Effects of pairing, continuum and deformation on particles in the classically forbidden areas

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Abstract

Particles in the classically forbidden areas are studied based on the deformed relativistic Hartree-Bogoliubov theory in continuum with PC-PK1 for magnesium isotopes. It is shown the deformation effect makes the number of particles in the classically forbidden areas increase. By analyzing the neutron and proton radii, it is found that the largest deviations from the empirical values appear at the predicted neutron halo nuclei $^{42}$Mg and $^{44}$Mg. Consistently, a notable increase at $^{42}$Mg and $^{44}$Mg is found in the total number of neutrons in the classically forbidden areas that includes the number of neutrons in continuum.

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I. INTRODUCTION

The development of radioactive ion beam facilities worldwide stimulates greatly the study of the so-called exotic nuclei far from the $\beta$ stability line [1–11]. Exciting discoveries in exotic nuclei including halo phenomena [12], pygmy resonances [13], and changes of magic numbers [14] have attracted a lot of attention.

As a microscopic quantum system, atomic nucleus has many quantum characteristics and exhibits rich quantum phenomena. The quantum tunneling effect allows nucleons to move in the classically forbidden (CF) areas and as a consequence has impacts on nuclear density distributions. For exotic nuclei that are very weakly bound systems, and particularly for halo nuclei that have very extended spatial density distributions, the tunneling effect is extremely important. Therefore, it is of particular interest to investigate particles in the CF areas for exotic nuclei.

In Refs. [15, 16], particles in the CF areas for calcium isotopes were investigated with the spherical Skyrme Hartree-Fock theory. It was found that with increasing mass number $A$, the neutron number in the CF areas increases due to the increase of occupied neutrons in open shell while the proton number in the CF areas decreases due to proton orbits becoming more tightly bound. As the difference between the numbers of proton and neutron in the CF areas is very similar to the difference of the density distributions of proton and neutron, the particle number in the CF areas can give a signal for the halo or skin [16].

For exotic nuclei, pairing correlations and the coupling to continuum need to be taken into account properly [17, 18]. Meanwhile, for open shell nuclei, one has to further deal with the deformation effect carefully. To better understand the quantum tunneling effect, it is necessary to investigate particles in the CF areas within a theoretical model that includes simultaneously the effects of pairing, continuum and deformation.

The covariant density functional theory (CDFT) describes nucleons as Dirac spinors which interact by exchanging effective mesons or point-coupling in a microscopic and covariant way. The CDFT naturally includes the nucleonic spin degree of freedom and automatically results in nuclear spin-orbit potential with the empirical strength. It can give naturally the pseudospin symmetry in the nucleon spectrum [19–24] and the spin symmetry in anti-nucleon spectrum [24, 25]. Furthermore, the CDFT can include the nuclear magnetism [26], which plays an important role in nuclear magnetic moments [27–31] and nuclear rotations [32–41].
Due to its successful description of many nuclear phenomena, the CDFT has become one of the most important microscopic methods in theoretical nuclear physics and has attracted wide attention [2, 9, 10, 32, 42–44].

Based on the CDFT, taking advantages of the Bogoliubov transformation and solving the relativistic Hartree-Bogoliubov equations in the coordinate space, the relativistic continuum Hartree-Bogoliubov (RCHB) theory was constructed to consider pairing correlations and continuum in a unify and self-consistent way [18, 45]. The RCHB theory has provided an interpretation of the halo in $^{11}$Li [18], predicted the giant halos [46–48], reproduced the interaction cross section and the charge-changing cross sections in light exotic nuclei in combination with the Glauber theory [49, 50], better restored the pseudo-spin symmetry in exotic nuclei [20, 21], and made predictions of exotic phenomena in hypernuclei [51] and new magic numbers in superheavy nuclei [52].

In order to describe deformed nuclei properly, the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) was developed by solving the deformed relativistic Hartree-Bogoliubov equation in a Dirac Woods-Saxon basis [53–55]. The DRHBc theory was applied to study the chain of magnesium isotopes and an interesting shape decoupling between the core and the halo was predicted in $^{44}$Mg and $^{42}$Mg [53, 54]. Later, the DRHBc theory has been extended to incorporate the blocking effect which is required for the description of odd-nucleon systems [55], and the density-dependent meson-nucleon couplings [56]. Recently, using the DRHBc theory, the puzzles concerning the radius and configuration of valence neutrons in $^{22}$C were resolved and $^{22}$C was predicted to be a new candidate of deformed halo nuclei with shape decoupling effects [57].

In this work, the DRHBc theory is applied to investigate particles in the CF areas for the magnesium isotopes. The results are compared with those from the RCHB theory and the RCHB calculations without pairing. The effects of pairing, continuum and deformation on particles in the CF areas are explored. The neutrons in continuum are included to discuss the relevant quantum effects. Particles in the CF areas for a given single-particle state are also investigated.
II. THEORETICAL FRAMEWORK

The starting point of the CDFT is a Lagrangian density where nucleons are described as Dirac spinors which interact via exchange of effective mesons or point-coupling. With the mean-field and the no-sea approximations, one can obtain the energy density functional for the nuclear system. According to the variational principle, one obtains the equation of motion for the nucleons by minimizing the energy density functional with respect to the densities. Without pairing correlations, the relativistic Hartree equation can be solved either in the basis space or in the coordinate space [42, 58–60].

In the RCHB theory, the pairing is taken into account by Bogoliubov transformation and the relativistic Hartree-Bogoliubov equations are solved in the coordinate space with spherical symmetry [18, 45]. The details of the RCHB theory can be found in Ref. [45].

In the DRHBc theory, the potentials and densities are expanded in terms of the Legendre polynomials,

\[ f(r) = \sum_{\lambda} f_{\lambda}(r) P_{\lambda}(\cos \theta), \quad \lambda = 0, 2, 4, \ldots, \] (1)

to include the deformation degree of freedom. The deformed relativistic Hartree-Bogoliubov equations have been solved in a Dirac Woods-Saxon basis, in which the radial wave functions have a proper asymptotic behavior in large \( r \) [53–55]. The details of the DRHBc theory can be found in Ref. [54].

Following Ref. [16], the number of particles in the CF areas for a single-particle state \( \beta \), \( N_{\text{CF}}^{\beta} \), is defined by

\[ N_{\text{CF}}^{\beta} = \int_{R_{\text{CF}}^{\beta}} \rho_{\beta}(r) d^3r, \] (2)

in which \( R_{\text{CF}}^{\beta} \) is the position where the mean field potential is equal to the single-particle energy \( e_{\beta} \), i.e., \( V(R_{\text{CF}}^{\beta}) = e_{\beta} \), and \( \rho_{\beta} \) is the density of the single-particle state \( \beta \). The number of particles in the CF areas are calculated by

\[ N_{\text{CF}} = \sum_{\beta} v_{\beta}^2 \cdot d_{\beta} \cdot N_{\text{CF}}^{\beta}, \] (3)

where \( v_{\beta}^2, d_{\beta} \) are the occupation probability and the degeneracy of single-particle state \( \beta \), respectively. The summation runs over all of the bound single-particle states.
In the spherical RCHB theory, $N_{\text{CF}}^\beta$ can be calculated by

$$N_{\text{CF}}^\beta = \int_{R_{\text{CF}}^\beta}^{\infty} \rho_\beta(r) d^3r$$

$$= \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \int_{R_{\text{CF}}^\beta}^{\infty} r^2 \rho_\beta(r) dr$$

$$= 4\pi \int_{R_{\text{CF}}^\beta}^{\infty} r^2 \rho_\beta(r) dr,$$

in which $R_{\text{CF}}^\beta$ is the radial coordinate where the mean field potential is equal to the single-particle energy, i.e., $V(R_{\text{CF}}^\beta) = e_\beta$. The boundary of the CF areas is a spherical surface with radius $R_{\text{CF}}^\beta$ correspondingly.

In the DRHBc model, the boundary of the CF areas is no longer a sphere but a surface determined numerically. For every fixed $\theta$, there exists a radial position $R_{\text{CF}}^\beta(\theta)$, and they satisfy

$$V[R_{\text{CF}}^\beta(\theta), \theta] = e_\beta. \quad (5)$$

As a result, $N_{\text{CF}}^\beta$ is calculated by

$$N_{\text{CF}}^\beta = \int_{R_{\text{CF}}^\beta}^{\infty} \rho_\beta(r) d^3r$$

$$= \sum_\lambda \int_0^{2\pi} d\phi \int_0^\pi P_\lambda(\cos \theta) \sin \theta \left[ \int_{R_{\text{CF}}^\beta(\theta)}^{\infty} r^2 \rho_\beta^\lambda(r) dr \right] d\theta$$

$$= 2\pi \sum_\lambda \int_0^\pi P_\lambda(\cos \theta) \sin \theta \left[ \int_{R_{\text{CF}}^\beta(\theta)}^{\infty} r^2 \rho_\beta^\lambda(r) dr \right] d\theta. \quad (6)$$

### III. NUMERICAL DETAILS

To explore the effects of pairing, continuum and deformation, the even-even Mg nuclei from proton drip line to neutron drip line are investigated by using the DRHBc theory and the RCHB theory. For the particle-hole channel, the relativistic density functional PC-PK1 [61], which has turned out to be very successful in providing good descriptions for the isospin dependence of the binding energy along either the isotopic or the isotonic chain [62, 63], is adopted. For the particle-particle channel, the pairing is taken into account by using a density-dependent zero-range pairing force. In the present calculations, we fix the box size $R_{\text{box}} = 20$ fm, the mesh size $\Delta r = 0.1$ fm, and the angular momentum cutoff $J_{\text{max}} = 23/2 \hbar$. It was shown that these numerical conditions give results accurately enough
in energies and radii for light nuclei [54, 58, 64]. In the DRHBc calculations, the maximal order $\lambda_{\text{max}} = 4$ is adopted in the Legendre expansion Eq. (1) of the deformed potentials and densities. For the determination of the Woods-Saxon basis an energy cutoff $E_{\text{cut}}^+ = 300$ MeV for positive-energy states is used, and the number of negative-energy states in the Dirac sea is the same as that of positive-energy states above the Dirac gap [58].

IV. RESULTS AND DISCUSSION

FIG. 1: Binding energies per nucleon from the DRHBc calculations for Mg as functions of neutron number. (a): the size of each point is proportional to the deviation between the calculated neutron root-mean-square radius $R_n$ and the empirical value $r_0^nN^{1/3}$, in which $r_0^n = 1.197$ fm, determined from $^{26}$Mg (star), is the smallest ratio $R_n/N^{1/3}$ in Mg isotopic chain. (b): same to (a) but for proton, with the empirical value $r_0^pZ^{1/3}$, in which $r_0^p = 1.222$ fm, also determined from $^{26}$Mg (star).

In Fig. 1, the binding energies per nucleon for magnesium isotopes from the DRHBc calculations are shown as functions of neutron number. It can be seen that the binding energies per nucleon decrease as neutron number moves away from 12, i.e. $^{24}$Mg, which is the
most stable nucleus in Mg isotopes. The deviations between the calculated neutron (proton) root-mean-square (rms) radii $R_n(R_p)$ and the empirical values $r_0^n N^{1/3}(r_0^p Z^{1/3})$ denoted by the size of each point are shown. $r_0^n$ and $r_0^p$ are the smallest ratios $R_n/N^{1/3}$ and $R_p/Z^{1/3}$ determined from $^{26}$Mg (star). In general, as nucleus moves away from $^{26}$Mg, the deviation from the empirical value becomes larger for both neutron and proton. For neutron, the largest deviations from the empirical values appear at $^{42}$Mg and $^{44}$Mg; this is consistent with the suggested halo phenomena in Refs. [53, 54]. For proton, the empirical value $r_0^p Z^{1/3}$ is a constant, and after $^{26}$Mg the proton radius increases gradually except for $^{46}$Mg. Instead of the increase of neutron radius from $^{44}$Mg to $^{46}$Mg, the proton radius is slightly reduced, as $^{44}$Mg has a prolate shape whereas $^{46}$Mg is spherical in the DRHBc calculations.

FIG. 2: The number of particles in the CF areas for neutron, proton and matter from (a) the RCHB calculations without pairing, (b) the RCHB calculations, and (c) the DRHBc calculations as functions of neutron number for magnesium isotopes.

It was suggested that particles in the CF areas can also provide information on the
appearance of halos or skins \cite{15, 16}. Figure 2 shows the number of particles in the CF areas for neutron, proton and matter as functions of neutron number for magnesium isotopes. In general, with the neutron number, the evolution trends from the different calculations are consistent. The number of protons in the CF areas ($N_{\text{CF}}^p$) gradually decreases with the neutron number, whereas the number of neutrons in the CF areas ($N_{\text{CF}}^n$) rapidly increases. As a result, the number of nucleons in the CF areas ($N_{\text{CF}}^m$) also increases with the neutron number. The similar results have been found in previous study with Skyrme Hartree-Fock model \cite{16}. For the nuclei near the neutron drip line, the difference $N_{\text{CF}}^n - N_{\text{CF}}^p$ becomes as large as 2. $N_{\text{CF}}^m$ increases with the neutron number due to the increase of occupied neutrons in weakly bound single-particle levels whereas $N_{\text{CF}}^p$ decreases due to proton orbits becoming more tightly bound, which is the reason for the big difference and has been analyzed carefully in Ref. \cite{16}. Although consistent in general, there are some differences between the results from the DRHBc theory and the RCHB theory. A prominent bump can be seen near $^{24}\text{Mg}$ in the DRHBc calculations.

In order to see more clearly the differences and the possible deformation effect, for Mg isotopes, the number of neutrons in the CF areas calculated by the DRHBc theory and the RCHB theory, and the ground state deformations from the DRHBc calculations are shown in Fig. 3. As seen in Fig. 3(b), the ground states of $^{20}\text{Mg}$, $^{32}\text{Mg}$ and $^{46}\text{Mg}$ are spherical in the DRHBc calculations. As the neutron number increases from 8 to 20 and from 20 to 34, the shape of nucleus goes from spherical to prolate, and then back to spherical. The ground state of $^{24}\text{Mg}$ is well deformed with the largest quadrupole deformation $\beta_2 \approx 0.60$, which is consistent with the experimental value $\beta_2 = 0.609(6) \ [65]$. By comparing (a) and (b), one can find the appearance of the bump near $^{24}\text{Mg}$ is caused by the strong deformation effect. Moreover, the Mg isotopes with $20 < N < 34$ are also deformed with large deformations $\beta_2 \approx 0.3 \sim 0.5$, and $N_{\text{CF}}^n$ from the DRHBc theory are larger than those from the RCHB theory in this region. Then it is concluded that the deformation effect makes the number of particles in the CF areas increase.

To better understand the deformation effect on the number of particles in the CF areas, taking $^{24}\text{Mg}$ as an example, the constraint DRHBc calculations with $\beta_2 = 0.1, 0.2, 0.3, 0.4, 0.5$ and 0.6 are performed. Here pairing correlations are not taken into account to exclude the influence of the pairing effect. It is found that both the neutron number and proton number in the CF areas increase with increasing $\beta_2$ and the increases in $N_{\text{CF}}^n$ and $N_{\text{CF}}^p$ are
FIG. 3: (a) The number of neutrons in the CF areas calculated by the RCHB theory without pairing, the RCHB theory and the DRHBc theory as functions of neutron number for magnesium isotopes. (b) The ground state quadrupole deformation $\beta_2$ for magnesium isotopes as a function of neutron number within the DRHBc calculations. The experimental values ("EXP.") are taken from Ref. [65].

very close. From $\beta_2 = 0.1$ to $\beta_2 = 0.6$, the numbers of neutrons in the CF areas are 1.331, 1.393, 1.542, 1.639, 1.761 and 1.847, respectively. To be more explicit, the contributions of different single-neutron states are further investigated. Here each state is labeled with $\Omega_i^\pi$ where $\Omega$ is the projection of angular momentum on the symmetry axis, $\pi$ is the parity, and $i$ is used to order the level in the $\Omega^\pi$–block, as $\Omega$ and $\pi$ are good quantum
numbers in the axially deformed system. It is found that the increase of \( N_{\text{CF}} \) mainly (more than 85%) comes from the contributions of the two most deeply bound single-neutron states \((1/2)_1^+\) and \((1/2)_1^-\), whereas for other occupied states, the neutron numbers in the CF areas increase or decrease very little.

![Density distributions and the boundary of the classically forbidden areas (dashed line) of single-neutron states \((1/2)_1^+\), \((1/2)_1^-\), and \((1/2)_2^+\) from the constraint DRHBc calculations without pairing at the quadrupole deformation \(\beta_2 = 0.1, 0.3\) and 0.5. The \(z\) axis is the symmetry axis. In each panel, the corresponding single-neutron energy, the number of neutrons in the classically forbidden areas and the two largest spherical components are given.](image)

**FIG. 4:** For \(^{24}\text{Mg}\), density distributions and the boundary of the classically forbidden areas (dashed line) of single-neutron states \((1/2)_1^+\), \((1/2)_1^-\), and \((1/2)_2^+\) from the constraint DRHBc calculations without pairing at the quadrupole deformation \(\beta_2 = 0.1, 0.3\) and 0.5. The \(z\) axis is the symmetry axis. In each panel, the corresponding single-neutron energy, the number of neutrons in the classically forbidden areas and the two largest spherical components are given. It can be seen that the three states become more bound with the increasing deformation. For the states \((1/2)_1^+\) and \((1/2)_1^-\), the numbers of neutrons in CF areas increase by more than 0.2, but for the state \((1/2)_2^+\), the number of neutrons in
CF areas decreases only by about 0.03. When the deformation increases, as seen in Fig. 4, on one hand, the intersection point between the boundary of the CF areas and the z axis moves away from the center, whereas that between the boundary and the x axis approaches the center, as a result the CF areas expand with the deformation. On the other hand, the density distributions of neutron states also evolve with the deformation as a result of the changes of mean field potential, the single-neutron energies and the component mixing. For the most deeply bound states ($1/2^+_1$ and $1/2^-_1$), not only the CF areas expand, but also the neutron densities at the boundary of the CF areas increase a bit, and then their numbers of neutrons in the CF areas increase a lot and dominate the increase of $N_{CF}^n$. For other states like $(1/2)_2^+$, the boundaries of CF areas are farther away from the center and the density distributions are more diffuse, therefore the deformation effect on them is weak and their numbers of neutrons in the CF areas slightly change with deformation. Then it is concluded that, the deformation will increase the particle number in the CF areas and the most deeply bound single-particle states play the dominate roles in this effect.

As seen in Fig. 3(a), there also exist some differences between $N_{CF}^n$ from the RCHB calculations with and without pairing. It can be seen that, for the isotopes with $8 \leq N \leq 20$, their results are very close, but for the neutron-rich nuclei, $N_{CF}^n$ from the RCHB calculations without pairing are larger than those from the RCHB calculations obviously. For the stable isotopes with $8 \leq N \leq 20$, neutrons occupy the well bound single-particle levels which are slightly affected by pairing correlations. For the neutron-rich side, pairing correlations can scatter valance neutrons into continuum, which are not taken into account in $N_{CF}^n$ temporarily.

It is noted that the states in continuum have energies higher than the threshold, which means they can not be occupied from the classical perspective, therefore the number of particles in continuum ($N_{continuum}$) should contribute also to the number of particles in the CF areas. In order to give a reasonable investigation of the relevant quantum effects, Fig. 5 shows the total number of neutrons in the CF areas including neutrons in continuum ($N_{continuum}^n$). For the nuclei with $8 \leq N \leq 20$, the numbers of neutrons in continuum are very small or even zero. For the neutron-rich side, the numbers of neutrons in continuum are remarkable. By comparing $N_{CF}^n + N_{continuum}^n$ from the DRHBc theory and those from the RCHB theory, one can find that they are comparable, although $N_{CF}^n$ from the DRHBc theory are larger than $N_{CF}^n$ from the RCHB theory. In the DRHBc calculations, a notable
FIG. 5: The total number of neutrons in the CF areas including neutrons in continuum from the RCHB calculations and the DRHBc calculations as functions of neutron number for magnesium isotopes. The number of neutrons in the CF areas without neutrons in continuum as functions of neutron number are shown with dashed lines and the shaded region represents neutrons in continuum.

increase of $N_{\text{CF}}^n + N_{\text{continuum}}^n$ can be seen at $^{42}\text{Mg}$ and $^{44}\text{Mg}$ and the increase mainly comes from the increase of $N_{\text{continuum}}^n$. This phenomenon is consistent with the previous predictions of halo phenomena in nuclei $^{42}\text{Mg}$ [54] and $^{44}\text{Mg}$ [53].

To further study the relation between halo phenomenon and particles in the CF areas, taking the neutron-rich nucleus $^{44}\text{Mg}$ as an example, the number of particles in the CF areas for each single-particle state $\beta$ ($N_{\text{CF}}^\beta$) from the RCHB calculations and the DRHBc calculations as functions of single-particle energy are shown in Fig. 6. Similar trend of $N_{\text{CF}}^\beta$ can be found for neutron and proton, as they share the same mean field self-consistently. However, one can not find a monotonic relationship between $N_{\text{CF}}^\beta$ and the single-particle energy $e_\beta$ in both theoretical calculations. In Fig. 6(a), by comparing the $N_{\text{CF}}^\beta$ with the
corresponding orbital angular momentum $l$ of the single-particle state, one can find a smaller $N_{\text{CF}}^\beta$ for the single-particle state with a larger $l$. This feature has been also seen in Ref. [16] as a state with large $l$ has a high centrifugal barrier. A weakly bound single-particle state with low orbital angular momentum $l$ is helpful to the formation of halos [18, 46]. It is seen that the weakly bound 2$p$ states contribute more $N_{\text{CF}}$ than the others.

In Fig. 6(b), the evolutions of $N_{\text{CF}}^\beta$ in the DRHBc calculations are similar to those in the RCHB calculations. It can be seen, the $(1/2)_5^-$ state and the $(3/2)_3^-$ state, that are near the threshold, contribute the largest $N_{\text{CF}}^\beta$. These two weakly bound orbitals were suggested to give rise to the formation of the halo in $^{44}\text{Mg}$ [53] and we find the $p$ wave components for the $(1/2)_5^-$ state and the $(3/2)_3^-$ state are 69.6% and 81.5%, respectively. On the other hand, the weakly bound $(5/2)_1^-$ state and the $(3/2)_2^-$ state have much smaller $N_{\text{CF}}^\beta$, as their dominant
components are 97.4% and 80.1% $f$ wave with a high centrifugal barrier. Therefore, it is concluded that a weakly bound single-particle state with low centrifugal barrier contributes more $N_{\text{CF}}$.

V. SUMMARY

In summary, particles in the classically forbidden areas for magnesium isotopes are investigated within the relativistic continuum Hartree-Bogoliubov theory and the deformed relativistic Hartree-Bogoliubov theory in continuum with PC-PK1. The effects of deformation, pairing and continuum on particles in the classically forbidden areas are studied. Particles in the classically forbidden areas for a given single-particle state have been investigated and the similar conclusion as in Ref. [16] has been obtained, i.e., a weakly bound single-particle state with low centrifugal barrier contributes more particles in the classically forbidden areas.

With the neutron number increasing, as in Ref. [16], the number of neutrons in the classically forbidden areas rapidly increases, whereas the number of protons in the classically forbidden areas gradually decreases. Comparing the results from the DRHBc theory and the RCHB theory, it is found that the deformation effect enhances the number of neutrons in the classically forbidden areas. The most deeply bound single-particle states play the dominate roles in the increase caused by deformation.

From the stable isotopes to the proton-rich side or the neutron-rich side, the deviations from the empirical values of radii increase and the largest deviations appear at $^{42}$Mg and $^{44}$Mg. Including neutrons in continuum, a notable increase of the total number of neutrons in the classically forbidden areas at $^{42}$Mg and $^{44}$Mg has been found; this is consistent with the largest deviations from empirical values of radii at $^{42}$Mg and $^{44}$Mg shown in Fig. 1 and the predictions of halo phenomena in $^{42}$Mg [54] and $^{44}$Mg [53].

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