Extending the nuclear chart by continuum: from oxygen to titanium

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Nuclear masses ranging from O to Ti isotopes are systematically investigated with relativistic continuum Hartree-Bogoliubov (RCHB) theory, which can provide a proper treatment of pairing correlations in the presence of the continuum. From O to Ti isotopes, there are 402 nuclei predicted to be bound by the density functional PC-PK1. For the 234 nuclei with mass measured, the root mean square (rms) deviation is 2.23 MeV. It is found that the proton drip-lines predicted with various mass models are roughly the same and basically agree with the observation. The neutron drip-lines predicted, however, are quite different. Due to the continuum couplings, the neutron drip-line nuclei predicted are extended further neutron-rich than other mass models. By comparison with finite-range droplet model (FRDM), the neutron drip-line nucleus predicted by RCHB theory has respectively 2(O), 10(Ne), 10(Na), 6(Mg), 8(Al), 8(Si), 8(P), 6(S), 14(K), 10(Ca), 10(Sc), and 12(Ti) more neutrons.

Relativistic continuum Hartree-Bogoliubov theory; Nuclear mass table; O to Ti isotopes

In recent decades, unstable nuclear beams have extended our knowledge of nuclear physics from the stable nuclei to the exotic nuclei far away from the stability. The properties of these exotic nuclei, for instance, masses and decay-lives, are essential in understanding the nucleosynthesis via rapid neutron capture (r-process) [1-6]. Although considerable achievements in mass measurements have been made due to the development of new experimental techniques and facilities, most of the neutron-rich nuclei of relevance to the r-process are still beyond the experimental capability in the foreseeable future and therefore, we need to rely on robust theoretical nuclear models.

The widely-used global nuclear mass models can be classified into the following two categories. The first consists of macroscopic-microscopic models, such as finite-range droplet model (FRDM) [7] and Weizsäcker-Skyrme (WS) model [8], which are proved to work pretty well in the description of known nuclides, but its extrapolation to very neutron-rich nuclides is generally questionable. The second consists of microscopic mass models, for example, the Hartree-Fock-Bogoliubov (HFB) method based on nonrelativistic density functional theory (DFT) [9-11], which treats the macroscopic part and the microscopic corrections in a unified framework, and is believed to have a more reliable extrapolation to the unknown regions.

Apart from the nonrelativistic DFT, the covariant density functional theory (CDFT) has attracted research focus because of the successful description of many nuclear phenomena [12-16]. It can also include the nucleon spin degree of freedom naturally and result in the nuclear spin-orbit potential automatically with the empirical strength in a covariant way. It can reproduce well the isotopic shifts in the Pb region [17], and give naturally the origin of the pseudospin symmetry [18,19] as a relativistic symmetry [20-25] and the spin symmetry in the anti-nucleon spectrum [26,27]. It can include the nuclear magnetism [28], that is, a consistent description of currents and time-odd fields, which has an important role in the nuclear magnetic moments [29-33] and nuclear rotations [34-37]. Therefore, it is natural to investigate the nuclear masses based on CDFT.

The first CDFT mass table was reported for 2000 even-even nuclei with 8 ≤ Z ≤ 120 [38], but without including pairing correlations. Later, by including the pairing correlations with Bardeen-Cooper-Schrieffer (BCS) method, the ground-state properties of 1315 even-even nuclei with 10 ≤ Z ≤ 98 were calculated [39]. In 2005, by employing the state-dependent BCS method with a delta pairing force, the first systematic study of the ground-state properties for over 7000 nuclei was performed [40].

It is well known that, the pairing correlation has a critical role in open shell nuclei. In particular, for the exotic nuclei close to the nucleon drip-lines, where the Fermi levels are very close to the continuum threshold, pairing correlation can scatter the valence nucleons between the bound states and continuum, and therefore provide a significant coupling between them. As a result, some unbound nuclei predicted without pairing correlation can become bound. For example, Meng et al. [41] found that after taking into account the pairing correlation and the contribution from the continuum, the neutron-rich nuclei 60-72Ca predicted unbound without pair-
ing correlation are found to be bound. Therefore, the couplings between the bound states and the continuum due to the pairing correlation can strongly affect the drip-line position.

The BCS method is a popular method in dealing with pairing correlations, but not justified for exotic nuclei as it cannot include the contribution of continuum states properly. Conversely, Bogoliubov quasiparticle transformation can provide a unified description of the mean field and pairing correlation, and include the continuum appropriately when treated in coordinate representation.

In Refs. [15,42-45], the relativistic Hartree-Bogoliubov (RHB) theories in coordinate space have been developed for spherical nuclei. With the relativistic continuum Hartree-Bogoliubov (RCHB) theory [15,44], the first microscopic self-consistent description of halo in $^{11}$Li has been provided [42] and the giant halos in light and medium-heavy nuclei have been predicted [41,46,47]. The RCHB theory has been generalized to treat the odd particle system [48] and combined with the Glauder model, the charge-changing cross sections for C to F isotopes on a carbon target have been reproduced well [49]. For deformed nuclei, much effort has been made to develop a deformed RHB theory in continuum [50-54] and an interesting shape decoupling between the core and the halo was predicted [52,54]. Later, the deformed RHB theory in continuum has been extended to incorporate the blocking effect to treat odd nucleon system [55] and the density-dependent meson-nucleon couplings [56].

As the first step to investigate the impact of the continuum for the nuclear chart, the relativistic continuum Hartree-Bogoliubov (RCHB) theory will be used in this paper to explore the nucleon drip-lines by assuming spherical symmetry. Because of the huge numerical computational efforts involved, we focus on the nuclear chart ranging from O to Ti as examples.

The starting point of the CDFT is a general effective zero-range point-coupling Lagrangian density [57],

$$\mathcal{L} = \bar{\psi}(i\gamma_\mu \partial^\mu - M)\psi - \frac{1}{4} F^\mu\nu F_{\mu\nu} - e \frac{1}{2} \bar{\psi} \gamma^\mu \psi A_\mu - \frac{1}{2} \sigma_S (\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2} \sigma_{TV} (\bar{\psi}\gamma^\mu \psi)(\bar{\psi}\gamma^\mu \psi) - \frac{1}{2} \sigma_T S (\bar{\psi}\psi)^3 - \frac{1}{4} \gamma_S (\bar{\psi}\psi)^3 - \frac{1}{4} \gamma_{TV} (\bar{\psi}\gamma^\mu \psi)(\bar{\psi}\gamma^\mu \psi)^2$$

$$- \frac{1}{2} \delta_S \partial_\mu (\bar{\psi}\partial^\mu \psi) - \frac{1}{2} \delta_{TV} \partial_\mu (\bar{\psi}\gamma^\mu \psi)$$

$$- \frac{1}{2} \delta_T S \partial_\mu (\bar{\psi}\gamma^\mu \psi)$$

$$- \frac{1}{2} \delta_{TV} \partial_\mu (\bar{\psi}\partial^\mu \psi)$$

where $M$ is the nucleon mass, and $\sigma_S$, $\sigma_{TV}$, $\sigma_T$, $\beta_S$, $\gamma_S$, $\gamma_{TV}$, $\delta_S$, $\delta_{TV}$, $\delta_T$ are the coupling constants. $A_\mu$ and $F_{\mu\nu}$ are respectively the four-vector potential and field strength tensor of the electromagnetic field.

Starting from the Lagrangian density in Eq. (1), one can derive the RHB equation for the nucleons [58],

$$\left( \frac{h_D - \lambda}{-\Delta^s} + \frac{\Delta}{h_D^s + \lambda} \right) \left( \frac{U_k}{V_k} \right) = E_k \left( \frac{U_k}{V_k} \right),$$

where $E_k$ is the quasiparticle energy, $\lambda$ is the Fermi level. The Dirac Hamiltonian $h_D$ is

$$h_D = \alpha \cdot \cdot \cdot + \beta(M + S(r)) + V(r),$$

where the scalar and vector potentials are, respectively,

$$S(r) = \alpha_S \rho_S + \beta_S \rho_S^3 + \gamma_S \rho_S^3 + \delta_S \Delta \rho_S,$$

$$V(r) = \alpha_T \rho_T + \beta_T \rho_T^3 + \gamma_T \rho_T + \delta_T \rho_T + \Delta \rho_T + \epsilon \rho_0$$

with the local densities

$$\rho_S(r) = \sum_{k=0}^{\infty} \tilde{V}_k(r) \tilde{V}_k(r),$$

$$\rho_T(r) = \sum_{k=0}^{\infty} \tilde{V}_k(r) \tilde{V}_k(r),$$

$$\rho_{TV}(r) = \sum_{k=0}^{\infty} \tilde{V}_k(r) \tilde{V}_k(r).$$

The pairing potential reads,

$$\Delta_{k\bar{k}}(r, r') = \sum_{k=\bar{k}} \sum_{\lambda\lambda'} V_{kk'\bar{k}\bar{k}'}(r, r') \rho_{\lambda\lambda'}(r, r'),$$

with the pairing tensor $\kappa = U^T V^T$ and a density-dependent delta pairing force

$$\Delta_{kk}(r, r') = \sum_{\lambda=0}^{\infty} V_{kk'\bar{k}\bar{k}'}(r, r')\rho_{\lambda\lambda'}(r, r').$$

The RCHB theory [42,44] solves the RHB equations in coordinate representation, thus it provides a fully self-consistent description of both the continuum and the bound states as well as the coupling between them.

Following the procedures as described in Ref. [44], the RHB equations are solved in a box with a size of $R = 20$ fm and a step size of 0.1 fm. In the present work, we use the density functional PC-PK1 [57] for particle-hole channel, which particularly improves the description for isospin dependence of the nuclear masses [59] and has been successfully used in describing the Coulomb displacement energies between mirror nuclei [60], fission barriers [61] as well as nuclear rotations [35-37]. For particle-particle channel, the density-dependent delta pairing force with the saturation density $\rho_0 = 0.152$ fm$^{-3}$ is used and the strength $V_0 = 685.0$ MeV fm$^{-3}$ is fixed by reproducing experimental odd-even mass differences of Ca isotopes obtained with a three-point formula. The contribution from the continuum is restricted within a cutoff energy $E_{\text{cut}} \sim 100$ MeV.

The particular purpose of the present work is to investigate the extension of the nuclear chart by the continuum couplings. Therefore, we focus on the location of the nucleon drip-lines. On one hand, both the one-nucleon separation energy

$$S_\nu(Z, N) = B(Z, N) - B(Z, N - 1),$$

(8a)
402 nuclei from O to Ti predicted to be bound by the RCHB theory with the covariant density functional PC-PK1. For 234 nuclei with the available data, the binding energy differences \( E_{\text{Exp}} - E_{\text{Cal}} \) between the data [62] and present calculation are shown as different color. Furthermore, the nucleon drip-lines predicted by the mass tables TMA, HFB-21, FRDM and WS3 are plotted for comparison.

In Fig. 1, the bound nuclei region from O to Ti isotopes predicted by RCHB theory with the density functional PC-PK1 are shown as squares. It is found that 402 bound nuclei are predicted. The squares with cross represent the predicted by RCHB theory with the density functional PC-PK1.

\[
S_p(Z, N) = B(Z, N) - B(Z - 1, N), \quad (8b)
\]

and two-nucleon separation energy

\[
S_{2p}(Z, N) = B(Z, N) - B(Z, N - 2), \quad (9a)
\]

\[
S_{2p}(Z, N) = B(Z, N) - B(Z - 2, N), \quad (9b)
\]

can provide the information on nucleon drip-lines. On the other hand, the Fermi level, \( \lambda_n \) and \( \lambda_p \), can provide the bound information of the nucleus. In the present work, only if the nucleon separation energy is positive and the Fermi level is negative, the nucleus is considered to be bound.

In Fig. 1, the bound nuclei region from O to Ti isotopes predicted by RCHB theory with the density functional PC-PK1 are shown as squares. It is found that 402 bound nuclei are predicted. The squares with cross represent the predicted by RCHB theory with the density functional PC-PK1. Furthermore, the nucleon drip-lines predicted by the mass tables TMA, HFB-21, FRDM and WS3 are plotted for comparison.

In order to evaluate the agreement of the present calculated masses with the available data, we show the binding energy differences \( E_{\text{Exp}} - E_{\text{Cal}} \) with different colors in Fig. 1. One can find that most deviations are in the range of \(-2.5 \sim 2.5\) MeV, resulting in the rms deviation \( \sigma \) in this nuclear region is 2.23 MeV. There are two nuclear regions with the deviation \(|E_{\text{Exp}} - E_{\text{Cal}}| > 3.5\) MeV. One is around the mass number \( N = Z = 12 \) region, and the other is near \( N = 20 \) and \( Z = 10 \) region. The reasons for such large deviation areas may result from the following reasons: firstly, the proton-neutron pairing correlation, which can provide additional binding in \( N \sim Z \) nuclei [64], is not taken into account; secondly, the deformation effect is not included. Indeed, when we restrict ourselves to the spherical nuclei, for instance, O and Ca isotopes, the results achieve good agreement with the data and the corresponding rms deviation \( \sigma \) reduces to 1.67 and 1.09 MeV, respectively.

Following the definition of the nucleon drip-line, in Fig. 1 one can easily recognize the proton and neutron drip-lines for O to Ti isotope chains predicted with the RCHB theory. For comparison, we also show the predictions from the mass tables FRDM [7], WS3 [65], HFB-21 [11] and TMA [40] in Fig. 1. On the neutron-deficient side, owing to the repulsive electrostatic interaction between the protons, the proton drip-line lies relatively close to the valley of stability. The predictions from different theoretical models are roughly the same as the experimental observations.

On the neutron-rich side, as neutrons do not carry the electric charge, the neutron drip-line is located far from the val-
In conclusion, the nuclear masses are systematically investigated in nuclear region from O to Ti isotopes with relativistic continuum Hartree-Bogoliubov (RCHB) theory, which can provide an appropriate treatment of pairing correlations in the presence of the continuum. By applying the density functional PC-PK1, 402 bound nuclei are predicted in this nuclear area, including 100 neutron-deficient and 287 neutron-rich bound nuclei. For the 234 nuclei with mass measured, the RCHB results can reproduce the data with the rms deviation 2.23 MeV. For the spherical O and Ca isotopes, the results can achieve good agreement with the data and the corresponding rms deviation is reduced to 1.67 and 1.09 MeV, respectively. It is found that the drip-lines predicted by various mass models are roughly the same as the experimental observation on neutron-deficient side. For the neutron-rich side, because of the continuum couplings, the neutron drip-line predicted by RCHB theory is extended further neutron-rich than other mass models. By comparison with FRDM, the neutron drip-line nucleus predicted by RCHB theory has respectively 2(O), 10(Ne), 10(Na), 6(Mg), 8(Al), 6(Si), 8(P), 6(S), 14(K), 10(Ca), 10(Sc), and 12(Ti) neutrons more.

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