

First order shape transition and critical point nuclei in Sm isotopes from relativistic mean field approach (Postprint)

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Date: 2017-08-22T00:00:00+00:00

Abstract

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Full Text

Preamble

First Order Shape Transition and Critical Point Nuclei in Sm Isotopes from Relativistic Mean Field Approach

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(Dated: August 1, 2017)

The critical point nuclei in Sm isotopes, which mark the first-order phase transition between spherical U(5) and axially deformed SU(3) shapes, have been investigated using the microscopic quadrupole-constrained relativistic mean field (RMF) model plus BCS method with all the most commonly used interactions: NL1, NL3, NLSH, and TM1. The calculated potential energy surfaces show a clear shape transition for the even-even Sm isotopes with $N = 82-96$, and the critical point nuclei are found to be ^{144}Sm , ^{146}Sm , and ^{148}Sm . Similar conclusions can also be drawn from the microscopic neutron and proton single-particle spectra.

PACS numbers: 21.10-k, 21.60.Jz, 21.60.Fw, 21.10.Re

The equilibrium shapes of finite many-body systems such as nuclei, atoms, and molecules have been a topic of intense interest for several decades. These shapes are typically not rigid and evolve as a function of their constituent particles. Sometimes these changes can be quite abrupt, exhibiting phase transitional and critical point behavior analogous to that found in a wide variety of many-body systems, although the concepts of phase transitions are only approximate for finite systems. Properties of the system in the transition region and, in particular, at the critical point can be obtained by numerically solving the eigenvalue problem for the Hamiltonian. However, transition regions are difficult to interpret because they exhibit a complicated interplay of competing degrees of freedom. Yet such systems are in many respects the most important, as their structure defines the nature of the transition region itself.

Recently, the concept of critical point solutions has been introduced in the framework of algebraic models, in which different shapes (phases) correspond to dynamical symmetries of some algebraic structure G , and the phase transition corresponds to the breaking of these dynamical symmetries. In the Interacting Boson Model [?], $G = U(6)$ and there are three dynamical symmetries characterized by the first algebra in the chain originating from $U(6)$: namely $U(5)$, $SU(3)$, and $SO(6)$, corresponding to spherical, axially deformed, and γ -unstable shapes, respectively. Experimental examples of all three types of symmetries can be found in nuclei: $U(5)$ nuclei occur near closed shells, $SU(3)$ nuclei appear in the middle of shells, and the $O(6)$ limit tends to occur in nuclei with particle-hole configurations. The phase transition between spherical $U(5)$ and axially deformed $SU(3)$ shapes is first order [?, ?]. The phase/shape transition region is characterized by pronounced γ -softness [?]. This characteristic led to an analytic solution for critical point nuclei, called $X(5)$ for the axially symmetric case, which is based on analytic solutions of the Schrödinger equation corresponding to a geometric (Bohr) Hamiltonian with a square-well potential [?]. It has been shown that ^{148}Sm [?] and other $N = 90$ isotones [?] represent the first empirical manifestation of the predicted nuclei at the critical point of the vibrator (spherical shape) to axial rotor (axially deformed shape) phase transition.

Critical-point symmetries provide a classification of states and analytic expressions for observables in regions where the structure changes most rapidly. These ideas can be visualized in terms of two coexisting potentials—spherical and de-

formed—whose energy separation varies with nucleon number. Although phase transitions and critical points have been discussed in atomic nuclei for many years, there have been no microscopic investigations to date. As an important complementary approach, a microscopic study could be very helpful for understanding where and how nuclei exhibiting structures close to these symmetries occur. The main purpose of this Letter is to close this gap in the study of symmetry. The relativistic mean field (RMF) theory [?] has received wide attention due to its successful description of many nuclear phenomena in recent years [?]. In particular, exotic halo phenomena can be understood self-consistently in this microscopic model after proper treatment of continuum effects [?, ?, ?]. Here we discuss the realization of the critical point concept in atomic nuclei using microscopic quadrupole-constrained RMF theory with pairing treated by the BCS method, which will show that ^{116}Xe , ^{124}Ba , ^{132}Xe are excellent empirical manifestations of this critical point structure.

The basic ansatz of RMF theory is a Lagrangian density where nucleons are described as Dirac particles that interact via the exchange of various mesons including the isoscalar-scalar meson, the isoscalar-vector meson, and the isovector-vector meson. The effective Lagrangian density considered is written in the form:

$$\mathcal{L} = \bar{\psi}_i(i\gamma^\mu\partial_\mu - M)\psi_i + \frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2 - g_\sigma\bar{\psi}_i\sigma\psi_i - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_\omega^2\omega^\mu\omega_\mu - g_\omega\bar{\psi}_i\gamma^\mu\omega_\mu\psi_i - \frac{1}{4}\vec{R}^{\mu\nu}\cdot\vec{R}_{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^\mu\cdot\vec{\rho}_\mu$$

where $\bar{\psi} = \psi^\dagger\gamma^0$ and ψ is the Dirac spinor. Other symbols have their usual meanings.

The Dirac equation for the nucleons and the Klein-Gordon type equations for the mesons and the photon are obtained from the variational principle and can be solved by expanding the wavefunctions in terms of the eigenfunctions of a deformed axially symmetric harmonic-oscillator potential [?] or a Woods-Saxon potential [?]. Further details can be found in Ref. [?] and references therein.

The potential energy curve can be calculated microscopically by constrained RMF theory. The binding energy at a certain deformation value is obtained by constraining the quadrupole moment to a given value μ_2 in the expectation value of the Hamiltonian:

$$\langle H \rangle + C_q(\langle \hat{Q}_2 \rangle - \mu_2)^2,$$

where C_q is the constraint multiplier.

For the nuclei studied in this paper, the full $N = 20$ deformed harmonic oscillator shells are taken into account and the convergence of the numerical calculation on the binding energy and deformation is very good. The converged deformations corresponding to different μ_2 values are not sensitive to the deformation

parameter β_0 of the harmonic oscillator basis in a reasonable range due to the large basis. Different choices of β_0 lead to different iteration numbers in the self-consistent calculation and different computational time costs, but physical quantities such as binding energy and deformation change very little. Thus the deformation parameter β_0 of the harmonic oscillator basis is chosen near the expected deformation to obtain high accuracy with low computational cost. By varying μ_2 , the binding energy at different deformations can be obtained. Pairing is treated using the constant gap approximation (BCS) in which the pairing gap is taken as $\Delta = 12/\sqrt{A}$ MeV for even-even nuclei.

[TABLE I]

The binding energies and quadrupole deformations for the ground states are listed in Table I from constrained RMF theory with the NL1 [?], NLSH [?], TM1 [?], and NL3 [?] parameter sets. For the binding energies, the data are well reproduced within 0.5%. Particularly for NL3, excellent agreement (within 1 MeV) is observed for the binding energy in ^{1-1}Sm . Even for the neutron magic nucleus ^{1-1}Sm , the difference between the RMF calculation and the data is less than 3 MeV, i.e., relatively less than 0.3%. The spherical shapes in ^{1-1}Sm and the weakly deformed ^{1-1}Sm are well reproduced. The deformations in ^{1-1}Sm are slightly overestimated by the theoretical calculations. In general, the data are well reproduced by constrained RMF theory.

Figures 1, 2, 3, and 4 show the potential energy curves for ^{1-1}Sm from constrained RMF theory with NL1, NL3, NLSH, and TM1 parameters, where the energy for the ground state is taken as a reference. Similar patterns are found for all parameter sets. The ground state of ^{1-1}Sm is found to be spherical and has about a 12 MeV stiff barrier against deformation. Although the ground state of ^{1-1}Sm is still spherical, its barrier becomes around 8 MeV against deformation. With increasing neutron number, the ground state gradually moves toward the deformed side and the potential energy curve becomes softer. Finally, well-deformed ^{1-1}Sm are observed.

To examine how the shape of the Sm isotopes changes with neutron number, the differences in binding energy between the ground state and the spherical state for Sm isotopes are presented in Table II from constrained RMF theory with the NL1, NL3, NLSH, and TM1 parameter sets. These differences indicate how soft the nucleus is against deformation and may provide insight into the nuclear shape phase transition. From ^{1-1}Sm , the energy differences between the ground state and the spherical shape change from 0 to 15 MeV. There are two jumps in the energy differences: the first appears at ^{1-1}Sm and the second at ^{1-1}Sm , which suggests the shape transition from spherical to critical point nuclei, and finally to axially deformed nuclei. The potential energy curves for ^{1-1}Sm , ^{1-1}Sm , and ^{1-1}Sm are relatively flat, i.e., they are β -soft nuclei in the transition between spherical and axially symmetric deformed nuclei.

One of the merits of microscopic nuclear models such as RMF theory is that they can provide detailed information on single-particle levels, shell structure,

etc., which are very important for discussing nuclear structure and examining the deformation-driving effect. In Fig. 5 [Figure 5: see original paper] and Fig. 6 [Figure 6: see original paper], the single neutron and proton levels for ^{1-1}Sm lying between 0–15 MeV are shown, respectively. The Fermi levels are indicated by dashed lines. These figures present results calculated with the TM1 parameter set; the other three parameter sets give similar single-particle structure and are therefore not presented here.

From Figs. 5 and 6, one finds consistency between the shell structure evolution and the shape evolution in Sm isotopes with increasing neutron number. For ^{1-1}Sm , spherical symmetry is better restored. The deformation develops with increasing N. The deformation in ^{1-1}Sm is still small and the energy gap with $N = 82$ can be clearly seen from the single-particle spectra. The nuclei ^{1-1}Sm belong to a transition region where the $N = 82$ gaps still exist but are much smaller than in ^{1-1}Sm . Starting from ^{1-1}Sm , the gap with $N = 82$ disappears. Meanwhile, a deformed gap for $Z = 62$ develops, as does that for $N = 94$. Correspondingly, we observe the well-deformed ^{1-1}Sm .

In summary, the shape transition between spherical and axially deformed nuclei in ^{1-1}Sm has been investigated using microscopic quadrupole-constrained relativistic mean field theory with all the most commonly used interactions: NL1, NL3, NLSH, and TM1. The RMF calculations reproduce the ground-state binding energy and deformation data very well. By examining the potential energy curves and single-particle levels obtained from this microscopic approach, ^{1-1}Sm , ^{1-1}Sm , and ^{1-2}Sm are found to be soft against deformation and are identified as critical point candidate nuclei, marking the first-order phase transition between spherical U(5) and axially deformed SU(3) shapes.

We thank Victor Zamfir for helpful discussions and useful comments. This work was partly supported by the Major State Basic Research Development Program under Contract Number G2000077407 and the National Natural Science Foundation of China under Grant Nos. 10025522, 10221003, and 10047001.

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