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Abstract. Phase transitions are often associated with the breaking of a symmetry in the low-temperature phase described by non-vanishing values of certain order parameters. However, in finite-size systems the correlated equilibrium configuration preserves the symmetries of the underlying Hamiltonian. We discuss a method to calculate the statistical distribution of the order parameters without breaking the corresponding symmetries. The maxima of these statistical distributions mimic the phase transitions that are found in a mean-field approximation. We demonstrate the method for the case of shape transitions in atomic nuclei.

INTRODUCTION

Phase transitions in bulk systems are often associated with the spontaneous breaking of certain symmetries. Such symmetry breaking is typical in a thermal mean-field approximation below a certain critical temperature. In Landau theory [1], the system is described by a set of order parameters that do not all vanish in the symmetry-breaking phase.

Strictly speaking, phase transitions do not occur in a finite-size system. Fluctuations in the order parameters smooth the singularities that characterize the phase transition. The exact equilibrium configuration of such a system possesses the same symmetries of the underlying Hamiltonian. Here we discuss a method to calculate the exact statistical distribution of the order parameters in a finite-size system within a symmetry-conserving framework. The main idea is based on a Landau-like expansion of the logarithm of this distribution in combinations of the order parameters that are invariant under the symmetries of the system. We demonstrate the method for the case of shape transitions in an isotopic chain of even-mass samarium nuclei $^{148-154}$Sm [2, 3, 4]. In the interacting boson model [5], the chain of samarium isotopes describes a shape transition between the spherical $U(5)$ and the axially deformed $SU(3)$ limits [6]. In a classification of critical symmetries of shape transitions, introduced by Iachello, ^{152}Sm is known as an $X(5)$ nucleus [7, 8], describing the critical point of the spherical to axially deformed transition.

MEAN-FIELD THEORY OF PHASE TRANSITIONS

The grand-canonical ensemble, describing the equilibrium density of a system at fixed temperature and chemical potential, is obtained from a variational principle in which the grand potential is minimized with respect to a variation of a general many-particle density operator. In a mean-field theory, such as the finite-temperature Hartree-Fock (HF) and the Hartree-Fock-Bogoliubov (HFB) approximations, the grand potential is minimized with respect to an uncorrelated trial density.

Landau theory is a mean-field theory in which the free energy a a given temperature is minimized with respect to a set of variables known as the order parameters. This theory describes a symmetry-breaking phase transition where the low-temperature phase is characterized by non-vanishing values of the order parameters. The free energy is

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invariant under the corresponding symmetries and can therefore be expanded in combinations of the order parameters that are invariants of the corresponding symmetries. Usually the expansion is carried out to the lowest order necessary to describe the phase transition of interest.

Landau theory of Shape Transitions

As an example, we briefly discuss a Landau theory of shape transitions in nuclei [9, 10].

Order Parameters

The order parameters are taken to be the mass quadrupole tensor $q_{2\mu}$, a second-rank tensor. Alternatively, we can use the quadrupole deformation parameters $\alpha_{2\mu}$ as the order parameters. They are related to $q_{2\mu}$ via the liquid drop relation $q_{2\mu} = \frac{3}{\sqrt{5\pi}} r_0^2 A^{5/3} \alpha_{2\mu}$, where A is the mass number of the nucleus and $r_0 = 1.2$ fm.

The transition from a spherical to a deformed nucleus breaks rotational symmetry. The higher symmetry phase describes a spherical nucleus $\alpha_{2\mu} = 0$, while the lower symmetry phase describes a deformed nucleus with $\alpha_{2\mu} \neq 0$. We define intrinsic quadrupole deformation parameters $\tilde{\alpha}_{2\mu}$ by a rotation to an intrinsic frame in which $\tilde{\alpha}_{21} = \tilde{\alpha}_{2-1} = 0$ and $\tilde{\alpha}_{22} = \tilde{\alpha}_{2-2} =$ real. The intrinsic deformation parameters β, γ are then defined by the standard relations

$$\tilde{\alpha}_{20} = \beta \cos\gamma \; ; \quad \tilde{\alpha}_{22} = \tilde{\alpha}_{2,-2} = \frac{1}{\sqrt{2}} \beta \sin\gamma \; . \tag{1}$$

The three rotation angles Ω together with β, γ characterize the intrinsic-frame variables. The free energy is a scalar and therefore is a function only of β, γ, i.e., $F(T, \alpha_{2\mu}) = F(T, \beta, \gamma)$.

Quadrupole Invariants

The free energy at temperature T can be expanded in invariant combinations of $\alpha_{2\mu}$, known as quadrupole invariants [11, 12]. There are two basic quadrupole invariants

$$\alpha \cdot \alpha = \beta^2 \; ; \quad [\alpha \times \alpha]_2 \cdot \alpha = -\sqrt{\frac{2}{7}} \beta^3 \cos(3\gamma) \; , \tag{2}$$

and all other invariants are of the form $(\beta^2)^m [\beta^3 \cos(3\gamma)]^n$, where $m, n \geq 0$ are integers.

Landau Expansion

In the Landau theory of shape transitions, we expand the free energy $F(T, \beta, \gamma)$ to fourth order in deformation [9, 10]. There are only three invariants β^2, $\beta^3 \cos(3\gamma)$, and β^4 to fourth order, and the free energy is given by

$$F(T, \beta, \gamma) = F_0(T) + A(T)\beta^2 + B(T)\beta^3 \cos(3\gamma) + C(T)\beta^4 \; , \tag{3}$$

where F_0, A, B, C are temperature-dependent constants.

The equilibrium shape at temperature T is determined by minimizing F with respect to β, γ. The topography of the free energy surface in the $\beta - \gamma$ plane depends on a single parameter $\tau = AC/B^2$ [9]. As a function of increasing τ, we find a first-order phase shape transition from a deformed nucleus for $\tau < 0$ to a spherical nucleus for $\tau > 9/32$. The region $0 < \tau < 9/32$ is a coexistence region with a first-order transition occurring for $\tau = 1/4$.

LANDAU-LIKE THEORY IN A SYMMETRY-CONSERVING FRAMEWORK

The Landau theory of shape transitions discussed in the previous section is valid in the thermodynamic limit. Rotational symmetry is spontaneously broken in the equilibrium configuration which is described by a non-vanishing deformation below a certain critical temperature. However, the nucleus is a finite-size system and the underlying symmetries are preserved in the exact equilibrium configuration. Here we describe a theory of deformation in which the underlying rotational symmetry is preserved.

We consider the distribution $P(T, \alpha_{2\mu})$ of the order parameters at temperature T. This distribution is invariant under rotations, and therefore depends only on the intrinsic shape parameters β, γ, i.e., $P(T, \alpha_{2\mu}) = P(T, \beta, \gamma)$. The volume element $\prod_\mu d\alpha_{2\mu}$ in the laboratory frame can be written in terms of the intrinsic parameters Ω, β, γ as $\prod_\mu d\alpha_{2\mu} = \frac{1}{2}\beta^4 |\sin(3\gamma)| \, d\beta \, d\gamma \, d\Omega$. Iintegrating over Ω, the distribution in β, γ is given by $4\pi^2 \beta^4 |\sin(3\gamma)| P(T, \beta, \gamma)$.

Landau-like Theory

The distribution $P(T, \alpha_{2\mu})$ is invariant under rotations, and therefore depends only on the quadrupole invariants. We expand the logarithm of $P(T, \beta, \gamma)$ in the quadrupole invariants to fourth order, leading to a distribution of the form [4]

$$P(T, \beta, \gamma) = \mathcal{N}(T) e^{-a(T)\beta^2 - b(T)\beta^3 \cos(3\gamma) - c(T)\beta^4} , \quad (4)$$

where a, b, c are temperature-dependent coefficients and $\mathcal{N}$ is a normalization constant.

The constants a, b, c can be determined from the expectation values of the three lowest-order invariants. Each of these invariants is unique at a given order and its expectation value can be related to corresponding moments of the axial quadrupole operator $\hat{Q}_{20}$ in the laboratory frame [2, 3]

$$\chi^2 \langle \beta^2 \rangle_L = 5 \langle \hat{Q}_{20}^2 \rangle ; \quad \chi^3 \langle \beta^3 \cos(3\gamma) \rangle_L = \frac{35}{2} \langle \hat{Q}_{20}^3 \rangle ; \quad \chi^4 \langle \beta^4 \rangle_L = \frac{35}{3} \langle \hat{Q}_{20}^4 \rangle . \quad (5)$$

where $\chi = \frac{3}{\sqrt{5\pi}} r_0^2 A^{5/3}$, and the expectation values

$$\langle f(\beta, \gamma) \rangle_L \equiv 4\pi^2 \int d\beta \, d\gamma \, \beta^4 | \sin(3\gamma) | f(\beta, \gamma) P(T, \beta, \gamma) . \quad (6)$$

are defined with respect to the Landau-like distribution $P(T, \beta, \gamma)$ in Eq. (4).

The coefficients a, b, c in Eq. (4) are determined from the moments $\langle \hat{Q}_{20}^n \rangle$ for $n = 2, 3, 4$ by solving Eqs. (5).

Distribution of the Axial Quadrupole in the Laboratory Frame

The axial quadrupole distribution $P(T, q_{20})$ of a nucleus with Hamiltonian $\hat{H}$ at temperature T is defined by

$$P(T, q_{20}) = \frac{1}{Z} \mathrm{Tr} \, [\delta(\hat{\mathrm{Q}}_{20} - \mathrm{q}_{20}) \mathrm{e}^{-\hat{\mathrm{H}}/\mathrm{T}}] , \quad (7)$$

where $Z = \mathrm{Tr} \, \mathrm{e}^{-\hat{\mathrm{H}}/\mathrm{T}}$ is the partition function.

The distribution in (7) can be calculated [2, 3] in the auxiliary-field quantum Monte Carlo (AFMC) method [13, 14, 15] using a discrete Fourier representation of the projection on the mass axial quadrupole operator $\hat{Q}_{20} = \sum_i [2\hat{z}_i^2 - (\hat{x}_i^2 + \hat{y}_i^2)]$ (the sum is over all nucleons), and a Hubbard-Stratonovich representation [16] of the Gibbs operator $e^{-\hat{H}/T}$ in Eq. (7).

We present results for the chain of even-mass samarium isotopes $^{148-154}$Sm using the framework of the configuration-interaction (CI) shell model. We assume a single-particle Woods-Saxon central potential with spin-orbit interaction and a two-body interactions with a monopole pairing term and multipole-multipole interaction that includes quadrupole, octupole and hexadecupole terms [17]. The single-particle model space and the various coupling parameters in the CI shell model Hamiltonian are given in Ref. [18].

In Fig. 1 we show distributions $P(T, q_{20})$ vs. the axial quadrupole deformation q_{20} for a chain of even-mass samarium isotopes $^{148-154}$Sm at several temperatures. For the nuclei that are deformed in their ground state in the HFB mean-field approximation, we find a skewed distribution at low temperatures with a crossover to a Gaussian-like distribution at high temperatures. For the nucleus ^{148}Sm whose HFB ground state is spherical, we find an almost Gaussian-like distribution already at low temperatures. The solid lines in the bottom row describe the lab-frame distribution of a rigid rotor whose intrinsic quadrupole moment is taken to be the ground state HFB quadrupole moment. They are qualitatively similar to the exact AFMC distributions. We conclude that the distribution of the axial quadrupole is a model-independent signature of deformation using a CI shell model framework that conserves rotational symmetry.

Validation of the Fourth-Order Landau-like Expansion

In deriving Eq. (4), the expansion of $\ln P$ in the quadrupole invariants was truncated in fourth order. To determine the validity of this assumption, we rewrite the distribution (4) in terms of the lab-frame components $\alpha_{2\mu}$

$$P(T, \alpha_{2\mu}) = \mathcal{N}(T) e^{-a(T)\alpha\cdot\alpha + b(T)\sqrt{\frac{7}{2}}[\alpha\times\alpha]_2\cdot\alpha - c(T)(\alpha\cdot\alpha)^2} , \quad (8)$$

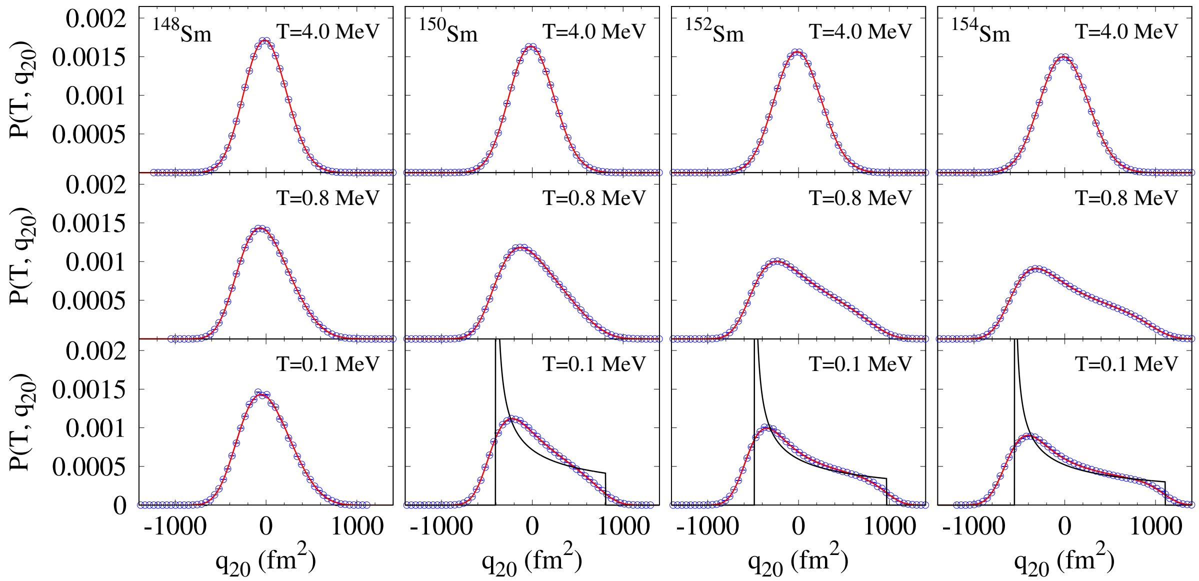

FIGURE 1. Axial quadrupole distributions $P(T, q_{20})$ for a chain of even-mass samarium isotopes $^{148-154}$Sm at several temperatures $T = 0.1$ MeV (bottom row), $T = 0.8$ MeV (middle row), and $T = 4$ MeV (top row). The distributions calculated with AFMC (open circles) are in excellent agreement with the marginal distributions calculated from the Landau-like distributions (4) (solid red lines). The solid black lines in the bottom row are the lab-frame distributions of a rigid rotor with an intrinsic quadrupole moment determined in the HFB approximation. Adapted from Ref. [3].

where we have used Eqs. (2). By integrating over $\alpha_{2\mu}$ for all four components with $\mu \neq 0$, we can find the marginal distribution $P(T, \alpha_{20})$, and compare it with the distribution of q_{20} calculated directly in AFMC. In Fig. 1, we compare the marginal distribution derived from the Landau-like distribution (4) (solid lines) with the distribution calculated directly in AFMC (solid circles). The excellent agreement confirms the validity of the fourth-order Landau expansion of $\ln P(T, \alpha_{2\mu})$.

QUADRUPOLE SHAPE DISTRIBUTIONS IN THE INTRINSIC FRAME

We used the AFMC axial quadrupole distributions to calculate the moments $\langle Q_{20}^n \rangle = \int dq_{20} q_{20}^n P(T, q_{20})$ for $n = 2, 3, 4$ and solved Eqs. (5) to determine the Landau coefficients a, b, c as a function of temperature. In Fig. 2, we show the distributions $P(T, \beta, \gamma)$ (using a logarithmic scale) in the $\beta - \gamma$ plane for the even-mass samarium isotopes $^{148-154}$Sm at the same temperatures as in Fig. 1.

The maxima of the distributions $P(T, \beta, \gamma)$ mimic the shape transitions that are usually observed in a mean-field approximation (e.g., HFB) but within the framework of the CI shell model that includes full correlations and preserves rotational symmetry. In the samarium isotopes for which these maxima at low temperatures is deformed, we observe as a function of increasing temperature a thermal shape transition from a deformed to a spherical configuration.

At the low temperature of $T = 0.1$ MeV (i.e., near the ground state), we observe shape transition from a spherical to a deformed configuration as the number of valence neutrons increases towards mid shell. Such ground-state transition occurring as a function a control parameter (here the number of neutrons) is known as a quantum shape transition. These transitions are qualitatively similar to what we find in the $T = 0$ HFB approximation: ^{148}Sm is spherical, ^{150}Sm has a small deformation while ^{154}Sm is strongly deformed. ^{152}Sm is known as an $X(5)$ nucleus [7, 8], at a critical point of a first-order shape transition from a spherical to an axially deformed nucleus.

As in the mean-field Landau theory, the topography of the distributions $P(T, \beta, \gamma)$ are determined by a single parameter $\tau = ac/b^2$. In Fig. 3 we show τ as a function of temperature for the four even-mass samarium isotopes. The maxima of these distributions describe a thermal shape transition at $\tau = 1/4$. This corresponds to transition temperatures of $T = 0.81$ MeV, $T = 1.03$ MeV, and $T = 1.29$ MeV in ^{150}Sm, ^{152}Sm and ^{154}Sm, respectively. The corresponding transition temperatures in HFB calculations are $T = 0.74$ MeV, $T = 0.94$ MeV, and $T = 1.10$ MeV [3].

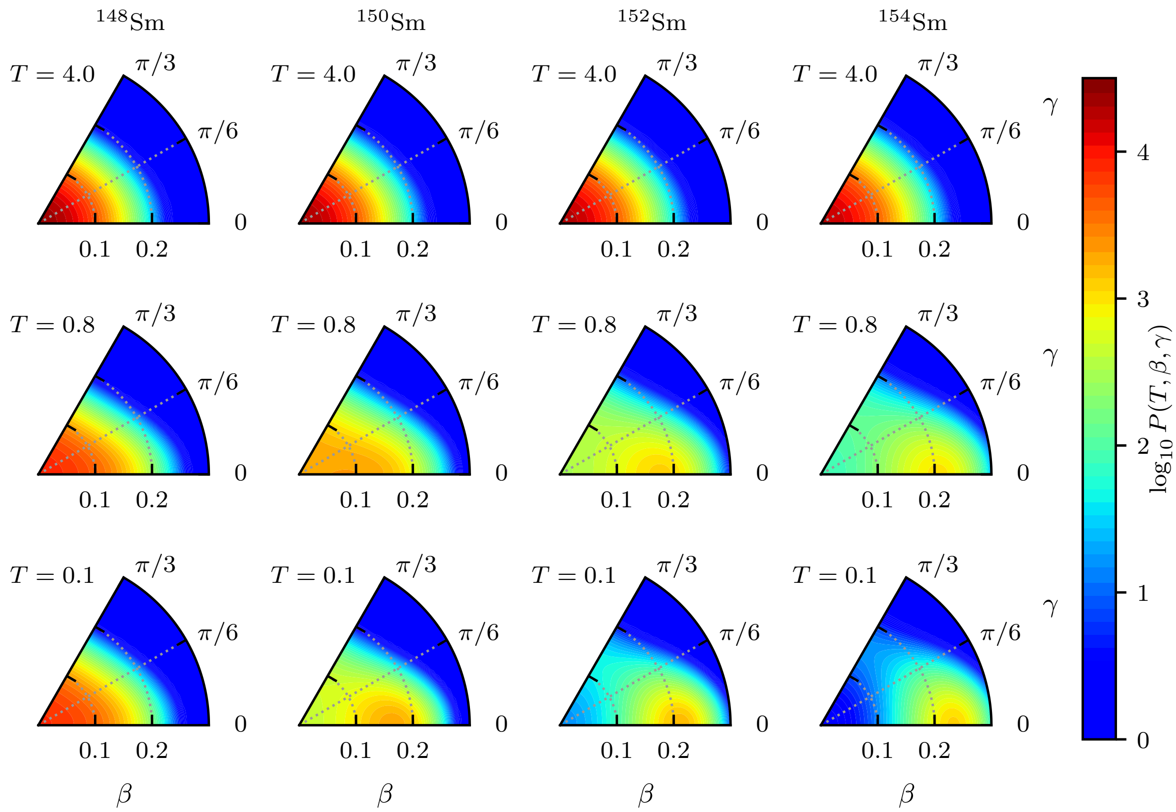

FIGURE 2. Quadrupole shape distributions $P(T,\beta,\gamma)$ in the $\beta-\gamma$ plane for the even-mass samarium isotopes $^{148-154}$Sm at the same temperatures as in Fig. 1. The maxima of these distributions mimic the thermal and quantum shape transitions that are usually found in a mean-field approximation. Adapted from Ref. [4].

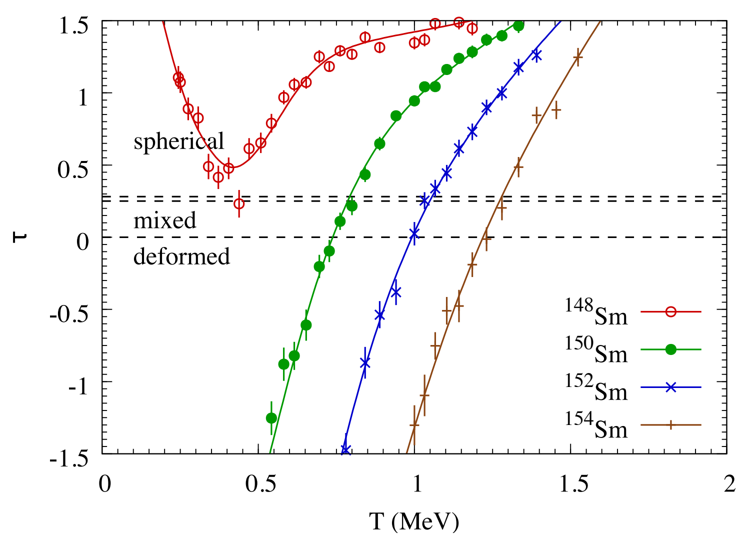

FIGURE 3. The parameter $\tau = ac/b^2$ characterizing the topography of the Landau-like distributions (4) as a function of temperature for the four even-mass samarium isotopes $^{148-154}$Sm. Taken from Ref. [4].

For ^{148}Sm, the parameter τ has a minimum as a function of temperature. This nucleus almost undergoes a shape transition around $T \sim 0.5$ MeV as the temperature decreases but this is prevented by the pairing interaction which favors a spherical configuration at lower temperatures.

CONCLUSION

We discussed a method to calculate the distribution of the order parameters in a finite-size system that undergoes a symmetry-breaking phase transition in the thermodynamic limit. Such a phase transition is usually found in a mean-field approximation, for which the equilibrium configuration breaks certain symmetries of the underlying Hamiltonian. Our method works in a framework that preserves the underlying symmetries. We demonstrated the method in the context of nuclear shape transitions. In particular, we calculated the quadrupole shape distributions in the intrinsic frame using the CI shell model approach without a mean-field approximation that breaks rotational symmetry. The results presented here are based on the AFMC approach for the CI shell model, but in principle our method can be used in the context of other approaches to the CI shell model or in other models that preserve rotational symmetry.

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