

Continuum Skyrme Hartree–Fock–Bogoliubov theory with Green’s function method for neutron-rich Ca, Ni, Zr, and Sn isotopes

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Abstract

The possible exotic nuclear properties in the neutron-rich Ca, Ni, Zr, and Sn isotopes are examined with the continuum Skyrme Hartree–Fock–Bogoliubov theory in the framework of the Green’s function method. The pairing correlation, the couplings with the continuum, and the blocking effects for the unpaired nucleon in odd- A nuclei are properly treated. The Skyrme interaction SLy4 is adopted for the ph channel and the density-dependent δ interaction is adopted for the pp channel, which well reproduce the experimental two-neutron separation energies S_{2n} and one-neutron separation energies S_n . It is found that the criterion $S_n > 0$ predicts a neutron drip line with neutron numbers far smaller than those for $S_{2n} > 0$. Owing to the unpaired odd neutron, the neutron pairing energies $-E_{\text{pair}}$ in odd- A nuclei are far lower than those in the neighboring even-even nuclei. By investigating the single-particle structures, the possible halo structures in the neutron-rich Ca, Ni, and Sn isotopes are predicted, where sharp increases in the root-mean-square (rms) radii with significant deviations from the traditional $r \propto A^{1/3}$ rule and diffuse spatial density distributions are observed. Analyzing the contributions of various partial waves to the total neutron density $|\psi_l(r)|^2$ reveals that the orbitals located around the Fermi surface—particularly those with small angular momenta—significantly affect the extended nuclear density and large rms radii. The number of neutrons N_λ (N_0) occupying above the Fermi surface λ_n (continuum threshold) is discussed, whose evolution as a function of the mass number A in each isotope is consistent with that of the pairing energy, supporting the key role of the pairing correlation in halo phenomena.

Full Text

Continuum Skyrme Hartree-Fock-Bogoliubov Theory with Green's Function Method for Neutron-Rich Ca, Ni, Zr, Sn Isotopes

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The possible exotic nuclear properties in neutron-rich Ca, Ni, Zr, and Sn isotopes are examined using continuum Skyrme Hartree-Fock-Bogoliubov theory within the framework of the Green's function method. The pairing correlation, couplings with continuum, and blocking effects for unpaired nucleons in odd- A nuclei are properly treated. The Skyrme interaction SLy4 is adopted for the ph channel and the pairing interaction DDDI is adopted for the pp channel, which well reproduce the experimental two-neutron separation energies S_{2n} and one-neutron separation energies S_n . It is found that the criterion $S_n > 0$ predicts a neutron drip line with much smaller neutron numbers than that of $S_{2n} > 0$. Due to the unpaired odd neutron, neutron pairing energies ΔE_{pair} in odd- A nuclei are much smaller than those in neighboring even-even nuclei. By investigating the single-particle structures, possible halo structures in neutron-rich Ca, Ni, and Sn isotopes are predicted, where a sharp increase of rms radii with significant deviations from the traditional $r \propto A^{1/3}$ rule and diffuse spatial distributions in densities are observed. By analyzing the contributions of various partial waves to the total neutron density $\rho_{lj}(r) = \rho(r)$, the orbitals located around the Fermi surface, especially those with low angular momenta, play significant roles in the extended nuclear density and large rms radii. The number of neutrons $N_>$ (N_0) occupying above the Fermi surface λ_n (continuum threshold) are discussed, the evolution of which as a function of mass number A in each isotopic chain is consistent with those of pairing energy, supporting the key role of pairing correlation in halo phenomena.

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Introduction

The study of exotic nuclei far from the β stability line is a very challenging frontier topic in nuclear physics, both experimentally [?] and theoretically [?]. Unstable nuclei with extreme N/Z ratios, which are weakly bound systems, have

shown many exotic properties different from stable nuclei, such as halo structures [?], changes of traditional magic numbers [?], and new nuclear excitation modes [?, ?], which may also herald new physics. The study of exotic nuclei is not only crucial for fully understanding rich nuclear structures and properties, but also important for investigations of element synthesis and nuclear astrophysics [?]. However, due to their extremely short lifespans, the cross sections for synthesizing exotic nuclei are extremely small, making it very difficult to create them experimentally. As a result, more and more advanced large-scale radioactive beam facilities and updated detector techniques have been built, upgraded, or planned worldwide [?]. Meanwhile, abundant theoretical studies of exotic nuclei provide a useful way for the layout of experiments and analysis of experimental results [?].

In exotic nuclei, especially drip-line nuclei, the neutron or proton Fermi surfaces are usually very close to the continuum threshold. With the effects of pairing correlation, valence nucleons have a certain probability to be scattered into the continuum and occupy resonant states therein, making nuclear density distributions very diffuse and extended. It is therefore essential to treat pairing correlations and couplings to continuum properly in theoretical descriptions of exotic nuclei [?]. Besides, in one-neutron halo nuclei such as ^{31}Ne [?] and ^{37}Mg [?], the blocking effect [?] should also be considered to treat the unpaired odd nucleon. The Hartree-Fock-Bogoliubov (HFB) theory has achieved great successes in describing exotic nuclei with a unified description of the mean field and pairing correlation via Bogoliubov transformation [?]. Different models based on HFB theory have been used to study exotic nuclei, such as the Gogny-HFB theory [?], the Skyrme-HFB theory [?], the relativistic continuum Hartree-Bogoliubov (RCHB) theory [?], and the density-dependent relativistic Hartree-Fock-Bogoliubov (RHFB) theory [?]. To explore halo phenomena in deformed nuclei, these models have been extended to the deformed framework, such as the deformed relativistic Hartree-Bogoliubov (DRHB) theory [?, ?, ?] and the coordinate-space Skyrme-HFB approach [?].

Traditionally, these H(F)B equations are often solved in configuration spaces using basis expansion methods [?]. However, the calculations are strongly related to the space size and shape of the expanded basis. For the harmonic oscillator basis, which has a Gaussian tail, although it is very efficient for describing stable nuclei, significant difficulties are encountered when applying it to exotic nuclei. Bases with proper shapes, such as the Woods-Saxon basis [?] and the transformed harmonic oscillator basis [?, ?], are often used for exotic nuclei. For example, to explore deformed halos [?, ?], the DRHB theory based on a Woods-Saxon basis [?, ?] has been developed. In contrast with the basis expansion method, solving the HFB equation in coordinate space is believed to be more effective.

In coordinate space, the discretized method with box boundary conditions has been widely used, by which a series of discrete quasiparticle levels can be obtained easily. However, some flaws have been identified for this method, such

as nonphysical drops of nuclear densities at the box boundary, discretization of continuum and resonant states, and inclusion of some unphysical states. In contrast, the Green's function (GF) method [?] in coordinate space can avoid these problems and offers great advantages: it can describe the asymptotic behaviors of wave functions properly, provide energies and widths of resonant states directly, and treat bound states and continua on the same footing.

Due to these advantages, the Green's function method has been applied extensively in nuclear physics to study the contribution of the continuum to nuclear structures and excitations. As early as 1987, Belyaev et al. constructed the Green's function for the HFB equation [?]. Afterwards, this HFB Green's function was applied to the quasiparticle random-phase approximation (QRPA) [?], which was further used to describe collective excitations coupled to the continuum [?]. In 2009, the continuum HFB theory in a coupled-channel representation was developed to explore the effects of continuum and pairing correlation in deformed neutron-rich Mg isotopes [?]. In 2011, Zhang et al. developed the fully self-consistent continuum Skyrme-HFB theory with Green's function method [?], which was further applied to investigate giant halos [?] and the effects of pairing correlation on quasiparticle resonances [?, ?]. In 2019, to explore halo phenomena in neutron-rich odd-A nuclei, the self-consistent continuum Skyrme-HFB theory was further extended by including the blocking effect [?].

In recent years, Green's function methods have also been adopted for covariant density functional theory (CDFT) [?] in studies of nuclear structure. For example, by introducing the Green's function method to relativistic mean field theory (GF-RMF), the single-particle level structures including bound states and resonant states and the pseudospin symmetries therein have been investigated for neutrons [?, ?], protons [?], and Λ hyperons [?]. Besides, it has been confirmed that exact values of energies and widths can be obtained by searching for poles of the Green's function or extremes of the density of states regardless of the widths of resonant states [?, ?]. By combining the Green's function method with RCHB theory, pairing correlation and continuum are well described in the giant halos of Zr isotopes [?]. By extending the GF-RMF model to the coupled-channel representation, the halo candidate nucleus ^{37}Mg reported experimentally is analyzed and confirmed to be a p-wave one-neutron halo according to the Nilsson levels [?]. In addition, the complex-scaled Green's function method [?] has been established as a powerful tool for exploration of resonant states, which was further extended to the framework of relativistic mean field [?] and deformed nuclei [?]. Besides, the RMF-CMR-GF approach has been developed by combining the complex momentum representation method with the Green's function method in the relativistic mean-field framework to study halo structures in neutron-rich nuclei [?]. All these works have proved the great success of Green's function methods in describing the continuum.

In this paper, neutron-rich Ca, Ni, Zr, and Sn isotopes are investigated systematically using continuum Skyrme-HFB theory formulated with the Green's function method in coordinate space, which treats pairing correlations, couplings

with continuum, and blocking effects for odd unpaired nucleons properly. The paper is organized as follows: In Sec. II, we briefly introduce the continuum Skyrme-HFB theory. Numerical details are presented in Sec. III. Results and discussions are given in Sec. IV, and conclusions are drawn in Sec. V.

Theoretical Framework

In Hartree-Fock-Bogoliubov (HFB) theory [?], a pair-correlated nuclear system is described in terms of independent quasiparticles by the Bogoliubov transformation. The HFB equation in coordinate space [?] is:

$$\begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h}^* & -h^* + \lambda \end{pmatrix} \phi_i(r\sigma) = E_i \phi_i(r\sigma),$$

where E_i is the quasiparticle energy, $\phi_i(r\sigma)$ is the quasiparticle wave function, and λ is the Fermi energy determined by constraining the expectation value of the nucleon number. The HF Hamiltonian $h(r\sigma, r'\sigma')$ and the pair Hamiltonian $\tilde{h}(r\sigma, r'\sigma')$ are obtained by variation of the total energy functional with respect to the particle density $\rho(r\sigma, r'\sigma')$ and the pair density $\tilde{\rho}(r\sigma, r'\sigma')$, respectively. The solutions of the HFB equations have two symmetric branches: one with positive energy ($E_i > 0$) and quasiparticle wave function $\phi_i(r\sigma)$, and the other with negative energy ($-E_i < 0$) with conjugate wave function $\tilde{\phi}_i(r\sigma)$. The wave functions $\phi_i(r\sigma)$ and $\tilde{\phi}_i(r\sigma)$ have two components and are related as:

$$\phi_i(r\sigma) = \begin{pmatrix} \phi_{1;i}(r\sigma) \\ \phi_{2;i}(r\sigma) \end{pmatrix}, \quad \tilde{\phi}_i(r\sigma) = \begin{pmatrix} \phi_{2;i}(r\tilde{\sigma}) \\ \phi_{1;i}(r\tilde{\sigma}) \end{pmatrix},$$

with $\phi(r\tilde{\sigma}) = -2\sigma\phi(r, -\sigma)$. Here and hereafter, we follow the notations in Ref. [?] for convenience.

For an even-even nucleus, the ground state $|\Phi_0\rangle$ is a quasiparticle vacuum with particle density $\rho(r\sigma, r'\sigma')$ and pairing density $\tilde{\rho}(r\sigma, r'\sigma')$ determined by:

$$\rho(r\sigma, r'\sigma') \equiv \langle \Phi_0 | c_{r'\sigma'}^\dagger c_{r\sigma} | \Phi_0 \rangle,$$

$$\tilde{\rho}(r\sigma, r'\sigma') \equiv \langle \Phi_0 | c_{r'\tilde{\sigma}'} c_{r\sigma} | \Phi_0 \rangle,$$

where $c_{r\sigma}^\dagger$ and $c_{r\sigma}$ are particle creation and annihilation operators, respectively. The densities can be unified as a generalized density matrix $R(r\sigma, r'\sigma')$, with $\rho(r\sigma, r'\sigma')$ and $\tilde{\rho}(r\sigma, r'\sigma')$ being the “11” and “22” elements, respectively. With the quasiparticle wave functions, $R(r\sigma, r'\sigma')$ can be written in a simple form:

$$R(r\sigma, r'\sigma') = \sum_i \bar{\phi}_i(r\sigma) \bar{\phi}_i^\dagger(r'\sigma').$$

For an odd-A nucleus, the last odd nucleon is unpaired, for which the blocking effect should be considered. The nuclear ground state in this case is a one-quasiparticle state $|\Phi_1\rangle$, which can be constructed based on an HFB vacuum $|\Phi_0\rangle$ as $|\Phi_1\rangle = \beta_{i_b}^\dagger |\Phi_0\rangle$, where $\beta_{i_b}^\dagger$ is the quasiparticle creation operator and i_b denotes the blocked quasiparticle level occupied by the odd nucleon. Accordingly, the particle density $\rho(r\sigma, r'\sigma')$ and pairing density $\tilde{\rho}(r\sigma, r'\sigma')$ are:

$$\rho(r\sigma, r'\sigma') \equiv \langle \Phi_1 | c_{r'\sigma'}^\dagger c_{r\sigma} | \Phi_1 \rangle,$$

$$\tilde{\rho}(r\sigma, r'\sigma') \equiv \langle \Phi_1 | c_{r'\sigma'} c_{r\sigma} | \Phi_1 \rangle,$$

and the generalized density matrix $R(r\sigma, r'\sigma')$ becomes:

$$R(r\sigma, r'\sigma') = \sum_{i:\text{all}} \bar{\phi}_i(r\sigma) \bar{\phi}_i^\dagger(r'\sigma') - \bar{\phi}_{i_b}(r\sigma) \bar{\phi}_{i_b}^\dagger(r'\sigma') + \phi_{i_b}(r\sigma) \phi_{i_b}^\dagger(r'\sigma'),$$

where two more terms are introduced compared with those for even-even nuclei.

In conventional Skyrme-HFB theory, the HFB equation in coordinate space is often solved with box boundary conditions, and a series of discretized eigen-solutions including quasiparticle energies E_i and corresponding wave functions $\phi_i(r\sigma)$ can be obtained. Then the generalized density matrix $R(r\sigma, r'\sigma')$ can be calculated by summing these discretized quasiparticle states. We call this method the box-discretized approach. However, the applicability of the box boundary condition is limited for exotic nuclei, especially those close to the drip line, as a large enough coordinate space (or box size) should be taken to describe the very extended density distribution.

The Green's function method can avoid these problems of the box-discretized approach by imposing correct asymptotic behaviors on the wave functions, especially for weakly bound states and the continuum. The Green's function $G(r\sigma, r'\sigma'; E)$ with arbitrary quasiparticle energy E defined for the coordinate-space HFB equation obeys:

$$\begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h}^* & -h^* + \lambda \end{pmatrix} G(r\sigma, r'\sigma'; E) = \delta(r - r') \delta_{\sigma\sigma'} \mathbf{1},$$

which is a 2×2 matrix. The generalized density matrix $R(r\sigma, r'\sigma')$ can be calculated by integrals of the Green's function performed on the complex quasiparticle energy plane as:

$$R(r\sigma, r'\sigma') = \frac{1}{2\pi i} \oint_{C_{E<0}} dE G(r\sigma, r'\sigma'; E) + \frac{1}{2\pi i} \oint_{C_{-b}} dE G(r\sigma, r'\sigma'; E) + \frac{1}{2\pi i} \oint_{C_{+b}} dE G(r\sigma, r'\sigma'; E),$$

where the contour path $C_{E<0}$ encloses all negative quasiparticle energies $-E_i < 0$, C_{-b} encloses only the pole of $-E_{i_b}$, and C_{+b} encloses only the pole of E_{i_b} .

In the spherical case, the quasiparticle wave functions $\phi_i(r\sigma)$ and $\bar{\phi}_i(r\sigma)$ depend only on radial parts and can be expanded as:

$$\begin{aligned} \phi_i(r\sigma) &= \phi_{nlj}(r) = \begin{pmatrix} \phi_{1;nlj}(r) \\ \phi_{2;nlj}(r) \end{pmatrix} Y_{jm}^l(\hat{r}\sigma), \\ \bar{\phi}_i(r\sigma) &= \bar{\phi}_{nlj}(r) = \begin{pmatrix} \phi_{2;nlj}(r) \\ \phi_{1;nlj}(r) \end{pmatrix} Y_{jm}^{l*}(\hat{r}\tilde{\sigma}), \end{aligned}$$

where $Y_{jm}^l(\hat{r}\sigma)$ is the spin spherical harmonic, and $Y_{jm}^l(\hat{r}\tilde{\sigma}) = -2\sigma Y_{jm}^l(\hat{r}, -\sigma)$. Similarly, the generalized density matrix $R(r\sigma, r'\sigma')$ and Green's function $G(r\sigma, r'\sigma'; E)$ can be expanded as:

$$\begin{aligned} R(r\sigma, r'\sigma') &= \sum_{ljm} Y_{jm}^l(\hat{r}\sigma) R_{lj}(r, r') Y_{jm}^{l*}(\hat{r}'\sigma'), \\ G(r\sigma, r'\sigma'; E) &= \sum_{ljm} Y_{jm}^l(\hat{r}\sigma) G_{lj}(r, r'; E) Y_{jm}^{l*}(\hat{r}'\sigma'), \end{aligned}$$

where $R_{lj}(r, r')$ and $G_{lj}(r, r'; E)$ are the radial parts of the generalized density matrix and Green's function, respectively.

As a result, the radial local generalized density matrix $R(r) = R(r, r)$ can be expressed by the radial HFB Green's function $G_{lj}(r, r'; E)$ as:

$$R(r) = \sum_{lj:\text{all}} (2j+1) \left[\frac{1}{2\pi i} \oint_{C_{E<0}} dE G_{lj}(r, r; E) - \frac{1}{2\pi i} \oint_{C_{-b}} dE G_{i_b j b}(r, r; E) + \frac{1}{2\pi i} \oint_{C_{+b}} dE G_{i_b j b}(r, r; E) \right].$$

From the radial generalized matrix $R(r)$, one can easily obtain the radial local particle density $\rho(r)$ and pair density $\tilde{\rho}(r)$, which are the "11" and "12" components of $R(r)$, respectively. In the same way, other radial local densities needed in the functional of the Skyrme interaction, such as the kinetic-energy density $\tau(r)$ and spin-orbit density $J(r)$, can be expressed in terms of the radial Green's function. For details on constructing the Green's function, see Refs. [?, ?].

Numerical Details

For the Skyrme interaction in the ph channel, the SLy4 parameter set [?] is adopted. For the pairing interaction in the pp channel, a density-dependent δ interaction (DDDI) is used:

$$v_{\text{pair}}(r, r') = \frac{1 - P_{\sigma}}{2} V_0 \left[1 - \eta \left(\frac{\rho(r)}{\rho_0} \right)^{\alpha} \right] \delta(r - r').$$

The pair Hamiltonian $\tilde{h}(r\sigma, r'\sigma')$ is then reduced to a local pair potential [?]:

$$\Delta(r) = \frac{V_0}{2} \left[1 - \eta \left(\frac{\rho(r)}{\rho_0} \right)^{\alpha} \right] \tilde{\rho}(r).$$

The strength of the pairing force is $V_0 = -458.4 \text{ MeV} \cdot \text{fm}^3$, the density $\rho_0 = 0.08 \text{ fm}^{-3}$, and other parameters $\eta = 0.71$, $\alpha = 0.59$, which are constrained by reproducing experimental neutron pairing gaps for Sn isotopes [?, ?, ?]. With these parameters, DDDI can reproduce the scattering length $a = -18.5 \text{ fm}$ in the 1S channel of the bare nuclear force in the low-density limit [?]. The cutoff of quasiparticle states is taken with maximal angular momentum $j_{\text{max}} = 25/2$ and maximal quasiparticle energy $E_{\text{cut}} = 60 \text{ MeV}$.

The HFB equation is solved in coordinate space with space size $R_{\text{box}} = 20 \text{ fm}$ and mesh size $dr = 0.1 \text{ fm}$. To calculate densities with the Green's function, integrals of the Green's functions are performed along a contour path $C_{E<0}$, which is chosen as a rectangle with height $\gamma = 0.1 \text{ MeV}$ and length $E_{\text{cut}} = 60 \text{ MeV}$ to enclose all quasiparticle states with negative energies. For odd- A nuclei, two additional contour paths C_{+b} and C_{-b} , which only enclose the blocked quasiparticle states at energies E_{i_b} and $-E_{i_b}$, are introduced due to the blocking effect of the odd unpaired nucleon. For these details, see Ref. [?]. For the contour integration, an energy step of $\Delta E = 0.01 \text{ MeV}$ on the contour path is adopted.

Results and Discussion

In Fig. 1 [Figure 1: see original paper], two-neutron separation energies $S_{2n}(N, Z) = E(N - 2, Z) - E(N, Z)$ are plotted for even-even and odd-even Ca, Ni, Zr, and Sn isotopes. Red circles represent results calculated by the continuum Skyrme-HFB theory with the SLy4 parameter set, in comparison with results from the discretized method (blue triangles) and available experimental data [?] (black squares). The differences between S_{2n} from the Green's function method and discretized method are slight. Good agreement with experimental data is observed, indicating the reliability of continuum Skyrme-HFB theory for predicting neutron drip lines. Traditional shell closures, i.e., $N = 28$ in Ca isotopes, $N = 50$ in Ni isotopes, $N = 50, 82$ in Zr isotopes, and $N = 82$ in Sn isotopes, can be identified where S_{2n} drops sharply. For example, in the

Sn chain, S_{2n} drops from 13.25 MeV at ^{132}Sn to 4.94 MeV at ^{134}Sn when the neutron number exceeds the magic number $N = 82$. In the Ca, Ni, and Zr chains, the two-neutron separation energies quickly reach zero at large mass range, resulting in relatively short neutron drip lines at ^{67}Ca , ^{89}Ni , and ^{123}Zr , respectively. In contrast, in the Sn chain, S_{2n} remains less than 1.0 MeV over a wide mass region after the $N = 82$ gap and finally becomes negative only at $A = 178$, suggesting ^{177}Sn is a neutron drip-line nucleus. These weakly bound nuclei are quite interesting due to possible neutron halos, although they are experimentally difficult to reach.

In addition, exploration of the neutron drip line and determination of the limits of the nuclear landscape are significantly important in nuclear physics. However, various theoretical studies show that predicted neutron drip lines are very model-dependent [?]. Moreover, different physical quantities or criteria also predict very different neutron drip lines.

To explore neutron drip lines in Ca, Ni, Zr, and Sn isotopes, single-neutron separation energies $S_n(N, Z) = E(N-1, Z) - E(N, Z)$ are plotted in Fig. 2 [Figure 2: see original paper]. Results from the continuum Skyrme-HFB theory with the SLy4 parameter set are denoted by red circles, which agree well with experimental data [?] (black squares). Strong odd-even staggering is observed in all isotopes. In general, S_n in even-even nuclei is about 2-3 MeV larger than in neighboring odd-A nuclei, attributed to the unpaired odd neutron with vanishing pairing energy. Consequently, compared with Fig. 1, neutron drip lines determined by one-neutron separation energy are greatly shortened. In Ca, Ni, Zr, and Sn isotopes, the drip-line nuclei are ^{60}Ca , ^{86}Ni , ^{122}Zr , and ^{148}Sn , respectively, indicated by black arrows. Outside the neutron drip line determined by S_n , bound even-even nuclei behave as interesting Borromean systems. For example, based on the bound nucleus ^{60}Ca , $^{60}\text{Ca}+n$ is unbound while $^{60}\text{Ca}+n+n$ is bound.

In Fig. 3 [Figure 3: see original paper], neutron pairing energy E_{pair} is plotted as a function of mass number A for Ca, Ni, Zr, and Sn isotopes, expressed as:

$$E_{\text{pair}} = \int dr \Delta(r) \tilde{\rho}(r).$$

Red solid symbols represent even-even nuclei and open symbols represent odd-A nuclei. Neutron pairing energies E_{pair} for odd-A nuclei are much smaller than those of neighboring even-even nuclei due to the absent contribution of pairing energy by the unpaired neutron. This also explains why the drip line determined by single-neutron separation energy S_n is much shorter than that obtained by two-neutron separation energy S_{2n} . In addition, obvious shell effects are shown in the pairing energy. For example, in Sn isotopes, zero pairing energies at $N = 82$ and $N = 126$ while reaching the largest value at half-shell $N = 102$ can be observed. As a result, traditional shell closures— $N = 28, 40$ in Ca isotopes, $N = 40, 50$ in Ni isotopes, $N = 50, 82$ in Zr isotopes, and $N = 82, 126$ in Sn

isotopes—are clearly observed, consistent with those obtained in Fig. 1. In addition, a sub-shell $N = 32$ is also observed in Ca isotopes.

To explore possible neutron halos in Ca, Ni, Zr, and Sn isotopes, especially in weakly bound nuclei close to the neutron drip line where Fermi surfaces are very close to the continuum threshold and valence neutrons can be easily scattered to the continuum, we examine neutron single-particle structures, root-mean-square radii, and density distributions.

In Fig. 4 [Figure 4: see original paper], neutron canonical single-particle levels around the Fermi surface are plotted as functions of mass number for (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes. For details on obtaining canonical single-particle levels, see Refs. [?, ?]. The neutron Fermi energy λ_n and canonical single-particle energies ε are shown. As neutron number increases, the Fermi energy λ_n in each chain rises and finally reaches the continuum threshold while all HF single-particle levels decrease. Traditional shell closures— $N = 28, 40$ in Ca isotopes, $N = 40, 50$ in Ni isotopes, $N = 82$ in Zr isotopes, and $N = 82$ in Sn isotopes—can be observed where big gaps are obvious. Different single-particle structures are revealed in Ca, Ni, Zr, and Sn chains, based on which halos may be formed. In the Ni chain, above the shell closure $N = 50$, there are several weakly bound states and low-lying positive canonical states in the continuum with small angular momenta, which favor halo formation. For example, in ^{86}Ni , around the Fermi surface there are two weakly bound states, $2d_{5/2}$ and $3s_{1/2}$, and one low-lying positive canonical state $2d_{3/2}$. The Sn chain is quite similar to the Ni chain but has more advantages for halo formation, where weakly bound states and low-lying positive states in the continuum exist above the $N = 82$ shell closure. Besides, the Fermi surface λ_n approaches zero gradually and Sn isotopes in a large mass region are weakly bound. In the Ca chain, above the shell closure $N = 40$, there is mainly the $1g_{9/2}$ state, which evolves from a canonical positive state in the continuum ($A \leq 62$) to a weakly bound level ($A \geq 64$). Although valence neutrons may occupy the $1g_{9/2}$ orbital, the contributed density is very localized due to the large central barrier. In neutron-rich Ca isotopes, low-lying positive canonical states in the continuum $3s_{1/2}$ and $2d_{5/2}$ also play important roles. Halo formation is most unlikely for the Zr chain where the shell closure $N = 82$ is located around the continuum threshold and it's hard for valence neutrons to overcome the large gap and occupy the continuum.

In Fig. 5 [Figure 5: see original paper], neutron root-mean-square (rms) radii $r_{\text{rms}} = \sqrt{\int dr 4\pi r^4 \rho(r) / \int dr 4\pi r^2 \rho(r)}$ are plotted for Ca, Ni, Zr, and Sn isotopes, obtained by Skyrme-HFB calculations both with the Green's function method (filled circles and solid lines) and box-discretized method (open triangles and dashed lines) employing the SLy4 parameter set. Radii $r = b_0 A^{1/3}$ from the traditional liquid-drop model (black lines) are also indicated, where coefficient b_0 is determined by radii of deeply bound nuclei. For Ca, Ni, Zr, and Sn chains, they are $r \approx 0.991A^{1/3}$, $0.984A^{1/3}$, $0.957A^{1/3}$, and $0.961A^{1/3}$, respectively. In each chain, by adding more neutrons, nuclear rms radii r_{rms}

increase steeply and deviate from the $A^{1/3}$ rule. For example, in the Ca chain, compared with the isotopic trend for $N \leq 20$ with $r \approx 0.991A^{1/3}$, neutron rms radii in ^{50}Ca and heavier isotopes display steep increases with N . In these mass regions, possible neutron halos may occur. Besides, obvious odd-even staggering of rms radii can be observed in the Sn chain, where odd- A nuclei $^{151-165}\text{Sn}$ have larger rms radii than neighboring even-even nuclei. Detailed explanations can be found in Ref. [?]. The odd-even staggering phenomena in nuclear radii and masses have attracted great interest in recent years and many efforts have been made, such as in Refs. [?].

In exotic nuclei, diffuse density distributions in coordinate space are often observed. Thus, in Fig. 6 [Figure 6: see original paper], to explore exotic structures in (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes, neutron density distributions $\rho(r)$ are plotted, where solid lines are obtained by the Green's function method and dashed lines represent results from the box-discretized method. It is a global trend that neutron density distributions extend further with increasing neutron number. Shell structures influence density distributions significantly: compared with bound nuclei, density distributions of neutron-rich nuclei with neutron numbers exceeding the closures $N = 28, 50, 82$ are much more extended, consistent with the behaviors of rms radii plotted in Fig. 5. In addition, compared with Ca and Zr chains, Ni and Sn chains exhibit more diffuse density distributions, explained by their small two-neutron separation energies S_{2n} over a large mass range shown in Fig. 1. In Zr isotopes, density distributions are relatively localized. Combined with the large S_{2n} values in Fig. 1, we are inclined to believe in the absence of halos in Zr isotopes. However, using RCHB theory with the NLSH parameter set [?] and continuum Skyrme-HFB theory with the SKI4 parameter set [?, ?], giant halos in Zr isotopes have been predicted. In all isotopes, compared with the box-discretized method predicting nonphysical sharp decreases of densities at the space boundary, the Green's function method describes extended density distributions well, especially for very neutron-rich isotopes. Besides, densities obtained by the Green's function method can be independent of space size as discussed in Ref. [?], being basically determined by proper boundary conditions for bound states, weakly bound states, and the continuum employed when constructing the Green's functions.

To explore contributions of different partial waves to the extended density distributions in Fig. 6, taking neutron-rich (a) ^{64}Ca , (b) ^{86}Ni , (c) ^{120}Zr , and (d) ^{174}Sn as examples, compositions $\rho_{lj}(r)/\rho(r)$ are plotted as functions of radial coordinate r in Fig. 7 [Figure 7: see original paper]. It can be clearly seen that outside the nuclear surface (referring to the right boundary of shallow regions of total nuclear density distributions), orbitals located around the Fermi surface play the main role in density distributions. For example, in neutron-rich ^{64}Ca , partial waves $p_{1/2}$, $f_{5/2}$, $g_{9/2}$, $s_{1/2}$, and $d_{5/2}$ contribute significantly to the total density in the region $5 \text{ fm} < r < 15 \text{ fm}$. These levels are located within ~ 5 MeV around the Fermi surface as shown in Fig. 8 [Figure 8: see original paper], where neutron canonical single-particle levels and occupation probabilities are presented. When going further in coordinate space with $r > 15 \text{ fm}$, contributions

from partial waves $s_{1/2}$ and $d_{5/2}$ with small angular momenta increase evidently while others reduce. In ^{86}Ni , single-particle levels $2d_{5/2}$, $3s_{1/2}$, and $2d_{3/2}$ are located above the neutron shell $N = 50$ and close to the Fermi surface, playing the main role in neutron density distribution. Although the positive state $1g_{7/2}$ is also very close to the Fermi surface, it contributes little to the density at large coordinate space due to the large centrifugal barrier. For nucleus ^{120}Zr with neutron number very close to the $N = 82$ closure, single-particle levels between closures $N = 50$ and $N = 82$ including $2d_{5/2}$, $1g_{7/2}$, $3s_{1/2}$, $2d_{3/2}$, and $1h_{11/2}$ contribute significantly to densities at large coordinate space. The insignificant occupation of the positive state $2f_{7/2}$ leads to little contribution to the density. Regarding neutron-rich ^{174}Sn with neutron number exceeding the $N = 82$ closure, weakly bound single-particle levels $2f_{7/2}$, $2f_{5/2}$, $3p_{3/2}$, and $3p_{1/2}$ with small angular momentum play the key role in extended density distributions at large coordinate space. From these analyses, we conclude that single-particle levels around the Fermi surface, particularly those with low angular momenta, are the main cause of extended nuclear density and large rms radii.

In Fig. 8 [Figure 8: see original paper], particle occupation probabilities v^2 on different canonical levels ε_{can} are presented and denoted by line lengths. Without pairing, occupation probabilities v^2 should be either one or zero separated by the Fermi surface. With pairing effects, nucleons occupying levels below the Fermi surface can be scattered to higher levels, resulting in occupations of weakly bound states above the Fermi surface and even levels in the continuum. In neutron-rich nuclei ^{64}Ca , ^{86}Ni , ^{120}Zr , and ^{174}Sn , the numbers of neutrons $N_{>} = \sum (2j + 1)v^2$ scattered above the Fermi surface λ_n are 4.33, 2.51, 0.159, and 0.173, respectively. In ^{64}Ca , the weakly bound single-particle $1g_{9/2}$ contributes about 3.7 neutrons.

To explore pairing effects, in Fig. 9 [Figure 9: see original paper] we plot the number of neutrons $N_{>}$ scattered above the Fermi surface for (a) Ca, (b) Ni, (c) Zr, and (d) Sn chains obtained by Skyrme-HFB theory with the Green's function method. It can be seen clearly that substantial neutrons have been scattered from single-particle levels below the Fermi surface to weakly bound states above the Fermi surface and even levels in the continuum due to pairing, especially in nuclei with neutron numbers filling half-full shells. Besides, very obvious shell structure can be observed. When neutron number reaches a magic number— $N = 28, 40$ in Ca isotopes, $N = 40, 50$ in Ni isotopes, $N = 50, 82$ in Zr isotopes, and $N = 82, 126$ in Sn isotopes— $N_{>}$ is almost zero due to absence of pairing in closed-shell nuclei. Besides, at points $N = 32$ in Ca isotopes, $N = 54, 68$ in Zr isotopes, and $N = 88$ in Sn isotopes, very small numbers of neutrons $N_{>}$ are obtained, indicating weak pairing in those nuclei. This can also predict possible existence of sub-shells and new magic numbers. Furthermore, the evolution of $N_{>}$ is basically consistent with the trend of pairing energy.

In Fig. 10 [Figure 10: see original paper], we further investigate the number of neutrons occupying the continuum with single-particle energies $\varepsilon > 0$ MeV, i.e., $N_0 = \sum (2j + 1)v^2$. Compared with $N_{>}$, the number of neutrons occupying

the continuum N_0 is drastically reduced. For example, in the Ca chain, N_0 is less than one in all isotopes except ^{62}Ca . In ^{62}Ca , the single-particle level $1g_{9/2}$ appears as a low-lying canonical positive state in the continuum with energy $\varepsilon = 0.198$ MeV and a high occupation probability of $v^2 = 0.197$, resulting in almost 1.979 neutrons occupying it. But in neighboring ^{60}Ca , very small occupation probability $v^2 = 0.015$ of $1g_{9/2}$ is obtained, while in ^{64}Ca the $1g_{9/2}$ state becomes a weakly bound level with energy $\varepsilon = -0.072$ MeV. After removing the neutron contribution from $1g_{9/2}$ in ^{62}Ca , only 0.38 neutrons are in the continuum, denoted by an empty circle in panel (a). Except for the Sn chain, the shape of N_0 is very close to those of pairing energy and pairing gap. Although the Sn chain becomes very complex, we can still observe shell structure at $N = 82$ and $N = 126$ where N_0 is almost zero.

Summary

In this work, exotic nuclear properties of neutron-rich Ca, Ni, Zr, and Sn isotopes are examined systematically using continuum Skyrme-HFB theory in coordinate space formulated with the Green's function method, in which pairing correlations, couplings to continuum, and blocking effects for unpaired nucleons in odd-A nuclei are treated properly.

First, both two-neutron separation energies S_{2n} and one-neutron separation energies S_n are calculated, which are consistent with experimental data. Significant differences exist for drip lines determined by S_{2n} and S_n . In Ca, Ni, Zr, and Sn isotopes, drip-line nuclei are ^{67}Ca , ^{89}Ni , ^{123}Zr , and ^{177}Sn judging by S_{2n} , while ^{60}Ca , ^{86}Ni , ^{122}Zr , and ^{148}Sn according to S_n . Due to absent pairing energy contribution from the single unpaired odd neutron, neutron pairing energies $-E_{\text{pair}}$ of odd-A nuclei are about 2 MeV smaller than those of neighboring even-even nuclei. This also explains why drip lines determined by S_n are much shorter than those by S_{2n} . In addition, from fluctuation trends of pairing energy, traditional neutron magic numbers are clearly displayed: $N = 28, 40$ in Ca isotopes, $N = 40, 50$ in Ni isotopes, $N = 50, 82$ in Zr isotopes, and $N = 82, 126$ in Sn isotopes.

Second, to explore possible halo structures in neutron-rich Ca, Ni, Zr, and Sn isotopes, neutron single-particle structures, root-mean-square radii, and density distributions are investigated. In neutron-rich Ca, Ni, and Sn nuclei, especially weakly bound nuclei close to the neutron drip line, rms radii show sharp increases with significant deviations from the traditional $r \propto A^{1/3}$ rule. Besides, very diffuse spatial density distributions are observed in those nuclei, reflecting possible halo phenomena. By analyzing contributions of different partial waves to total density, we find that orbitals located around the Fermi surface, particularly those with low angular momenta, are the main cause of extended nuclear density and large rms radii.

Finally, numbers of halo nucleons that reflect pairing effects are discussed. Two different numbers of neutrons are defined: $N_{>}$ occupying single-particle levels

above the Fermi surface λ_n and N_0 occupying the continuum. We find that evolutions of $N_>$ and N_0 with mass number A are basically consistent with the trend of pairing energy $-E_{\text{pair}}$, supporting the key role of pairing correlations in halo phenomena.

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