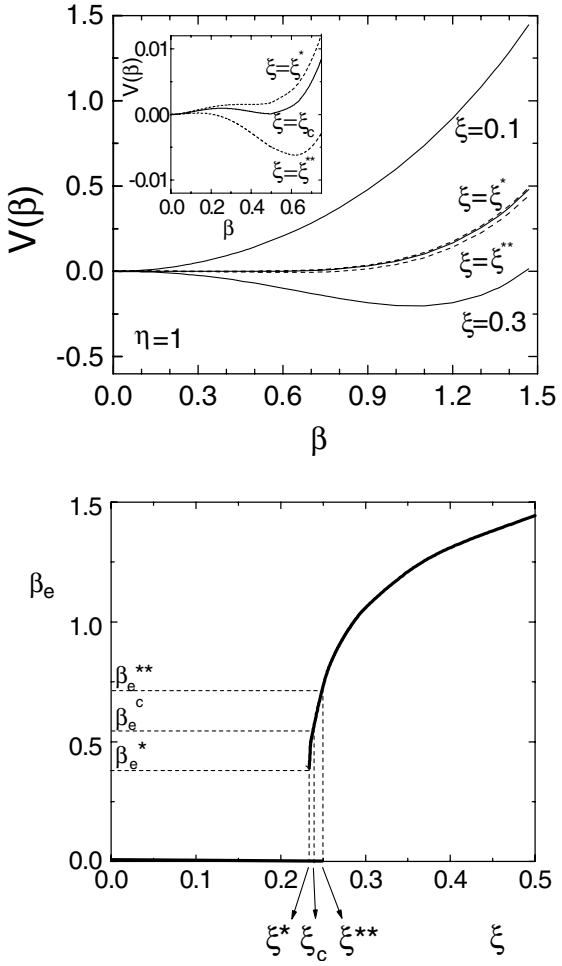

FIG. 1. Top: Landau potential for different values of the control parameter. The inset shows, on an expanded scale, the two shallow coexisting minima for a narrow range of values near the critical point. Bottom: Behavior of the order parameter β_e (values of the location of the minima of the Landau potential) as a function of the control parameter ξ.

Hamiltonian $H = \sum_\alpha \varepsilon_\alpha G_\alpha + \sum_{\alpha\beta} v_{\alpha\beta} G_\alpha G_\beta$, where $G_\alpha \in \mathcal{G}$ are elements of a Lie algebra. As an example, we consider the interacting boson model of nuclei, $\mathcal{G} \equiv U(6)$ [3]. The ingredients in this model are bosons with angular momentum $J = 0$ and 2 (s and d bosons) which represent Cooper-like pairs composed of two nucleons, either two protons or two neutrons. Only active pairs, i.e., pairs in the valence shell, are considered. Their number (typically 5–20) is denoted by N. The classical limit of this model is of the type discussed above. Specifically, we consider the Hamiltonian [7]

$$H = \epsilon_0 \left[(1 - \xi) n_d - \frac{\xi}{4N} Q^\chi \cdot Q^\chi \right], \tag{3}$$

where $n_d = (d^\dagger \cdot \tilde{d})$ and $Q^\chi = (d^\dagger \times \tilde{s} + s^\dagger \times \tilde{d})^{(2)} + \chi (d^\dagger \times \tilde{d})^{(2)}$ with $0 \geq \chi \geq -\sqrt{7}/2$ and $0 \leq \xi \leq 1$. The eigenvalues and eigenvectors of this Hamiltonian are controlled by two parameters (apart from a scale ϵ_0), ξ and χ. Its classical limit (Landau potential) can be obtained by the method of coherent states [1,8] in terms of two classical coordinates, β and γ. The scaled potential energy surface, $E(\beta, \gamma)/\epsilon_0 N$, is given by [9]

$$V(\beta, \gamma) = \frac{\beta^2}{1 + \beta^2} \left[(1 - \xi) - (\chi^2 + 1) \frac{\xi}{4N} \right] - \frac{5\xi}{4N(1 + \beta^2)} - \frac{\xi(N - 1)}{4N(1 + \beta^2)^2} \times \left[4\beta^2 - 4\sqrt{\frac{2}{7}} \chi \beta^3 \cos 3\gamma + \frac{2}{7} \chi^2 \beta^4 \right]. \tag{4}$$

This potential is either γ independent ($\chi = 0$) or has a minimum at $\gamma = 0^0$. We henceforth set $\gamma = 0^0$ and study only the β dependence. This is of the type given in Eq. (1). The quantum phase transitions of this model were extensively studied years ago and are summarized in the phase diagram of Fig. 2 [1,2]. There is a region of first order transitions ending in a point of second order transition. We note that an extended phase diagram has been recently introduced to include both prolate and oblate deformations [10]. This extended diagram has Z_2 symmetry, $\chi \rightarrow -\chi$. All quantities are either symmetric or antisymmetric under Z_2. A Landau analysis of second order transitions in the extended diagram has also been done [11]. Because of the Z_2 symmetry, we confine our discussion in this article to prolate deformations ($\chi \leq 0$). For oblate deformations, simply replace χ by $-\chi$.

One of the consequences of the finiteness of the system is that the potential contains energy denominators $(1 + \beta^2)$ and $(1 + \beta^2)^2$. In other words, $V(\beta)$ is finite as $\beta \rightarrow \infty$, contrary to the Landau potentials where $V \rightarrow \infty$ as $\beta \rightarrow \infty$. A detailed analysis of the phase transition reveals that nothing changes in the structure of the transitions by this "finiteness," except that the minima are slightly shifted.

We come now to the effects due to finite boson number N and introduce quantum order parameters. For second order transitions, it is easy to define an order parameter.

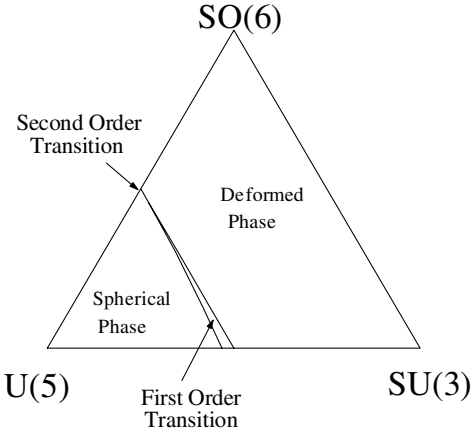

FIG. 2. Phase diagram of nuclei in the interacting boson model.

Here we use the normalized expectation value of the number of d bosons in the ground state, $\nu_1 = \langle 0_1|n_d|0_1\rangle/N$. The behavior of ν_1, as a function of the control parameter ξ, for the second order transition U(5)–SO(6), is shown in Fig. 3, obtained by numerical diagonalization of the quantum Hamiltonian (3) with $\chi = 0$. The classical limit (mean field) result is shown as $N \to \infty$. Even for moderate values of N, there is at the critical point a sudden increase in the order parameter. (A criterion for recognizing critical behavior is $\Delta\nu_1/\nu_1 \leq 1$ over an interval $\Delta\xi$ that is experimentally measurable [12].) The discontinuity in the slope is smoothed out but its effects are still visible. We can even estimate, from numerical simulation for various N, as shown in Fig. 3 (inset), the critical exponent μ defined above for the classical order parameter $\beta_e = \sqrt{\nu_1/(1-\nu_1)}$. We find $\mu = 0.53 \pm 0.03$ (mean field result $\mu = 0.5$). We conclude that *the concept of a second order quantum phase transition* (and its associated critical value and critical exponent) *persists even at moderate values of* $N \simeq 10$. An even more interesting situation occurs for a first order transition. For this transition we introduce an additional order parameter, the difference between the expectation value of n_d in the first excited 0^+ state and the ground state, $\nu_2 = [\langle 0_2|n_d|0_2\rangle - \langle 0_1|n_d|0_1\rangle]/N$. In Fig. 4, we plot the two order parameters, ν_1 and ν_2, characterizing the first order transition, obtained from a numerical diagonalization of H in Eq. (3) for the U(5)–SU(3) transition, $\chi = -\sqrt{7}/2$, as a function of the control parameter ξ. Again, one can see that the features of first order transitions persists even for moderate $N \simeq 10$. We extract, in the inset of Fig. 4 (top), the critical exponent at the spinodal point of the first order transition to be $\mu = 0.52 \pm 0.07$ (mean field result $\mu = 0.5$).

An important question is how to distinguish from model calculations for finite N (or from experiment) whether the phase transition is first or second order. The behavior of the order parameter ν_1 is the same for both transitions as the sudden increase is smoothed out by the finiteness of N. However, the behavior of the order parameter ν_2 can distinguish between first and second order, as can be seen in the inset of Fig. 4 (bottom). For first order transitions, ν_2 has a wiggling behavior changing sign in the region of the critical point due to the switching of the two coexisting phases. For second order transition, ν_2 has a smoother behavior.

In the final part of this article, we address the question of how to detect quantum phase transitions in mesoscopic systems. In the Ising model, this can be simply done by measuring a function of the order parameter, the susceptibility (a property of the ground state), as a function of the applied magnetic field. Mesoscopic systems have the disadvantage that the discontinuity is smoothed out (however, as shown in the paragraphs above, this effect does not appear to be dominant). They have conversely the great advantage that properties of both the ground state and of excited states can often be measured. In addition, mesoscopic systems described by Hamiltonians of the type of Eq. (3), that is, where the phase transition arises from a competition between one-body and two-body terms, have the advantage that the control parameter

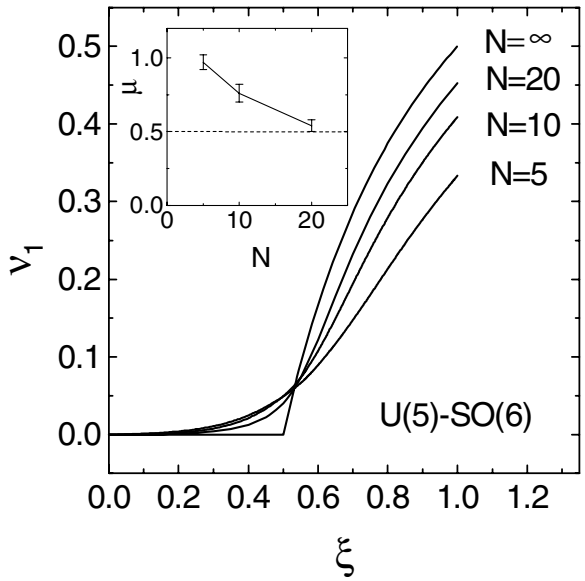

FIG. 3. Behavior of the order parameter ν_1 as a function of the control parameter ξ for second order phase transition in finite systems. The inset shows the "critical" exponent describing the behavior of the order parameter β_e in the critical point region.

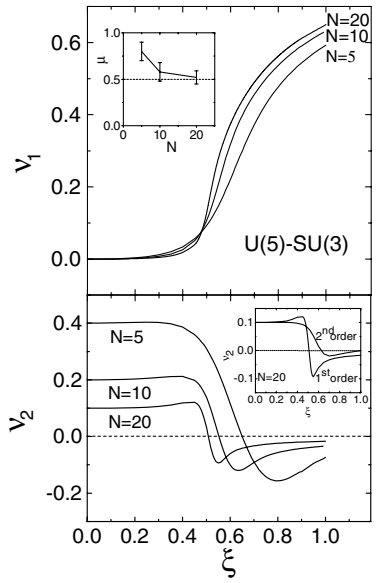

FIG. 4. Top: Behavior of the order parameter ν_1 as a function of the control parameter ξ for first order phase transition in finite systems. The inset shows the critical exponent describing the behavior of the order parameter β_e in the critical point region. Bottom: Behavior of the order parameter ν_2 as a function of the control parameter ξ for first order phase transition in finite systems. The inset shows a comparison between the first [U(5)–SU(3)] and second order [U(5)–SO(6)] phase transitions.

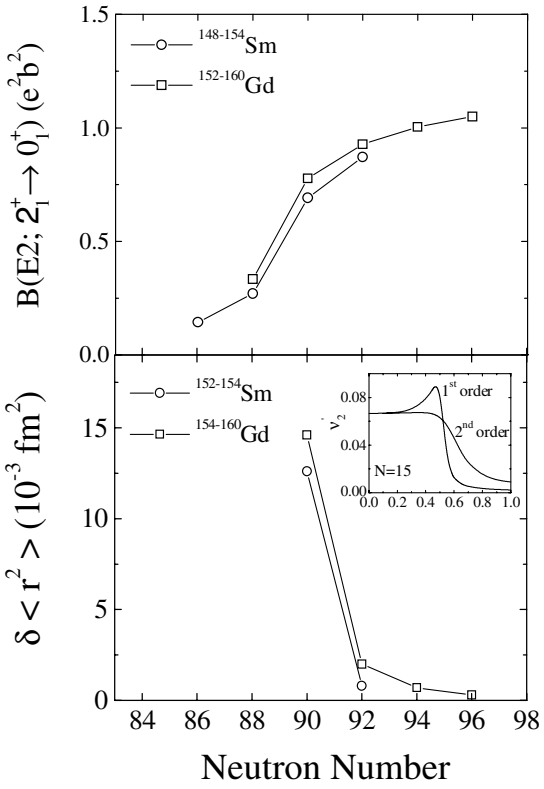

FIG. 5. Top: $B(E2; 0_1 \rightarrow 2_1)$ values (proportional to ν_1) in Sm and Gd isotopes plotted versus neutron number (proportional to the control parameter ξ). Bottom: Isomer shifts $\delta\langle r^2\rangle = \langle r^2\rangle_{2_1} - \langle r^2\rangle_{0_1}$ in Sm and Gd isotopes [13] plotted versus neutron number. The inset shows a comparison between first and second order phase transitions for ν_2'.

depends on the number of particles N. One can thus measure properties of the system as a function of N. In atomic nuclei, the order parameters ν_1 and ν_2 are directly related to the expectation value of the scalar operator r^2 [3]: $\nu_1 + c_1 = c_2\langle r^2\rangle_{0_1}$ and $\nu_2 = c_2[\langle r^2\rangle_{0_2} - \langle r^2\rangle_{0_1}]$, called the isomer shift, where c_1 and c_2 are parameters. These quantities are not easy to measure. A simpler quantity, proportional to $\langle n_d\rangle$ in the ground state, and thus to ν_1, is the intensity of electromagnetic radiation between the ground state, with $J = 0$, and the first excited state with $J = 2$, $B(E2; 0_1 \rightarrow 2_1)$. Figure 5 (top) shows the $B(E2; 0_1 \rightarrow 2_1)$ values for Sm-Gd isotopes, a known transitional region between spherical and axially deformed nuclei, U(5)–SU(3). The occurrence of a phase transition at neutron number 90 is evident. A similar situation occurs for ν_2. The isomer shift $\langle r^2\rangle_{0_2} - \langle r^2\rangle_{0_1}$ is not easily measurable. Rather one can measure the isomer shift $\delta\langle r^2\rangle = \langle r^2\rangle_{2_1} - \langle r^2\rangle_{0_1}$ between the first 2^+ state and the ground state. This is proportional to $\nu_2' = [\langle 2_1|n_d|2_1\rangle - \langle 0_1|n_d|0_1\rangle]/N$. The available data [13] on this isomer shift in Sm-Gd nuclei are shown in Fig. 5 (bottom). In addition to those mentioned above, other measurements can be used to distinguish first from second order transitions, in particular, two-nucleon separation energies, $S_{2n}(N) = E(N+1) - E(N)$, where $E(N)$ is the ground state energy of a nucleus with N bosons [3]. The phase transitional behavior of different quantities across the U(5)–SU(3) transition was also recently studied by Pan *et al.* [14].

In conclusion, mesoscopic systems that can be measured for various numbers of particles, offer a unique opportunity to study quantum phase transitions. The features of these transitions persist even to moderate values of N. An analysis *à la* Landau of first order transitions has been done and a critical exponent at the spinodal point of a first order transition has been defined. Systems where this study can be carried out and where all the tools are already in place are (i) shape phase transitions in atomic nuclei in terms of the interacting boson model [3], for example, the Sm-Gd-Dy nuclei; (ii) shape phase transitions in molecules in terms of the vibron model [4], for example, the hydride molecules *XYZ*-H and *XYZ*-D; (iii) conformation phase transitions in finite polymers in terms of the algebraic anharmonic model [5], for example, the paraffins $CH_3 - (CH_2)_n - CH_3$; and (iv) shape phase transitions in atomic clusters [15], for example, the alkaline clusters $(Na)_n$, $(K)_n$ (where, however, the formalism needs further development).

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