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 much 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 much 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 $\rho_n(r)/\rho(r)$ 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 $N_1 (N_2)$ occupying above the Fermi surface $\lambda_n$ (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.

Keywords Neutron-rich nuclei · Neutron halo · Skyrme Hartree–Fock–Bogoliubov theory · Green’s function method

1 Introduction
The study of exotic nuclei far from the $\beta$ stability line is a challenging frontier in experimental [1–4] and theoretical [5–10] nuclear physics. The unstable nuclei with extreme $N/Z$ ratios, which are weakly bound systems, have exhibited many exotic properties that differ from those of the stable nuclei, such as halo structures [11–17], changes in the traditional magic numbers [18–23], and new nuclear excitation modes [24, 25], which may herald new physics. The study of exotic nuclei is crucial for not only comprehensively understanding the rich nuclear structures and properties but also investigating element synthesis and nuclear astrophysics [26]. However, because of the short lifespan, the cross sections for synthesizing exotic nuclei are small, which makes it difficult to create them experimentally. Thus, advanced large-scale radioactive beam facilities and updated detector techniques have been developed, upgraded, or planned worldwide [27–34]. Meanwhile, abundant theoretical studies on exotic nuclei provide valuable guidance for the design of experiments and analysis of experimental results [35–37].

In the exotic nuclei—particularly the drip line nuclei—the neutron or proton Fermi surfaces are typically close to the...
continuum threshold. With the effects of the pairing correlation, the valence nucleons have a certain probability to be scattered into the continuum and occupy the resonant states therein, making the nuclear density distributions very diffuse and extended. It is therefore essential to treat the pairing correlations and the couplings to the continuum properly in the theoretical descriptions of exotic nuclei [38–42]. Additionally, for one-neutron halo nuclei, e.g., \(^{31}\text{Ne}\) [43] and \(^{37}\text{Mg}\) [44], the blocking effect [45] should be considered to treat the unpaired odd nucleon.

The Hartree–Fock–Bogoliubov (HFB) theory has achieved great success in describing exotic nuclei with a unified description of the mean field and pairing correlation via Bogoliubov transformation [45]. Different models based on the HFB theory have been used to study exotic nuclei, such as the Gogny–HFB theory [46], the Skyrme–HFB theory [47], the relativistic continuum Hartree–Bogoliubov (RCHB) theory [39], and the density-dependent relativistic Hartree–Fock–Bogoliubov (RHFB) theory [48]. To explore the halo phenomena in deformed nuclei, these models have been extended to the deformed framework, e.g., the deformed relativistic Hartree–Bogoliubov (DRHB) theory [16, 49, 50] and the coordinate-space Skyrme–HFB approach [51–54].

Traditionally, these H(F)B equations are often solved in configuration spaces, i.e., via the basis expansion method [55]. However, the calculations are closely related to the space size and the shape of the expanded basis. Although the harmonic oscillator basis, which has a tail in the shape of a Gaussian function, can efficiently describe stable nuclei, significant difficulties were encountered when it was applied to exotic nuclei. Bases with proper shapes, such as the Woods–Saxon basis [56] and the transformed harmonic oscillator basis [57, 58], are often used for the exotic nuclei. For example, to explore deformed halos [59, 60], the DRHB theory based on a Woods–Saxon basis [16, 49] was developed. In contrast to the basis expansion method, solving the HFB equation in the coordinate space is believed to be more effective. In the coordinate space, the discretized method with the box boundary condition has been widely used, whereby a series of discrete quasiparticle levels can be easily obtained. However, flaws in this method have been identified, such as the nonphysical drops in the nuclear densities at the box boundary, the discretization of continua and resonant states, and the inclusion of unphysical states. In contrast, the Green’s function (GF) method [61–63] in the coordinate space can avoid these problems and has significant advantages, i.e., it can describe the asymptotic behaviors of wave functions properly, provide the energies and widths of the resonant states directly, and treat the bound states and the continua on the same footing.

Owing to these advantages, the GF method has been applied extensively in nuclear physics to study the contribution of the continuum to the nuclear structures and excitations. In 1987, Belyaev et al. formulated the GF for the HFB equation [64]. Subsequently, this HFB GF was applied to the quasiparticle random-phase approximation [65], which was further used to describe the collective excitations coupled to the continuum [66–71]. In 2009, the continuum HFB theory in a coupled channel representation was developed to explore the effects of the continuum and pairing correlation in deformed neutron-rich Mg isotopes [72]. In 2011, Zhang et al. developed the fully self-consistent continuum Skyrme–HFB theory with the GF method [73], which was applied to investigate the giant halos [74] and the effects of the pairing correlation on the quasiparticle resonances [75, 76]. In 2019, to explore the halo phenomena in neutron-rich odd-A nuclei, the self-consistent continuum Skyrme–HFB theory was extended by including the blocking effect [77]. In recent years, the GF method has also been adopted for the covariant density functional theory [78–86] in studies on nuclear structure. For example, by introducing the GF method to the relativistic mean field theory (GF-RMF), the single-particle level structures, including the bound states and resonant states and the pseudospin symmetries therein, were investigated for neutrons [87, 88], protons [89], and A hyperons [90]. Additionally, it was confirmed that exact values of the energies and widths could be obtained by searching for the poles of the GF or the extremes of the density of states in disregard of the widths of resonant states [91, 92]. By combining the GF method with the RCHB theory, the pairing correlation and continuum are well described in the giant halos of the Zr isotopes [93]. By extending the GF-RMF model to the coupled channel representation, the halo candidate nucleus \(^{37}\text{Mg}\) reported experimentally was analyzed and confirmed to be a \(p\)-wave one-neutron halo according to the Nilsson levels [94]. In addition, the complex-scaled GF method [95] has been established as a powerful tool for the exploration of resonant states, which was extended to the framework of the relativistic mean field [96] and deformed nuclei [97]. Additionally, the RMF-CMR-GF approach was developed by combining the complex momentum representation method with the GF method in the relativistic mean field framework to study the halo structures in neutron-rich nuclei [98]. These studies proved the effectiveness of the GF method for the description of the continuum.

In this study, the neutron-rich Ca, Ni, Zr, and Sn isotopes are investigated systematically using the continuum Skyrme–HFB theory formulated with the GF method in the coordinate space, in which the pairing correlations, the couplings with the continuum, and the blocking effect for the odd unpaired nucleon are treated properly. The remainder of the paper is organized as follows. In Section 2, we briefly introduce the continuum Skyrme–HFB theory. Numerical details
Continuum Skyrme Hartree–Fock–Bogoliubov theory with Green's function method for neutron-rich…

2 Theoretical framework

In the Hartree–Fock–Bogoliubov (HFB) theory [45], the pair correlated nuclear system is described in terms of independent quasiparticles by the Bogoliubov transformation. The HFB equation in the coordinate space [38] is

\[
\left( \hat{h} - \lambda \right) \phi_\sigma(r) = E_\sigma \phi_\sigma(r),
\]

where \(E_\sigma\) represents the quasiparticle energy, \(\phi_\sigma(r)\) represents the quasiparticle wave function, and \(\lambda\) represents the Fermi energy, which is determined by constraining the expectation value of the nucleon number. The HF Hamiltonian \(\hat{h}(r, r', \sigma')\) and the pair Hamiltonian \(\hat{h}(r, r', \sigma')\) are obtained by the 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 is positive \((E_\sigma > 0)\) with the quasiparticle wave function \(\phi_\sigma(r)\) and the other is negative \((E_\sigma < 0)\) with the conjugate wave function \(\tilde{\phi}_\sigma(r)\).

\[
\phi_\sigma(r) = \left( \begin{array}{c} \varphi_{1\sigma}(r) \\ \varphi_{2\sigma}(r) \end{array} \right), \quad \tilde{\phi}_\sigma(r) = \left( \begin{array}{c} -\varphi^{*}_{2\sigma}(r) \\ \varphi^{*}_{1\sigma}(r) \end{array} \right),
\]

with \(\phi(r_\sigma) = -2\sigma\varphi(r, -\sigma)\). In this paper, we follow the notation used in Ref. [65] for convenience.

For an even–even nucleus, the ground state \(|\Phi_0\rangle\) is a quasiparticle vacuum with the particle density \(\rho(r_\sigma, r_\sigma')\) and pair density \(\tilde{\rho}(r_\sigma, r_\sigma')\) determined as follows:

\[
\rho(r_\sigma, r_\sigma') \equiv \langle \Phi_0 | c_{r_\sigma}^\dagger c_{r_\sigma'} | \Phi_0 \rangle,
\]

\[
\tilde{\rho}(r_\sigma, r_\sigma') \equiv \langle \Phi_0 | c_{r_\sigma'}^\dagger c_{r_\sigma} | \Phi_0 \rangle,
\]

where \(c_{r_\sigma}^\dagger\) and \(c_{r_\sigma'}\) are the 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:

\[
R(r_\sigma, r_\sigma') = \sum_i \tilde{\phi}_i(r_\sigma) \phi_i^\dagger(r_\sigma').
\]

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 on the basis of a HFB vacuum \(|\Phi_0\rangle\) as

\[
|\Phi_1\rangle = \beta^\dagger \Phi_0 | \Phi_0 \rangle,
\]

where \(\beta^\dagger\) is the quasiparticle creation operator and \(\Phi_0\) denotes the blocked quasiparticle level occupied by the odd nucleon. Accordingly, the particle density \(\rho(r_\sigma, r'_\sigma')\) and the pairing density \(\tilde{\rho}(r_\sigma, r'_\sigma')\) are

\[
\rho(r_\sigma, r'_\sigma') \equiv \langle \Phi_1 | c_{r_\sigma'}^\dagger c_{r_\sigma} | \Phi_1 \rangle,
\]

\[
\tilde{\rho}(r_\sigma, r'_\sigma') \equiv \langle \Phi_1 | c_{r'_\sigma'}^\dagger c_{r_\sigma} | \Phi_1 \rangle,
\]

and the generalized density matrix \(R(r_\sigma, r'_\sigma')\) becomes

\[
R(r_\sigma, r'_\sigma') = \sum_{i \text{ all}} \tilde{\phi}_i(r_\sigma) \phi_i^\dagger(r'_\sigma') - \tilde{\phi}_i(r_\sigma) \phi_i^\dagger(r'_\sigma') + \tilde{\phi}_i(r_\sigma) \phi_i^\dagger(r'_\sigma'),
\]

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

In the conventional Skyrme–HFB theory, the HFB equation (1) in the coordinate space is often solved with the box boundary condition, and a series of discretized eigensolutions including the quasiparticle energy \(E_\sigma\) and the corresponding wave functions \(\phi_\sigma(r)\) can be obtained. Then, the generalized density matrix \(R(r_\sigma, r'_\sigma')\) can be calculated by summing these discretized quasiparticle states, in accordance with Eqs. (4) and (7). We call this method the box-discretized approach. However, the applicability of the box boundary condition in the description of exotic nuclei—particularly those close to the drip line—is poor. A sufficiently large coordinate space (or box size) should be used to describe the extended density distribution.

The GF method can avoid these problems of the box-discretized approach, as it imposes the correct asymptotic behaviors on the wave functions—particularly for the weakly bound states and the continuum. The GF \(G(r_\sigma, r'_\sigma'; E)\) with an arbitrary quasiparticle energy \(E\) is defined for the coordinate-space HFB equation obeys

\[
\left[ E - \left( \frac{\hat{h} - \lambda}{\hat{h}^* - h^* + \lambda} \right) \right] G(r_\sigma, r'_\sigma'; E)
\]

\[
= \delta(r - r') \delta_{\sigma\sigma'},
\]

which is a \(2 \times 2\) matrix. The generalized density matrix \(R(r_\sigma, r'_\sigma')\) in Eq. (7) can be calculated by taking the integrals of the GFs on the complex quasiparticle energy plane, as follows:
\[ R(r, r'; r') = \frac{1}{2\pi i} \left[ \oint_{C_{E<0}} dE G(r, r'; r'; E) - \oint_{C_h} dE G(r, r'; r'; E) + \oint_{C_E^+} dE G(r, r'; r'; E) \right] , \]

where the contour path \( C_{E<0} \) encloses all the negative quasiparticle energies \(-E_i < 0\), \( C_h^- \) encloses only the pole of \(-E_h\), and \( C_E^+ \) encloses only the pole of \( E_h\).

In the spherical case, the quasiparticle wave functions \( \phi_i(r, \sigma) \) and \( \phi_i(r, \sigma') \) are only dependent on the radial parts, and they can be expanded as follows:

\[ \phi_i(r, \sigma) = \frac{1}{r} \phi_{nji}(r) Y_{jm}^l(r, \hat{\sigma}), \]

\[ \phi_i(r, \sigma') = \frac{1}{r} \phi_{nji}(r) Y_{jm}^{l'}(r, \hat{\sigma'}), \]

\[ \phi_{nlj}(r) = \begin{pmatrix} \phi_{1nlj}(r) \\ \phi_{2nlj}(r) \end{pmatrix} , \]

\[ \tilde{\phi}_{nlj}(r) = \begin{pmatrix} -\phi_{2nlj}(r) \\ \phi_{1nlj}(r) \end{pmatrix} , \]

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

\[ G(r, \sigma, r'; \sigma'; E) = \sum_{ljm} Y_{jm}^l(\hat{\sigma}) \tilde{G}_{lj}(r, r'; r', \sigma') Y_{jm}^{l*}(\hat{\sigma'}), \]

\[ R(r, r'; r') = \sum_{lj} Y_{jm}^l(\hat{\sigma}) R_{lj}(r, r') Y_{jm}^{l*}(\hat{\sigma'}), \]

where \( R_{lj}(r, r') \) and \( \tilde{G}_{lj}(r, r'; r', \sigma') \) are the radial parts of the generalized density matrix and GF, respectively.

Thus, the radial local generalized density matrix \( R(r, r) \) can be expressed by the radial HFB GF \( \tilde{G}_{lj}(r, r'; r', \sigma') \) as follows:

\[ R(r) = \sum_{lj} R_{lj}(r, r) \]

\[ = \frac{1}{4\pi r^2} \sum_{lj; all} \sum_{nlj} (2j + 1) \left[ \tilde{\phi}_{nlj}(r) - \tilde{\phi}_{nlj}(r) \right] \]

\[ + \tilde{\phi}_{nlj}(r) \]

\[ = \frac{1}{4\pi r^2} \sum_{lj; all} \sum_{nlj} (2j + 1) \int_{C_{E<0}} dE G_{lj}(r, r; E) \]

\[ - \oint_{C_h} dE G_{h}(r, r; E) + \oint_{C_E^+} dE G_{h}(r, r; E) \].

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, one can express other radial local densities needed in the functional of the Skyrme interaction, such as the kinetic-energy density \( T(r) \) and the spin–orbit density \( J(r) \), in terms of the radial GF. For the construction of the GF, see Refs. [73, 77].

### 3 Numerical details

For the Skyrme interaction in the \( ph \) channel, the SLy4 parameter set [100] is adopted. For the pairing interaction in the \( pp \) channel, a density-dependent \( \delta \) interaction (DDDI) is used:

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

The pair Hamiltonian \( \tilde{h}(r, r; \sigma') \) is then reduced to a local pair potential [47]:

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

The strength of the pairing force \( V_0 = -458.4 \text{ MeV fm}^3 \), density \( \rho_0 = 0.08 \text{ fm}^{-3} \), and parameters \( \eta = 0.71 \) and \( \alpha = 0.59 \) are constrained by reproducing the experimental neutron pairing gaps for the Sn isotopes [68, 101, 102]. With these parameters, the 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 [101]. The cutoff of the quasiparticle states is set to a maximal angular momentum of \( j_{\text{max}} = 25/2 \) and a maximal quasiparticle energy of \( E_{\text{cut}} = 60 \text{ MeV} \).

The HFB equation is solved in the coordinate space with the space size \( R_{\text{box}} = 20 \text{ fm} \) and mesh size \( dr = 0.1 \text{ fm} \). To calculate the densities with the GF, the integrals of the GFs are performed along a contour path \( C_{E<0} \), which is set as a rectangle with height \( \gamma = 0.1 \text{ MeV} \) and length
$E_{\text{cut}} = 60$ MeV to enclose all the quasiparticle states with negative energies. For the odd-$A$ nuclei, two more contour paths $C_b^+$ and $C_b^-$, which only enclose the blocked quasiparticle states at energies $E_b^+$ and $-E_b^-$, are introduced owing to the blocking effect of the odd unpaired nucleon. Details are presented in Ref. [77]. To perform the contour integration, an energy step of $\Delta E = 0.01$ MeV on the contour path is adopted.

4 Results and discussion

In Fig. 1, the two-neutron separation energies $S_{2n}(N,Z) = E(N-2,Z) - E(N,Z)$ are plotted for the even–even and odd–even Ca, Ni, Zr, and Sn isotopes. Red circles indicate those calculated according to the continuum Skyrme–HFB theory with the SLy4 parameter set, blue triangles indicate the results of the discretized method, and black squares indicate the available experimental data [99]. The differences between the $S_{2n}$ values obtained via the GF method and discretized method are small. Good agreement with the experimental data is observed, indicating the reliability of the continuum Skyrme–HFB theory for the prediction of neutron drip line. The 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 the $S_{2n}$ decreases sharply. For example, in the Sn chain, $S_{2n}$ decreases from 13.25 MeV at $^{132}$Sn to 4.94 MeV at $^{134}$Sn with the neutron number exceeding the magic number $N \geq 82$. In the Ca, Ni, and Zr chains, the two-neutron separation energies quickly reach 0 as mass increasing, resulting in relatively short neutron drip lines, which are $^{67}$Ca, $^{89}$Ni, and $^{122}$Zr, respectively. In contrast, in the Sn chain, $S_{2n}$ remains below 1.0 MeV in a wide mass region after the gap of $N = 82$ and finally becomes negative until $A = 178$, suggesting that $^{177}$Sn is a neutron drip line nucleus. These weakly bound nuclei are interesting owing to the possible appearance of neutron halos, although this is experimentally difficult to achieve. In addition, the exploration of the neutron drip line and the determination of the limit of the nuclear landscape are important in nuclear physics. However, various theoretical studies indicate that the predicted neutron drip line is very model dependent [103]. Moreover, different physical quantities and criteria yield different neutron drip line predictions.

To explore the neutron drip lines in the Ca, Ni, Zr, and Sn isotopes, in Fig. 2 the single-neutron separation energies $S_n(N,Z) = E(N-1,Z) - E(N,Z)$ are plotted. The results obtained using the continuum Skyrme–HFB theory with the SLy4 parameter set are indicated by red circles, which are consistent with the experimental data [99] indicated by the black squares. Strong odd–even staggering is observed in all isotopes. In general, the $S_n$ in the even–even nucleus is approximately $2 \sim 3$ MeV larger than those in the neighboring odd-$A$ nuclei, which is attributed to the unpaired odd neutron with vanishing pairing energy. Consequently, compared with those in Fig. 1, the neutron drip lines determined via the one-neutron separation energy are significantly shortened. In the Ca, Ni, Zr, and Sn isotopes, the drip line nuclei are $^{60}$Ca, $^{60}$Ni, $^{122}$Zr, and $^{148}$Sn, respectively, whose positions are indicated by the black arrows. Outside the neutron drip line determined by $S_n$, the bound even–even nuclei behave as interesting Borromean systems. For example, considering the bound nucleus $^{60}$Ca, $^{60}$Ca+$n$ is unbound, while $^{60}$Ca+$n + n$ is bound.

In Fig. 3, we plot the neutron pairing energy $E_{\text{pair}}$, which is expressed as

![Fig. 1 (Color online) Two-neutron separation energies $S_{2n}$ in the Ca, Ni, Zr, and Sn isotopes as a function of the mass number $A$ calculated according to the continuum Skyrme–HFB theory with the SLy4 parameter set (filled red circles), in comparison with the results of the discretized method (open blue triangles) and experimental data (filled black squares) [99]](image)
Fig. 2  (Color online) Single-neutron separation energies $S_n$ as a function of the mass number $A$ in the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes calculated according to the continuum Skyrme–HFB theory with the SLy4 parameter set (filled red circles), in comparison with the results of the discretized method (open blue triangles) and experimental data (filled black squares) [99].

Fig. 3  (Color online) Neutron pairing energy $-E_{\text{pair}}$ as a function of the mass number $A$ in the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes calculated according to the continuum Skyrme–HFB theory with the SLy4 parameter set. The filled and open squares indicate the results for the even–even and odd–even nuclei, respectively.
Continuum Skyrme Hartree–Fock–Bogoliubov theory with Green’s function method for neutron-rich...

The red solid symbols correspond to the even–even nuclei, and the open symbols correspond to the odd-\(A\) nuclei. The neutron pairing energies \(E_{\text{pair}}\) of the odd-\(A\) nuclei are obviously lower than those of the neighboring even–even nuclei, owing to the absent contribution of pairing energy from the unpaired neutron. This also explains why the drip line determined via the single-neutron separation energy \(S_n\) is much shorter than that obtained via the two-neutron separation energy \(S_{2n}\). In addition, obvious shell effects are observed in the pairing energy. For example, in Sn isotopes, the pairing energy is 0 at \(N = 82\) and \(N = 126\), and it is maximized at the half-shell \(N = 102\). As a result, the traditional shell closures, i.e., \(N = 28, 40\) in Ca isotopes, \(N = 40, 50\) in Ni isotopes, \(N = 50, 82\) in Zr isotopes, and \(N = 82, 126\) in Sn isotopes, can also be clearly observed, which are consistent with those shown in Fig. 1. In addition, a sub-shell \(N = 32\) is observed in Ca isotopes.

\[
E_{\text{pair}} = \frac{1}{2} \int dr \Delta(r) \tilde{\rho}(r). \tag{15}
\]

In the following, the possible neutron halos in the Ca, Ni, Zr, and Sn isotopes are examined—particularly those in the weakly bound nuclei close to the neutron drip line, where the Fermi surfaces are very close to the continuum threshold and the valence neutrons can be easily scattered to the continuum by the pairing correlation.

In Fig. 4, the neutron canonical single-particle structure as a function of the mass number is plotted for the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes. Details on obtaining the canonical single-particle levels are presented in Refs. [104, 105]. The neutron Fermi energy \(\lambda_n\) and the canonical single-particle energies \(\epsilon\) are shown. As the neutron number increases, the Fermi energy \(\lambda_n\) in each chain increases, finally reaching the continuum threshold, while all the HF single-particle levels decrease. The traditional shell closures, i.e., \(N = 28, 40\) in Ca isotopes, \(N = 40, 50\) in Ni isotopes, \(N = 82\) in Zr isotopes, and \(N = 82\) in Sn isotopes, can be observed, exhibiting large gaps. Different single-particle structures are revealed in the Ca, Ni, Zr, and Sn chains, whereby halos may be formed. In the Ni chain, above the shell closure of \(N = 50\), there are several weakly bound states and low-lying...
positive canonical states in the continuum with small angular momenta, which favor the formation of halos. For example, in $^{86}$Ni, around the Fermi surface, there are two weakly bound states, i.e., $2d_{5/2}$ and $3s_{1/2}$, and one low-lying positive canonical state, i.e., $2d_{3/2}$. The Sn chain is similar to the Ni chain but has more advantages for halo formation, where weakly bound states and the low-lying positive states in the continuum exist above the $N = 82$ shell closure. Additionally, the Fermi surface $\lambda_n$ gradually approaches 0, and the Sn isotopes in a large mass region are weakly bound. In the Ca chain, above the shell closure of $N = 40$, the main state is $1g_{9/2}$, which evolves from a canonical positive state in the continuum ($A \leq 62$) to a weakly bound level ($A \geq 64$). Although there is a possibility of valence neutrons occupying the $1g_{9/2}$ orbital, the contributed density is very localized owing to the large central barrier. In the neutron-rich Ca isotopes, the low-lying positive canonical states in the continuum $3s_{1/2}$ and $2d_{5/2}$ also play important roles. The formation of halos is most unlikely for the Zr chain, where the shell closure of $N = 82$ is located around the threshold of the continuum and it is difficult for the valence neutrons to overcome the large gap and occupy the continuum.

In Fig. 5, the neutron root-mean-square (rms) radii

$$r_{\text{rms}} = \sqrt{\frac{\int dr 4\pi r^4 \rho(r)}{\int dr 4\pi r^2 \rho(r)}}$$  \hspace{1cm} (16)

are plotted for the Ca, Ni, Zr, and Sn isotopes, which are based on Skyrme–HFB calculations with the GF method (filled circles and solid lines) and box-discretized method (open triangles and dashed lines) employing the SLy4 parameter set. The radii $r = b_0 A^{1/3}$ in the traditional liquid-drop model (black lines) are shown as well, with the coefficient $b_0$ determined via the radii of deeply bound nuclei. In the 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, with the addition of neutrons, the nuclear rms radii $r_{\text{rms}}$ increase steeply and deviate from the radii $A^{1/3}$ rule. For example, in the Ca chain, compared with the isotopic trend in $N \leq 20$ with $r \approx 0.991A^{1/3}$, the neutron rms radii in $^{50}$Ca and the heavier isotopes exhibit steep increases with an increase in $N$. In this mass range, possible neutron halos may occur. Additionally, odd–even staggering of rms radii can be clearly observed in the Sn chain, where the odd-$A$ nuclei $^{151–165}$Sn have larger rms radii than the neighboring two even–even nuclei. Details are presented in Ref. [77]. The odd–even staggering phenomena in nuclear radii and nuclear mass have attracted considerable research interest in recent years [106–112].

In exotic nuclei, diffuse density distributions in the coordinate space are often observed. Thus, in Fig. 6, to explore the exotic structures in the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes, we also plot the neutron density distributions $\rho(r)$, where the solid and dashed lines indicate...
those obtained via the GF method and the box-discretized method, respectively. As a global trend, the neutron density distributions are extended with an increase in the neutron number. The shell structures significantly affect the density distribution; i.e., compared with the bound nuclei, the density distributions of the neutron-rich nuclei in the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes with the neutron number exceeding the neutron closure $N = 28, 50, 50, 82$ are far more extended, which is consistent with the behaviors of the rms radii plotted in Fig. 5. In addition, compared with the Ca and Zr chains, the Ni and Sn chains exhibit more diffuse density distributions, which can be explained by their small two-neutron separation energies $S_{2n}$ in a large mass range, as shown in Fig. 1. For the Zr isotopes, the density distributions are relatively localized. The large $S_{2n}$ shown in Fig. 1 suggests the absence of halos in Zr isotopes. However, according to the RCHB theory with the NLSH parameter set [113] and the continuum Skyrme–HFB theory with the SK14 parameter set [74, 114], giant halos in Zr isotopes have been predicted. In all isotopes, compared with the box-discretized method predicting nonphysical sharp reductions in density at the space boundary, the GF method can better describe the extended density distributions—particularly for very neutron-rich isotopes. Additionally, the densities obtained via the GF method can be independent of the space sizes, as discussed in Ref. [77], which are mainly determined by the proper boundary conditions of the bound states, weakly bound states, and the continuum employed when constructing the GFs.

To explore the contributions of different partial waves to the extended density distributions in Fig. 6, taking the neutron-rich (a) $^{64}$Ca, (b) $^{86}$Ni, (c) $^{120}$Zr, and (d) $^{174}$Sn as examples, we plot in Fig. 7 the compositions $\frac{\rho_{0}(r)}{\rho(r)}$ as functions of the radial coordinate $r$. As shown, outside the nuclear surface referring to the right boundary of the shallow regions of the total nuclear density distributions, the orbitals located around the Fermi surface have the most significant effect on the density distributions. For example, in neutron-rich $^{64}$Ca, the partial waves $p_{1/2}$, $f_{5/2}$, $g_{9/2}$, $h_{11/2}$, and $d_{5/2}$ contribute significantly to the total density in the area of $5 \text{ fm} < r < 15 \text{ fm}$. These levels are located within $\sim 5 \text{ MeV}$ around the Fermi surface, as shown in Fig. 8, where the neutron canonical single-particle levels as well as the occupation probabilities are presented. As we move further in the coordinate space with $r > 15 \text{ fm}$, the contributions of the partial waves $s_{1/2}$ and $d_{5/2}$ with small angular momenta increase significantly, while the contributions of other partial waves decrease. In the case of $^{86}$Ni, the single-particle levels $2d_{5/2}$, $3g_{9/2}$, and $2d_{5/2}$ are located above the neutron shell of $N = 50$ and close to the Fermi surface, playing the main role in the neutron density distribution. Although the positive state $1g_{7/2}$ is also very close to the Fermi surface, it contributes little to the density in the large coordinate space owing to the large centrifugal barrier. For the nucleus $^{120}$Zr with the neutron number very close to the closure of $N = 82$,
the single-particle levels between the 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 the densities in the large coordinate space. The insignificant occupation of the positive state $2f_{7/2}$ leads to a small contribution to the density. Regarding the neutron-rich $^{174}$Sn with the neutron number exceeding the closure of $N = 82$, the weakly bound single-particle levels $2f_{7/2}$, $2f_{5/2}$, $3p_{3/2}$, and $3p_{1/2}$ with small angular momenta play the key role in the extended density distributions in the large coordinate space. From this analysis, we can conclude that the single-particle levels around the Fermi surface—particularly the waves with small angular momenta—are the main cause of the extended nuclear density distributions.

Fig. 7. Contributions of different partial waves to the total neutron density $\rho_{n}(r)/\rho(r)$ as a function of the radial coordinate $r$ for the neutron-rich nuclei (a) $^{64}$Ca, (b) $^{66}$Ni, (c) $^{120}$Zr, and (d) $^{174}$Sn. The shallow regions are for the nuclear density distributions $\rho(r)$, which are rescaled by multiplying by a factor of 5.

In Fig. 8, the particle occupation probabilities $v^2$ on different canonical levels $e^{can}_n$ are indicated by the lengths of the lines. Without pairing, the values of the occupation probabilities $v^2$ should be either 1 or 0, separated by the Fermi surface. With the effect of pairing, the nucleons occupying the levels below the Fermi surface can be scattered to higher levels, which results in the occupation of the weakly bound states above the Fermi surface and even levels in the continuum. In the neutron-rich nuclei $^{64}$Ca, $^{66}$Ni, $^{120}$Zr, and $^{174}$Sn, the numbers of neutrons $N_a = \sum_{\lambda_a > \lambda_f} (2j + 1)v^2$ scattered above the Fermi surface $\lambda_a$ are 4.33, 2.51, 0.159, and 0.173, respectively. In the case of $^{64}$Ca, the weakly bound single-particle $1g_{9/2}$ contributes approximately 3.7 neutrons.

To explore the effects of pairing, we plot in Fig. 9 the numbers of neutrons $N_n$ scattered above the Fermi surface for the (a) Ca, (b) Ni, (c) Zr, and (d) Sn chains obtained via the Skyrme–HFB theory with the GF method. As shown, large numbers of neutrons are scattered from the single-particle levels below the Fermi surface to the weakly bound states above the Fermi surface and even levels in the continuum owing to the pairing—particularly in the nuclei with the neutron number filling the half-full shells. Additionally, an obvious shell structure is observed. When the number of neutrons reaches a magic number, i.e., $N = 28, 40$ in Ca isotopes, $N = 50, 82$ in Ni isotopes, and $N = 50, 82, 126$ in Sn isotopes, $N_a$ is almost 0 owing to the absence of the pairing for the closed-shell nuclei. Additionally, at the points of $N = 32$ in the Ca isotopes, $N = 54, 68$ in the Zr isotopes, and $N = 88$ in the Sn isotopes, very small numbers of neutrons ($N_a$) are obtained, indicating weak pairing in these nuclei, along with the possible existence of subshells and new magic numbers. Furthermore, the evolution of $N_a$ is consistent with the trend of the pair energy $-E_{\text{pair}}$ in Fig. 3.
In Fig. 10, we further investigate the number of neutrons occupying the continuum with single-particle energies of $\varepsilon > 0$ MeV, i.e., $N_0 = \sum_{\varepsilon_k > 0} (2j + 1) v_k^2$. Compared with the number of neutrons $N_f$ occupying the levels above the Fermi surface, the number of neutrons occupying the continuum $N_0$ is significantly smaller. For example, in the Ca chain, $N_0$ is less than 1 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 of $\varepsilon = 0.198$ MeV and a high occupation probability of $v^2 = 0.197$, resulting in almost 1.979 neutrons occupying it. However, in the neighboring $^{60}$Ca, a very low occupation probability $v^2 = 0.015$ of $1g_{9/2}$ is obtained, and in $^{64}$Ca, the $1g_{9/2}$ state drops to a weakly bound level with energy of $\varepsilon = -0.072$ MeV. After the neutron contribution is removed...
Fig. 9 (Color online) Number of neutrons $N_j$ occupying the single-particle levels above the Fermi surface $\lambda_0$ as a function of the mass number $A$ for the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes calculated according to the Skyrme–HFB theory with the GF method.

Fig. 10 (Color online) Number of neutrons $N_0$ occupying in the continuum (above the threshold $\epsilon = 0$ MeV) as a function of the mass number $A$ for the (a) Ca, (b) Ni, (c) Zr, and (d) Sn isotopes calculated according to the Skyrme–HFB theory with the GF method.
from $1g_{s/2}$ in $^{62}$Ca, only 0.38 neutrons are in the continuum, which is denoted by an empty circle in panel (a). Except for the Sn chain, the shape of the evolution of $N_0$ is very close to those of the pairing energy and pairing gap. Although the case of the Sn chain becomes very complex, we can observe the shell structure at $N = 82$ and $N = 126$, where $N_0$ is almost 0.

5 Summary

In this study, the exotic nuclear properties of neutron-rich Ca, Ni, Zr, and Sn isotopes were examined systematically according to the continuum Skyrme–HFB theory in the coordinate space formulated with the GF method, in which the pairing correlations, the couplings to the continuum, and the blocking effects for the unpaired nucleon in odd-$A$ nuclei are treated properly.

First, the two-neutron separation energies $S_{2n}$ and one-neutron separation energies $S_n$ were calculated, which were consistent with experimental data. Significant differences exist for the drip lines determined by $S_{2n}$ and $S_n$. In the Ca, Ni, Zr, and Sn isotopes, the drip line nuclei are $^{67}$Ca, $^{89}$Ni, $^{120}$Zr, and $^{177}$Sn according to $S_{2n}$ and $^{60}$Ca, $^{86}$Ni, $^{120}$Zr, and $^{148}$Sn according to $S_n$. Owing to the absent contribution of pairing energy from the single unpaired odd neutron, the neutron pairing energies ($E_{pair}$) of the odd-$A$ nuclei are approximately 2 MeV lower than those of the neighboring even–even nuclei. This explains why the drip lines determined via $S_n$ are much shorter than those determined via $S_{2n}$.

In addition, from the fluctuation trends of the pairing energy, the traditional neutron magic numbers are clearly displayed, i.e., $N = 28, 40$ 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 the possible halo structures in the neutron-rich Ca, Ni, Zr, and Sn isotopes, the neutron single-particle structures, the rms radii, and the density distributions were investigated. In the neutron-rich Ca, Ni, Sn nuclei—particularly the weakly bound nuclei close to neutron drip line—the rms radii increase sharply, with significant deviations from the traditional $r \propto A^{1/3}$ rule. Additionally, very diffuse spatial density distributions are observed in these nuclei, possibly indicating a halo phenomenon therein. By analyzing the contributions of different partial waves to the total density, we found that the orbitals located around the Fermi surface—particularly those with small angular momenta—are the main cause of the extended nuclear density and large rms radii.

Finally, the numbers of halo nucleons that can reflect the effects of pairing were examined. Two different numbers of neutrons were defined: $N_A$ neutrons occupying the single-particle levels above the Fermi surface $\lambda_A$ and $N_0$ neutrons occupying the continuum. We found that the evolutions of $N_A$ and $N_0$ with respect to the mass number $A$ are consistent with the trend of the pairing energy $-E_{pair}$, which supports the key role of the pairing correlations in the halo phenomena.

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Data Availability The data that support the findings of this study are openly available in Science Data Bank at https://www.doi.org/10.57760/sciedb.j00186.00106 and https://cstr.cn/31253.11.sciedb.j00186.00106.

Declarations

Conflict of interest The authors declare that they have no competing interests.

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