Triple Point of Nuclear Deformations

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We show that the second-order phase transition between spherical and deformed shapes of atomic nuclei is an isolated point following from the Landau theory of phase transitions. This point can occur only at the junction of two or more first-order phase transitions which explains why it is associated with one special type of structure and requires the recently proposed first-order phase transition between prolate and oblate nuclear shapes. Finally, we suggest the first empirical example of a nucleus located at the isolated triple-point.

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Phase transitions in finite quantal systems are a challenge to theoreticians and experimenters [1]. One of the reasons is that it is not clear how they manifest themselves empirically. This is especially true for phase transitions involving a small number of interacting bodies, such as the constituents of an atomic nucleus. Quantum phase transitions in nuclei concern, for example, the geometric shape associated with the ground state. These transitions take place at zero temperature and depend on the number of nucleons.

Nuclear shape phase transitions came again to the forefront of nuclear structure physics when recent β-decay studies [2] led to a new interpretation [3,4] of the spherical-deformed transitional region ($N \approx 90$ nuclei) as a first-order phase transition. Soon thereafter, Iachello developed new symmetries that describe atomic nuclei at the critical points [5,6]. These symmetries, called X(5) and E(5), are obtained within the framework of the collective model [7] under some simplifying approximations. Remarkably, the parameter-free predictions provided by the new symmetries are closely realized in some nuclei, such as ^{152}Sm and ^{134}Ba, respectively [8,9].

The geometric shape of the ground state can be conveniently described by three Euler angles defining the orientation of the deformed nucleus in space, and by the quadrupole deformation parameters β and γ [7]. Many models for nuclear structure therefore express the potential in terms of an expansion in β and γ. Although the results to be obtained below follow from any such model, for specificity, we will use the interacting boson model (IBM) [10], since it allows the treatment of the finite number of nucleons in the nuclear many-body problem. The IBM describes even-even nuclei in terms of interacting valence nucleon pairs with angular momenta $L = 0$ (s bosons) and 2 (d bosons) and incorporates an explicit dependence on the number of valence nucleons. Phase transitions in such systems were intensively studied in the early 1980s in the pioneering works by Dieperink [11], Ginocchio [12], Feng [13], and their collaborators. Feng, Gilmore, and Deans [13] discussed the IBM phase structure in terms of a first-order phase transition terminating in an isolated point of a second-order phase transition. Recently, it was shown [14,15] that the model exhibits an additional, previously unrecognized, first-order prolate-oblate phase transition.

It is the purpose of the present Letter to analyze the nuclear shape phase diagram in terms of the Landau theory of continuous (second-order) phase transitions [16,17]. We will show that, in the realistic nuclear case, a second-order phase transition can occur only as an isolated point where there is a junction of at least two first-order shape phase transitions and that, therefore, the nuclear shape phase diagram must have both spherical-deformed and prolate-oblate first-order phase transitions. Thus, the Landau theory of continuous phase transitions, constructed almost 70 years ago for infinite classical systems, is shown to be a useful approach also for finite quantal systems such as the atomic nucleus. (Note that the

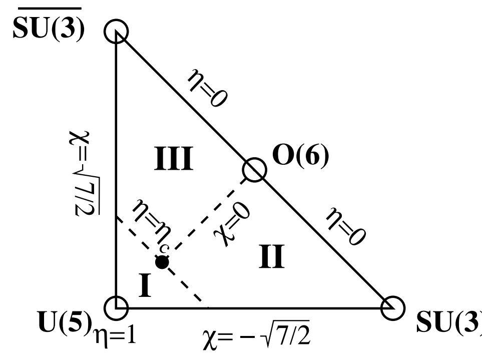

FIG. 1. The extended Casten triangle [15] and its different phases. The circles indicate the location of the IBM dynamical symmetries. The solid dot in the center represent the second-order transition between spherical nuclei (phase I) and deformed nuclei with prolate (phase II) and oblate (phase III) forms. The dashed lines correspond to first-order phase transitions.

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Landau theory of phase transitions was already applied in nuclear physics in another context, hot rotating nuclei, by Alhassid *et al.* [18]). Our observations will also allow the introduction of the concept of a triple point for nuclear deformation and the identification of a corresponding triple-point nucleus.

Let us consider a standard two-dimensional parametrization of the IBM-1 Hamiltonian:

$$\hat{H}(N, \eta, \chi) = \eta\, \hat{n}_d + \frac{\eta - 1}{N}\, \hat{Q}_\chi \cdot \hat{Q}_\chi, \qquad (1)$$

where $\hat{n}_d = d^\dagger \cdot \tilde{d}$ is the d-boson number operator and $\hat{Q}_\chi = [d^\dagger s + s^\dagger \tilde{d}]^{(2)} + \chi[d^\dagger \times \tilde{d}]^{(2)}$ the quadrupole operator. N in the denominator stands for the total number of bosons (integral of motion) and ensures a convenient scaling. Control parameters η and χ vary within the range $\eta \in [0, 1]$ and $\chi \in [-\sqrt{7}/2, +\sqrt{7}/2]$. The parameter space can be naturally represented by the extended Casten triangle [15] (see Fig. 1) whose $\eta = 1$ vertex corresponds to the U(5) dynamical symmetry (spherical shape), while the dynamical symmetries SU(3) (prolate), O(6) (γ-soft), and $\overline{\text{SU(3)}}$ (oblate) are located on the $\eta = 0$ side: SU(3) and $\overline{\text{SU(3)}}$ at the $\chi = -\sqrt{7}/2$ and $\chi = +\sqrt{7}/2$ vertices, respectively, O(6) at $\chi = 0$. The halves of the triangle with positive and negative χ are related by the $\chi \leftrightarrow -\chi$ parameter symmetry [19].

The geometric interpretation of the Hamiltonian (1) can be derived by the method of Gilmore [20] using the s, d-boson condensate states $|N\beta\gamma\rangle$ defined in Ref. [21]. The energy functional $E(N, \eta, \chi; \beta, \gamma) = \langle N\beta\gamma|\hat{H}(N, \eta, \chi)|N\beta\gamma\rangle$:

$$E(N, \eta, \chi; \beta, \gamma) = -5(1-\eta) + \frac{1}{(1+\beta^2)^2}\Bigg[\{N\eta - (1-\eta)(4N + \chi^2 - 8)\}\beta^2 + 4N(1-\eta)\sqrt{\frac{2}{7}}\chi\beta^3 \cos 3\gamma + \left\{N\eta - (1-\eta)\left(\frac{2N+5}{7}\chi^2 - 4\right)\right\}\beta^4\Bigg], \qquad (2)$$

encodes several phase-transitional phenomena [22] described in a general framework within the Landau theory of phase transitions [16,17]. Instead of the thermodynamic potential $\Phi(P, T; \xi)$ that depends on external parameters (pressure P and temperature T) and the order parameter ξ, as investigated by Landau, we have $E(N, \eta, \chi; \beta, \gamma)$ depending on the external parameters η and χ, and on the order parameters β and γ. The task is to minimize the functional by varying β and γ for each η and χ—the optimal values being denoted $\beta_0(N, \eta, \chi)$ and $\gamma_0(N, \eta, \chi)$. The simple form of the dependence on γ in Eq. (2) yields either $\gamma_0 = 0$ (for negative χ), or $\pi/3$ (for positive χ). The latter case can be equivalently described by a substitution $\gamma_0 \to 0$ and $\beta_0 \to -\beta_0$ which allows us to omit the parameter γ from further considerations by imposing the constraints $\beta_0 > 0$ for $\chi < 0$ and $\beta_0 < 0$ for $\chi > 0$. These values distinguish prolate and oblate deformations, respectively, while $\beta_0 = 0$ corresponds to the spherical symmetry.

The ground-state energy obtained from the global minimum of the energy functional $E(N, \eta, \chi; \beta_0)$ must be a continuous function of η and χ, similarly as the thermodynamic potential in the equilibrium configuration ξ_0 is a continuous function of P and T. However, the derivatives of $E(N, \eta, \chi; \beta_0)$ or $\Phi(P, T; \xi_0)$ with respect to the control parameters do *not* have to be continuous. Discontinuities in the first or second derivatives result in first- or second-order phase transitions, respectively, the latter case being also called a continuous phase transition [16,17]. Thus, first-order transitions are characterized by a singularity in the specific heat $C_P = -T\partial^2\Phi/\partial T^2$, giving a nonzero latent heat. This corresponds to a situation when the optimal order parameter ξ_0 or β_0 jumps discontinuously from one value to another at the phase transition. For the second-order transitions the latent heat vanishes and the optimal configuration changes continuously (although not smoothly).

In Landau theory, the potential Φ is expanded as

$$\Phi(P, T; \xi) = \Phi_0 + A(P, T)\xi^2 + B(P, T)\xi^3 + C(P, T)\xi^4 + \dots. \qquad (3)$$

Analyzing the behavior of this function for transitions between more symmetric ($\xi_0 = 0$) and less symmetric ($\xi_0 \neq 0$) phases, it is found that first-order phase transitions form continuous lines in the $P \times T$ plane, while second-order transitions occur either along continuous lines or at isolated points. The former is the case only if the coefficient B vanishes identically for all P and T. If this is not so, the conditions for the second-order transition read as $A = 0$, $B = 0$, and $C > 0$, giving isolated solutions $P = P_c$ and $T = T_c$. These points can only be located at intersections of two or more curves corresponding to first-order phase transitions. In the simplest case, the second-order transition takes place at the triple point of three phases—see Fig. 65(a) in Ref. [17]. Phase I has the higher symmetry ($\xi_0 = 0$) while phases II and III with lower symmetry differ just by the sign of ξ_0. Landau remarks that such isolated points forming a second-order phase transition had not been observed in nature. However, as we will see below, atomic nuclei provide evidence for their existence.

Landau theory is perfectly applicable to the energy functional (2). Expanding $(1 + \beta^2)^{-2} = 1 - 2\beta^2 + 3\beta^4 - 4\beta^6 + \dots$, and adopting the convention with

$\gamma = 0$ we can write

$$E(N, \eta, \chi; \beta, \gamma) = E_0(\eta) + A(N, \eta, \chi)\beta^2 + B(N, \eta, \chi)\beta^3 + C(N, \eta, \chi)\beta^4 + \ldots, \quad (4)$$

where, clearly, $B(\eta, \chi)$ is generally nonzero. Thus, from the above discussion, the second-order phase transition between spherical and deformed nuclear phases can take place only at isolated points of the $\eta \times \chi$ plane. Indeed, there is just one such point, located on the connection of the U(5) and O(6) dynamical symmetries, namely, at $\chi = 0$ and $\eta = \eta_{\rm trip}(N) = (4N - 8)/(5N - 8)$ in the parametrization of Eq. (1). As shown in Fig. 1, this is the triple point of the nuclear shape phase diagram since the spherical phase ($\beta_0 = 0$) exists for $\eta > \eta_{\rm trip}$ while for $\eta < \eta_{\rm trip}$ two deformed phases (prolate, $\beta_0 > 0$, and oblate, $\beta_0 < 0$) are separated by the line $\chi = 0$. Except at the triple point, the transitions between spherical and deformed (prolate/oblate), and between deformed prolate and oblate phases are of the first-order, conforming to Landau theory.

For $\chi \neq 0$, that is, anywhere except along the U(5)-O(6) line in Fig. 1, the deformed-to-spherical transition proceeds in the following way: When η increases to the value $(4N + \chi^2 - 8)/(5N + \chi^2 - 8) = 4/5 + \mathcal{O}(1/N)$, the potential develops a minimum at $\beta = 0$ (A becomes positive). At first, however, this minimum is only local, the global minimum being still situated at $\beta_0 \neq 0$. Both minima become degenerate at $\eta = \eta_c(N, \chi)$:

$$\eta_c(N, \chi) = \frac{4 + 2\chi^2/7}{5 + 2\chi^2/7} + \mathcal{O}\left(\frac{1}{N}\right), \quad (5)$$

which defines the real phase separatrix between spherical and deformed (prolate or oblate) shapes for the Hamiltonian (1). For $\chi = 0$ we have $\eta_c(N, 0) = \eta_{\rm trip}(N)$. In this case, the deformed minimum β_0 converges to 0 for $\eta \to \eta_{\rm trip}$ conforming to the law $\beta_{0|\chi=0\pm} \propto \mp\sqrt{\varepsilon}[1 + \mathcal{O}(\varepsilon)]$, where $\varepsilon = (\eta_{\rm trip} - \eta)/\eta_{\rm trip}$. Thus the critical exponent [23,24] for β_0 at the triple point is $\lambda = 1/2$. Note that this behavior is in perfect agreement with general predictions derived in Ref. [16]. At the triple point, the potential does not develop the double-well form. Indeed, as a general rule, phase coexistence can be found only in first-order phase transitions [17,23,24].

Concerning the prolate-oblate transition $\beta_0 \to -\beta_0$ at $\chi = 0$ and $\eta < \eta_{\rm trip}$ we recall that the negative-β part of the energy functional just represents the $\gamma = \pi/3$ cut of the energy surface (2). To speak about a double-well form of the energy functional in β would be misleading, because the higher minimum is only an unstable saddle point in the $\beta \times \gamma$ plane. When crossing $\chi = 0$ the surface becomes totally flat in γ and then the saddle points and real minima are exchanged. The prolate-oblate phase transition is a first-order phase transition since for $\eta < \eta_{\rm trip}$ the energy minimum moves discontinuously from β_0 to $-\beta_0$. At the triple point, again, the transition becomes of the second order. The behavior of the deformed minimum along the spherical-deformed phase separatrix $\eta = \eta_c(N, \chi)$ reads as $\beta_0|_{\eta=\eta_c-} \propto -\chi + \mathcal{O}(\chi^2)$ for small χ.

The difference between second- and first-order phase transitions between spherical and deformed nuclei is founded in the different behavior of the energy surface near the phase transition. For the second-order transition, it evolves as in Fig. 2(a) (similar to Fig. 63 of Ref. [17]).

Such a phase transition occurs (at low energy and spin) only when gamma softness is preserved throughout. In the first-order transition, as noted above, a lower symmetry (deformed) metastable minimum exists "before" the phase transition while, "after," the higher symmetry (spherical) minimum is the metastable state. This is illustrated in Fig. 2(b).

Microscopically, the first-order phase transition between spherical and deformed nuclei typically arises when there is a subshell gap such that the particle-hole excitations across the gap produce a more deformed configuration (at a cost in energy). The energy of this configuration is lowered as more valence nucleons are added due to the eradication of the gap by attractive monopole *p-n* interactions [25,26]. Equilibrium deformation ensues when the deformed configuration crosses the spherical (dashed curve in Fig. 2(b)). The clearest first-order phase transitions are quite rapid as a function of nucleon number (e.g., near $N = 60, 90$), especially compared to second-order phase transitions (such as those near $A \approx 130$), but this need not be the case.

The above analysis of the nuclear phase diagram allowed us to clarify the results of Refs. [14,15] directly from the Landau theory. It provides a new perspective on the evolution of nuclear structure and gives new meaning to the earlier association of ^{134}Ba with the E(5) symmetry [9] (whose predictions for an infinite potential well are the analog of the IBM results close to the second-order phase-transitional point). In the new view ^{134}Ba is, in fact, the first example of a triple-point nucleus. Other candidates occur in the $A \approx 100$ mass region.

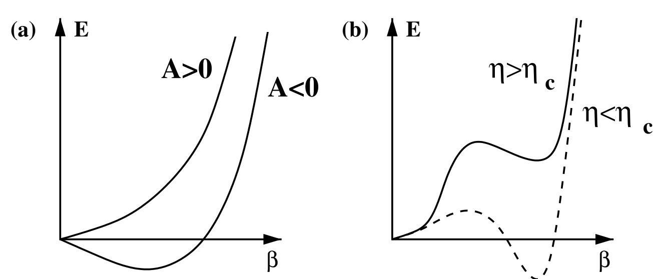

FIG. 2. Energy surfaces (in the $\gamma = 0$ plane) before and after the phase transition as a function of β for (a) second-order and (b) first-order phase transitions.

In conclusion, we have explained, using Landau theory of second-order (continuous) phase transitions, why the nuclei at low spin exhibit an isolated second-order phase transition and why they therefore exhibit two lines of first-order phase transitions meeting at the second-order transition. In agreement with the Landau theory, these transitions are between higher and lower symmetries (spherical and deformed) and between symmetries characterized by opposite signs of the order parameter (prolate and oblate). We stress that, although we have used the IBM, all these results are quite general for any collective model where the energy functional can be expanded as in Eq. (4). Thus, the classical results also apply to the quantum mechanical case. This study allows the definition of a triple point for nuclear shape transitions and suggests ^{134}Ba as the first example of a triple-point nucleus.

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