

Ground States of Odd-mass Nuclei in Nuclear Density-functional Theory under a Time-odd External Field

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Nuclear density-functional theory (DFT) is a microscopic framework that provides crucial nuclear data for astrophysical simulations out of experimentalists' reach. Only a few studies, however, have been done on odd-mass nuclei, though they occupy three-quarters of the nuclear chart. Nuclear superfluidity makes the treatment of odd-mass nuclei different from that of even-even nuclei. Proposed is a novel method to describe the ground state of odd-mass nuclei in a similar way to even-even ones as the lowest energy state under an appropriate external field. We apply this method to the neutron-rich Mg isotopes and show it produces the unique property, deformed halo structure, of ³⁷Mg.

KEYWORDS: Density functional theory, Superfluidity and deformation, Nuclear data

1. Introduction

As a microscopic input for astrophysical simulations, desired are highly accurate and reliable nuclear data for thousands of nuclides. For exotic nuclei those are not accessible experimentally, one should rely on a microscopic calculation. Density functional theory (DFT) is an approach that describes ground-state properties of quantum many-body systems such as atomic nuclei in terms of the particle density. Since the computational cost does not depend on the number of constituent nucleons, it can be applied to light, medium-mass, heavy, and superheavy nuclei in principle. In practice, however, there have been few DFT studies on odd-mass nuclei, while the nature of even-even nuclei has been studied a lot. This is because the conventional description of odd-mass nuclei in DFT is complicated. We propose a new method to describe odd-mass nuclei with the same procedure as for even-even ones in the framework of DFT.

2. Basics of DFT for describing superfluid systems

Superfluidity of nuclei is a key to the nuclear structure. A method that can explicitly deal with the superfluidity in DFT is known as the Hartree-Fock-Bogoliubov (HFB) method in nuclear physics. The heart of HFB arrives at solving the eigenvalue equation, which can be written in a matrix form as [1]

$$\begin{pmatrix} h - \lambda I & \Delta \\ -\Delta^* & -h^* + \lambda I \end{pmatrix} \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \quad (1)$$

where E is a diagonal matrix ordering the eigenvalues, and both the single-particle Hamiltonian h and the pair potential Δ are square matrixes with the dimension of the single-particle configuration space, λ is the chemical potential, and I is the identity matrix. Since h and Δ include the information of the solution U_k, V_k , the HFB equation (1) is a nonlinear equation, which can be solved iteratively. Note that when $(U_k \ V_k)^T$ is an eigenvector with an eigenvalue E_k , $(V_k^* \ U_k^*)^T$ is also an eigenvector with an

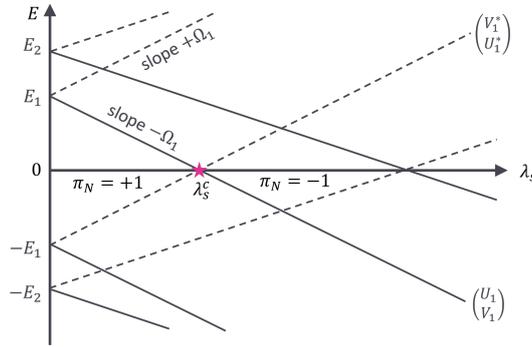


Fig. 1. Single-particle energy levels under an external field $-\lambda_s S$. Solid and dashed lines represent $(U_k V_k)^T$ and $(V_k^* U_k^*)^T$ orbits, respectively. When $\lambda_s < \lambda_s^c$, the number parity of the ground state is even, and if $\lambda_s > \lambda_s^c$, the orbits $(U_1 V_1)^T$ and $(V_1^* U_1^*)^T$ are automatically swapped leading to the number parity odd.

eigenvalue $-E_k$. The ground state wave function of the many-body system in the HFB method, or the HFB vacuum, $|\Phi\rangle$ can be explicitly written as [1]

$$|\Phi\rangle = \prod_{i=1}^{N_1} c_i^\dagger \prod_{p=1}^{N_2} (u_p + v_p c_p^\dagger c_p^\dagger) |0\rangle. \quad (2)$$

Here $|0\rangle$ is the (true) vacuum state defined as $c_i |0\rangle = 0$, with c_i (c_i^\dagger) being the single-particle annihilation (creation) operator. The state $|\Phi\rangle$ is a linear superposition of components with different particle numbers. While the particle number is not conserved, the parity of the particle number, or the *number parity* $\pi_N = (-1)^{N_1}$, is conserved [1]. In other words, the HFB vacuum $|\Phi\rangle$ consists of states with either even or odd particle number depending on whether N_1 is even or odd. It is evident that a wave function $|\Phi\rangle$ with even number parity can only describe a system with even particle number, and vice versa. The unitary matrix

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad (3)$$

has all the information about $|\Phi\rangle$, and one finds $\det \mathcal{W} = (-1)^{N_1} = \pi_N$. This means if $\det \mathcal{W} = +1$, then $|\Phi\rangle$ is a superposition of even-particle-number states, and if $\det \mathcal{W} = -1$, $|\Phi\rangle$ is a superposition of odd-particle-number states. For systems with the time-reversal symmetry, it turns out that $\det \mathcal{W}$ is always +1 because of the Kramerse degeneracy. In other words, the ground state of a system with the time-reversal symmetry includes the even-particle-number states only.

3. Method for describing the odd-mass nuclei in HFB

If one wants to solve the HFB equation for odd-mass nuclei or odd-number-parity states, one starts conventionally the calculation for the neighboring even-even nuclei, whose number parity is +1, or $\det \mathcal{W} = +1$. One can get such an even-number-parity state easily as the lowest energy state in a system with the time-reversal symmetry. Swapping columns of the matrix \mathcal{W} gives a new matrix \mathcal{W}' that satisfies $\det \mathcal{W}' = -1$. The state represented by \mathcal{W}' is the very state one wants. This procedure looks simple, but practically it takes a lot of trouble. One has to select the appropriate one-particle orbit and interchange the corresponding columns in each step of the iteration. Since one has more involved procedures for describing odd-mass nuclei than for even-even ones, existing HFB codes for even-even nuclei need to be drastically modified to apply to odd-mass nuclei.

A new method we propose describes odd-mass nuclei as the ground state under an appropriate external field which breaks the time-reversal symmetry. Breaking the time-reversal symmetry from the beginning, we can get the ground states of odd-mass nuclei in the same way as for even-even nuclei. The idea of obtaining odd-mass nuclei by imposing a constraint was originally proposed by Bertsch *et al.* [2]. The x -signature was considered for the constraint [2]. We generalize this idea and encapsulate the essential point: Assuming a system under an external field proportional to S which has time-odd character, $TST^{-1} = -S$, the single-particle Hamiltonian h becomes $h' = h - \lambda_s S$, where λ_s is a parameter. The HFB equation under such an external field is written as follows:

$$\left[\begin{pmatrix} h - \lambda I & \Delta \\ -\Delta^* & -h^* + \lambda I \end{pmatrix} - \lambda_s \begin{pmatrix} S & 0 \\ 0 & -S^* \end{pmatrix} \right] \begin{pmatrix} U' & V'^* \\ V' & U'^* \end{pmatrix} = \begin{pmatrix} U' & V'^* \\ V' & U'^* \end{pmatrix} \begin{pmatrix} E' & 0 \\ 0 & -E' \end{pmatrix}. \quad (4)$$

We suppose the intrinsic system is symmetric under the operation of S . This means there are simultaneous eigenstates of the original HFB Hamiltonian and the mean-field representation of S . Therefore, the HFB equation as an eigenvalue equation for the simultaneous eigenstates reads

$$\left[\begin{pmatrix} h - \lambda I & \Delta \\ -\Delta^* & -h^* + \lambda I \end{pmatrix} - \lambda_s \Omega_k \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \right] \begin{pmatrix} U_k \\ V_k \end{pmatrix} = (E_k - \lambda_s \Omega_k) \begin{pmatrix} U_k \\ V_k \end{pmatrix}, \quad (5)$$

where Ω_k is an eigenvalue of S . The mean-field representation of S is proportional to the identity matrix, which does not change the eigenvectors of the original HFB Hamiltonian and just shifts the eigenvalues by $-\lambda_s \Omega_k$. Because of the time-odd character of S , the eigenenergies of the time-reversal states are shifted for the opposite directions. Figure 1 shows a schematic picture of the single-particle energy levels under an external field $-\lambda_s S$ against the parameter λ_s . When $\lambda_s = 0$, the system has the time-reversal symmetry, thus every orbit degenerates at least doubly. When $\lambda_s \neq 0$, the levels split into the opposite directions linearly with a slope $\pm \Omega_k$. When λ_s is bigger than the point at which the levels cross the horizontal axis for the first time, the two states $(U_k V_k)^T$ and $(V_k^* U_k^*)^T$ are swapped automatically. This means the number parity has been changed. In this way, the proper orbit is selected by the operator S automatically and swapping of columns occurs just by adjusting the parameter λ_s . Odd- and even-number-parity states are obtained in the same manner, hence one can treat odd-mass nuclei in the existing HFB codes just by adding the external field.

4. Results of the calculation for neutron-rich Mg isotopes

The new method was applied to neutron-rich Mg isotopes, and the binding energies and radii were calculated. We performed the axially deformed HFB calculation with the SLy4 functional [3] and the surface-type pairing interaction with the strength of -430 MeV fm^{-3} in the cylindrical coordinate. Figure 2(a) shows the one-neutron separation energies S_n for $^{34-40}\text{Mg}$, which is defined by $S_n(A) = B(A) - B(A - 1)$, where $B(A)$ is the binding energy of ^AMg . Whereas one-neutron separation energies calculated by the present procedure (calculation 1) reproduce the experimental data quite well, the calculation without considering the number-parity change but only with the chemical potential adjusted for producing the expectation value of particle number (calculation 2) misses completely the data. The latter describes the odd-mass nuclei as even-number-parity states, that is, a superposition of even-even nuclei.

Figure 2(b) shows the root-mean-square matter radii $\sqrt{\langle r^2 \rangle_m}$ for $^{34-40}\text{Mg}$. The results calculated with and without considering the number-parity change are almost the same except for ^{37}Mg . A sudden increase in the radius of ^{37}Mg measured at RIBF is considered due to the emergence of deformed halo [4]. Only if we consider properly the number parity, this unique structure can be explained in the framework of DFT. The density distribution of ^{37}Mg calculated with the present procedure is shown in Fig. 3, which clearly shows the neutrons extend spatially with deformation.

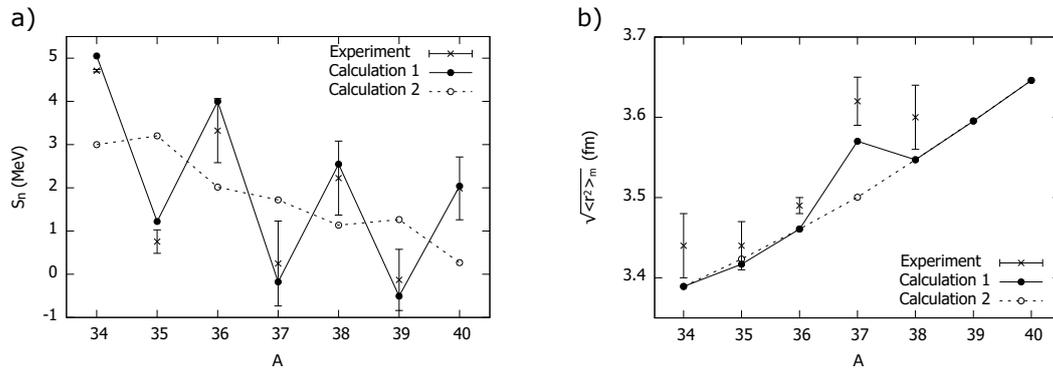


Fig. 2. (a) One-neutron separation energies and (b) root-mean-square matter radii for $^{34-40}\text{Mg}$. The experimental data are taken from Refs. [5, 6].

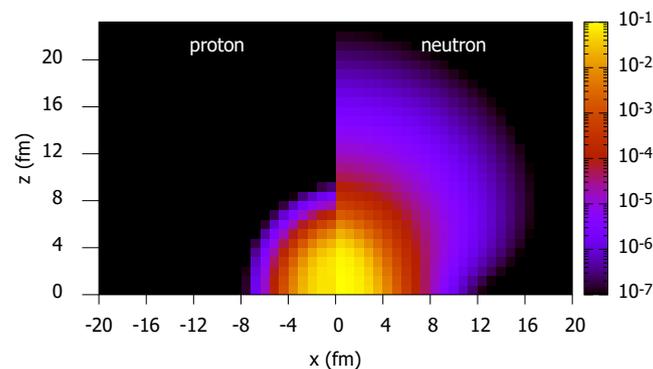


Fig. 3. Density distribution of ^{37}Mg with the z -axis as the symmetry axis. Protons and neutrons are shown for $x < 0$ and $x > 0$, respectively.

5. Summary

DFT is a promising avenue for constructing the computational nuclear data. However, there have been few DFT studies on odd-mass nuclei. We proposed a novel method to describe odd-mass nuclei as the ground state under an appropriate external field which breaks the time-reversal symmetry. Since odd- and even-number-parity states are treated in the same manner, it is easy to extend the existing framework for even-even nuclei to that for both even-even and odd-mass nuclei. We applied our method to the neutron-rich Mg isotopes and demonstrated the unique properties of odd-mass nuclei can be explained well.

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