NUCLEAR DEFORMATION AND THE LANDAU THEORY OF PHASE TRANSITIONS WITH A SPATIALLY INHOMOGENEOUS ORDER PARAMETER

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To study the shape of deformed nucleus, Landau-type theory of phase transitions with a spatially inhomogeneous order parameter is used. The order parameter is an angular function that describes the deviation of the shape of the nucleus from sphericity. The equilibrium order parameter minimizes the Landau-type energy functional containing various powers of order parameter and its derivatives. Information about collective forces the competition and compromise of which lead to the appearance of various stable deformations of nuclei is extracted from the experimental data. Analysis reveals crucial role of higher derivatives of order parameter and its higher harmonics of modulation.

PACS: 21.60.−n, 21.60.Cs, 21.60.Ev, 27.30.+t

INTRODUCTION

The complex, multi-particle nature of nuclear forces makes nuclear physics a largely eclectic science: to understand different observable properties of nuclei, it is often necessary to use different concepts from different areas of physics (see, e.g., Refs. [1, 2] or any textbook on nuclear physics). And any new idea is always welcome.

So, to understand the origin of nuclear deformation, the concept of phase transitions and the Landau theory of phase transitions, proposed and well developed for condensed matter physics [3], turned out to be useful (see, e.g., review [4] and references therein). Indeed, the very fact of the appearance of a deformation of the nucleus shape caused by a change in, say, the number of nucleons in the nucleus can be considered as a result of phase transition from a high-symmetry (spherical) phase to a low-symmetry (deformed) phase of a nucleus. Thus, spontaneous breaking of rotational symmetry of a spherical nucleus can be accepted as an origin of nuclear deformation. The Landau theory of phase transitions is well suited for describing such shape phase transitions in a phenomenological language.

The currently known applications of the Landau theory to shape phase transitions suggest that the potential energy of the nucleus (in the form of thermodynamic potentials, Helmholtz free energy, Gibbs free energy, etc.) has the form of a polynomial from rotationally invariant combinations of quadrupole deformation parameters introduced by Bohr and Mottelson [5]. Such a polynomial is either the by-product of microscopic or semi-microscopic calculations (as, e.g., in the interacting boson and boson-fermion models), or is parameterized directly (as, e.g., in geometric collective models) [4]. The coefficients of the polynomial depend on the control parameter associated with the number of nucleons in the nucleus. Equilibrium deformation parameters minimize potential energy. A change in the control parameter leads to a transition from a spherical phase, for which the equilibrium deformation parameters are zero, to deformed phases, for which the equilibrium deformation parameters differ from zero. Following this recipe, interesting data were described and phase transitions of the first and second order were identified (see, e.g., reviews [6–8] and references therein).

The briefly mentioned applications of the Landau theory are based on the decomposition of the radius of a nucleus, which depends on spherical angles, into a series of spherical functions [5]. Thus, the potential energy of the nucleus contains collective forces that act on the deformation parameters, but not on the angular variables. Strictly speaking, to predict the equilibrium shape of the nucleus, the theory must contain angular derivatives of various orders.

Spatial derivatives naturally arise in the Landau-type theory of phase transitions with a spatially inhomogeneous order parameter (see, e.g., Ref. [9] or any textbook on phase transitions). This theory turned out to be very effective in describing phase transitions in ferroelectrics and magnetics with incommensurate phases (see, e.g., Refs. [9–14]). The latter are states in which the period of spatial modulation of the order parameter is not commensurate with (or does not depend on) the period of the crystal lattice. In this case, the Landau-type potential is a functional of the order parameter and its derivatives. The competition and compromise of different powers of the order parameter and its derivatives lead to the appearance of various stable spatially inhomogeneous states of the system.

Assuming that the characteristic size at which the angular function describing the deviation of the nucleus shape from sphericity changes significantly, is not commensurate with both the size of the nucleon and the distance between the nucleons, the deformed nucleus can be considered as an incommensurate phase. Therefore, the Landau-type theory of phase transitions with a spatially inhomogeneous order parameter can be used to study the shape of a deformed nucleus.

In what follows, the order parameter is an angular function that describes the deviation of the shape of the nucleus (or the shape of the equipotential surface of the self-consistent potential of the nucleus) from sphericity. The equilibrium order parameter minimizes the Landau-type energy functional containing various powers of the order parameter and its derivatives. The coefficients of the functional depend on the control parameter associated with the number and/or states (configurations) of nucleons in the nucleus. Information about collective forces (i.e., the content of the energy functional), the competition and compromise of which lead to the appearance of various stable deformations of nuclei both in the ground states and in low-lying single-particle exited states, is extracted from the data on the energies, spins, and parities of these states, and also the probabilities of electromagnetic transitions between them. For definiteness and simplicity, we demonstrate our approach in action for well-studied ^{25}Al nuclei [15, 16]. Data analysis reveals the crucial role of the higher derivatives of the order parameter and its higher harmonics of modulation (i.e., deformation multipolarities).

1. LANDAU-TYPE ENERGY FUNCTIONAL

To simplify the presentation, we restrict ourselves to the case of an axially symmetric nucleus with an additional symmetry plane perpendicular to the symmetry axis. In this case, the Landau-type order parameter is a function of a single variable, the polar angle θ, $\theta\in[0,\pi/2]$. The Landau-type energy functional must contain various powers of the order parameter and its angular derivatives:

$$\Phi[\varphi] = \Phi_0 + \int_0^{\pi/2} d\theta \sin\theta \left[\sum_{n=1}^{N} \alpha_{2n}\varphi^{2n} + \sum_{m=1}^{M} \sum_{l=1}^{L} \beta_{m,l}\varphi^{(m)l} \right], \quad (1)$$

where $\varphi\equiv\varphi(\theta)$ is the order parameter and $\varphi^{(m),l}\equiv(d^m\varphi/d\theta^m)^l$. The necessary boundary conditions are: $d\varphi/d\theta\equiv 0$ at the points $\theta=0$ and $\theta=\pi/2$. Φ_0 corresponds to a spherical nucleus with $\varphi=0$. The first term in braces of Eq. (1) is the expansion, which in the original Landau theory guarantees the appearance of states with $\varphi=\pm\text{const}\neq 0$. To ensure that only the state with $\varphi=0$ corresponds to a spherical nucleus, we require that all parameters from the set $\{\alpha_{2n}\}$ be positive. Then the first term in braces of Eq. (1) describes the forces that retain (or restore) the spherical symmetry of the nucleus. The second term in braces of Eq. (1) is an expansion containing different powers of derivatives of different orders of the order parameter. Then this term describes the forces that violate the spherical symmetry of the nucleus. To eliminate the appearance of high-frequency modulations of the order parameter (that is, large deformation multipolarities), we require that L be even and $\beta_{\mu,L}>0$, where μ is the number for which $\mu L>ml$ for any $m\neq\mu$ and $l\neq L$. If necessary, the expansion in $\varphi^i\varphi^{(j)p}$ with i,j,p=1,2,3... can also be included in Eq. (1).

The equilibrium order parameter must minimize the functional (1). To solve this variational problem, we can use an evolutionary algorithm [17] that evolves a population of numerical solutions of the variational problem (see also Ref. [18]). Evolved solutions are model-independent, smooth, can have a given shape (if necessary), and satisfy the boundary or any other additional conditions (if they are superimposed). At the same time, the content of the functional (1) and the boundary conditions suggest a suitable form of a variational solution:

$$\varphi(\theta) = \sum_{k=0}^{\infty} \varphi_{2k} \cos(2k\theta), \quad (2)$$

whose parameters are determined by minimizing the functional (1) with respect to them. Note that this decomposition is equivalent to the widely used decomposition of the radius of an axially symmetric nucleus into a series of spherical harmonics (see, e.g., Ref. [5]). But in the case of functional (1), this decomposition naturally arises as a result of competition and compromise between collective forces represented by different powers of the order parameter and its derivatives, and the specific boundary conditions.

The values of the parameters α_{2n} and $\beta_{m,l}$ are determined from the analysis of experimental data. In general, the search process consists of two levels. On the first of them, for a given set $\{\alpha_{2n},\beta_{m,l}\}$ we are looking for a set $\{\varphi_{2k}\}$ that minimizes the functional (1). On the second level, we are looking for a set $\{\alpha_{2n},\beta_{m,l}\}$ (and the corresponding equilibrium set $\{\varphi_{2k}\}$) that minimizes the deviation between the calculated observables and the measured data. The method of multi-level optimization using a genetic algorithm specifically designed for this case is presented in Ref. [14]. After the parameters $\{\alpha_{2n},\beta_{m,l},\varphi_{2k}\}$ with which the data is replicated are found, those whose role in the fitting is overvalued should be removed. As a result, only those forces remain in the functional (1) and those harmonics in the decomposition (2) that are necessary and sufficient to fit the data.

In fact, all of the parameters $\{\alpha_{2n},\beta_{m,l}\}$ may depend on the nucleon configuration, i.e., the number and/or states of nucleons in the nucleus (the so-called control parameter; see, e.g., Ref. [4]). Therefore, we must additionally determine which parameters (forces) should depend on the configuration in order to fit the data.

2. DEFORMED-SHELL MODEL

Currently, the dynamics of nuclear shape caused by a change in the number of nucleons in the nucleus is mainly studied (see, e.g., review [4] and references therein). However, the same nucleus in different single-particle states also has different shapes. Regardless of the method of calculation, the shape of the nucleus in the single-particle state strongly influences its wave function. The wave functions of the initial and final states of the nucleus largely determine the probability of an electromagnetic transition between them. Therefore, the experimentally observed probabilities of electromagnetic transitions are a valuable source of information about the shape of the nucleus in various single-particle states.

To preserve the simplicity of the presentation, we chose an axially symmetric single-particle harmonic-oscillator potential with an additional symmetry plane perpendicular to the symmetry axis and the spin-orbit interaction (see, e.g., Refs. [19]). Making a direct generalization, we write the single-particle Hamiltonian in the form [20]:

$$H = \hbar\omega(H_0 + H_1),\ H_0 = \left(-\Delta + r^2\right)/2\ ,$$
$$H_1 = -r^2\varphi(\theta)/2 - 2\kappa(\mathbf{l}\cdot\mathbf{s})[1-\varphi(\theta)], \qquad (3)$$

where r is the reduced coordinate; $1\big/\sqrt{1-\varphi(\theta)}$ is the reduced radius of the equipotential surface of the nuclear potential; θ is the polar angle, $\theta \in [0;\pi/2]$; $\varphi(\theta)$ is the function that describes the shape of the equipotential surface, $\varphi(\pi-\theta) \equiv \varphi(\theta)$, $d\varphi/d\theta \equiv 0$ at the points $\theta = 0$ and $\theta = \pi/2$; $r^2\varphi(\theta)$ is the coupling of the particle with the symmetry axis; $(\mathbf{l}\cdot\mathbf{s})$ is the spin-orbit interaction; $(\mathbf{l}\cdot\mathbf{s})\varphi(\theta)$ is the coupling of the spin-orbit interaction with the symmetry axis; $\hbar\omega = 41A^{-1/3}(1+\varepsilon)$ MeV is the energy scale; $A = N + Z$ is the nucleus mass number; N and Z are the numbers of neutrons and protons in the nucleus; ε takes into account the deviation of the energy scale from its simple estimate.

The Hamiltonian (3) is diagonalized in the basis of the spherical harmonic oscillator (see Ref. [19] < for details). The single-particle wave function of the nucleus in a certain state is the Slater determinant constructed from the occupied single-particle states calculated using the Hamiltonian (3).

The explicite expressions for the reduced electric and magnetic multipole transition probabilities between the initial and final single-particle states are presented in Ref. [20].

3. DEFORMATION FORCES IN SINGLE-PARTICLE STATES

The following Landau-type energy functional in tandem with the deformed-shell model (3) allowed us to reproduce the experimentally measured data [15, 16] on the energies, spins, and parities of the low-lying single-particle states and the probabilities of electromagnetic transitions between them in ^{25}Al nuclei:

$$\Phi[\varphi] = \Phi_0 + C\int_0^{\pi/2} d\theta \sin\theta \left[\xi\varphi^{(2)4} + \eta\varphi^{(6)}\right.$$
$$\left. + \delta\varphi^{(4)} + \gamma\varphi^{(2)} + \alpha\varphi^2 + \varphi^4\right], \qquad (4)$$

where *C, ξ, α*>0 and *η, δ, γ* depend on the configuration of the nucleons. The variational solution for the functional (4) has the form:

$$\varphi(\theta) = \sum_{k=0}^{3}\varphi_{2k}\cos(2k\theta)\,. \qquad (5$$

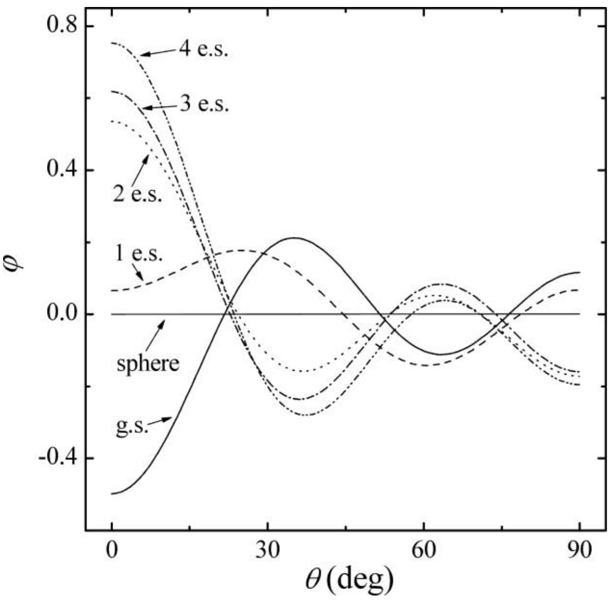
The schemes of occupation of single-particle states by protons (proton configurations) in the ground (g.s.) and first four single-particle excited states (1–4 e.s.) of the nucleus were chosen as follows:

g.s.	2	2	2	2	2	2	1	0	0	0	0
1 e.s.	2	2	2	2	2	2	0	1	0	0	0
2 e.s.	2	2	2	2	2	2	0	0	1	0	0
3 e.s.	2	2	2	2	2	2	0	0	0	0	1
4 e.s.	2	2	2	2	2	1	2	0	0	0	0

The schemes of occupation of single-particle states by neutrons (neutron configurations) were chosen to be independent of the nucleus state:

2 2 2 2 2 2 0 0 0 0 0

We have achieved very good consistency between the calculated and measured observables for the ^{25}Al nucleus. Figure shows the dynamics of the order parameter $\varphi(\theta)$ caused by the changes in the configuration of nucleons. Table contains the values of parameters of the variational solution (5).



Dynamics of the order parameter φ(θ) caused by the changes in the configuration of nucleons in ^{25}Al *nuclei. Curves with the words "sphere", g.s., and 1–4 e.s. correspond to the spherical state, the ground state, and 1-4 single-particle excited states, respectively*

According to our basic assumption, all forces that directly or indirectly affect the shape of the ^{25}Al nucleus and are necessary and sufficient to explain the experimental data are contained in functional (4) in the form of polynomials in $\varphi(\theta)$ and its angular derivatives. So, e.g., pairing (long-range) correlations that retain (or restore) the spherical shape of the nucleus are taken into account by the terms φ^2 and φ^4, quadrupole-quadrupole and more complex (short-range) correlations that violate the spherical shape contribute to the terms $\varphi^{(2)}$, $\varphi^{(4)}$, and $\varphi^{(6)}$, and correlations that limit the deformation multipolarity are modeled using the term $\varphi^{(2)4}$.

The appearance of higher derivatives in the functional (4) leads to the appearance of higher harmonics of modulation of the equilibrium order parameter (see Figure) and higher multipolarities of deformation of the equipotential surface of the single-particle harmonic oscillator.

Values of the parameters of the variational solution (5). The ground and four excited states are indicated by g.s. and 1–4 e.s.

	g.s.	1 e.s	2 e.s.	3 e.s.	4 e.s.
$\varphi_0(10^{-2})$	-3.763	2.988	3.950	3.931	3.416
$\varphi_2(10^{-1})$	-1.108	1.013	1.821	1.732	2.415
$\varphi_4(10^{-1})$	-1.533	0.368	1.422	1.904	2.449
$\varphi_6(10^{-1})$	-1.962	-1.025	1.713	2.157	2.325

It is usually assumed that quadrupole deformations are of the most importance, while hexadecupole deformations are good corrections to quadrupole deformations and may be important for describing the ground states of heavy nuclei (see, e.g., Refs. [1, 2] or any textbook on nuclear physics). As for the higher multipolarity deformations, they are not considered to have much physical significance especially for light and medium nuclei.

Contrary to this, our study shows that the fourth $\cos(4\theta)$ and sixth $\cos(6\theta)$ harmonics of modulation in Eq. (5), which correspond to hexadecapole λ=4 and hexacontatetrapole λ=6 multipolarity deformations, can play an equally important role as quadrupole deformation in explaining the experimental data for 1d2s-shell nuclei (see Figure and Table). In this case, the usual prolate and oblate shapes of the nucleus can no longer be identified.

The energy surfaces of the functional (4) in the space $\{\varphi_{2k}\}$ are determined by the values of the parameters (η,δ, and γ) depending on the configuration of the nucleons. For arbitrary values of η, δ, and γ, the energy surface is unique and has a unique minimum. When $\eta=\delta=\gamma=0$, the equilibrium order parameter is $\varphi(\theta)=0$, i.e., the shape is spherical. The phase diagram is very simple: the spherical phase exists in an isolated point, surrounded by a continuous deformed phase, and the transition from the spherical phase to the deformed phase is smooth, i.e., of the second order.

Looking at Table, one might think that our model has an excessive number of parameters to fit a very limited set of experimental data. But, as emphasized in Ref. [2], the belief that "anything can be fitted with a sufficient number of parameters", however, also oversimplifies the situation, because the data are usually strongly correlated. With this in mind, we conducted an extensive numerical study of our model and concluded that the set of fitting parameters given in Tables is necessary, sufficient, and unique in the sense that is usually assumed when the evolutionary algorithm is used as a key component of the fitting procedure (as in our case).

As indicated in Ref. [18], evolutionary algorithms, as a rule, represent a method of global optimization, which, however, cannot guarantee that the optimum found is global. Therefore, we must perform the procedure several times. In addition, it is impossible to know in advance what the minimum value of the objective function will be. Thus, it is useful to follow the dynamics of the best, worst and average values of the objective function and the standard deviation from the average value in the population during these several runs of the procedure. Such monitoring usually helps to localize the region of potentially low values of the objective function.

4. SUMMARY

The Landau-type theory of phase transitions with a spatially inhomogeneous order parameter has been applied to study the shape of a deformed nucleus.

In this application, the order parameter is an angular function that describes the deviation of the shape of the nucleus (or the shape of the equipotential surface of the self-consistent potential of the nucleus) from sphericity. The equilibrium order parameter minimizes the Landau-type energy functional containing various powers of the order parameter and its derivatives. The coefficients of the functional depend on the control parameter associated with the number and/or states (configurations) of nucleons in the nucleus. The modulation period of the order parameter is not commensurate with both the size of the nucleon and the distance between the nucleons.

Information about collective forces (i.e., the content of the energy functional), the competition and compromise of which lead to the appearance of various stable deformations of the nuclei both in the ground states and in low-lying single-particle exited states, is extracted from the data on the energies, spins, and parities of these states, and also the probabilities of electromagnetic transitions between them in well-studied ^{25}Al nuclei. Data analysis reveals the crucial role of the higher derivatives of the order parameter and its higher harmonics of modulation (i.e., deformation multipolarities).

If the analyses of experimental data requires, our approach can be generalized to the case when the order parameter is a function of both polar and azimuth angles.

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ЯДЕРНА ДЕФОРМАЦІЯ І ТЕОРІЯ ЛАНДАУ ФАЗОВИХ ПЕРЕХОДІВ ІЗ ПРОСТОРОВО НЕОДНОРІДНИМ ПАРАМЕТРОМ ПОРЯДКУ

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Для вивчення форми деформованого ядра використовується теорія фазових переходів типу Ландау з просторово неоднорідним параметром порядку. Параметр порядку – це кутова функція, яка описує відхилення форми ядра від сферичності. Рівноважний параметр порядку мінімізує функціонал енергії типу Ландау, що містить різні степені параметра порядку та його похідних. Інформація про колективні сили, конкуренція та компроміс яких призводять до появи різних стабільних деформацій ядер, визначається з експериментальних даних. Аналіз доводить вирішальну роль вищих похідних параметра порядку та його вищих гармонік модуляції.