Giant halo in relativistic and non-relativistic approaches (postprint)

Authors: J. Terasaki, S. Q. Zhang, S. G. Zhou, J. Meng

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The phenomena of giant halo and halo of neutron-rich even-Ca isotopes are investigated and compared in the framework of the relativistic continuum Hartree-Bogoliubov (RCHB) and non- relativistic Skyrme Hartree-Fock-Bogoliubov (HFB) calculations. With two parameter sets for each of the RCHB and the Skyrme HFB calculations, it is found that although halo phenomena exist for Ca isotopes near neutron drip line in both calculations, the halo of the Skyrme HFB calculations starts at a more neutron-rich nucleus than that of the RCHB calculations, and the RCHB calculations have larger neutron root-mean-square (rms) radii systematically in N 40 than those of the Skyrme HFB calculations. The former difference comes from difference in shell structure. The reasons for the latter can be partly explained by the neutron 3s1/2 orbit, which causes more than 50 % of the difference among the four calculations for neutron rms radii at 66Ca.

Full Text

Giant Halo in Relativistic and Non-Relativistic Approaches

J. Terasaki[1], S. Q. Zhang[1,2], S. G. Zhou[2,3] and J. Meng[1] [3]

[1]Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou 730000, China
[2]Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China
[3]School of Physics, Peking University, Beijing 100871, China
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Abstract

The phenomena of giant halo and halo in neutron-rich even-Ca isotopes are investigated and compared within the frameworks of relativistic continuum

Hartree-Bogoliubov (RCHB) and non-relativistic Skyrme Hartree-Fock-Bogoliubov (HFB) calculations. Using two parameter sets for each approach, we find that although halo phenomena exist for Ca isotopes near the neutron drip line in both calculations, the halo in Skyrme HFB calculations begins at more neutron-rich nuclei than in RCHB calculations. Furthermore, RCHB calculations systematically yield larger neutron root-mean-square (rms) radii for N 40 compared to Skyrme HFB results. The former difference originates from variations in shell structure, while the latter can be partially explained by the neutron 3s / orbit, which accounts for more than 50% of the difference in neutron rms radii among the four calculations for Ca.

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Introduction

The study of exotic nuclei with extreme N/Z ratios has attracted worldwide attention since the first discovery of halo in ^{11}Li [?]. For exotic nuclei, the Fermi surfaces are typically very close to the continuum threshold, and valence nucleons can be easily scattered into continuum states due to pairing correlations [?, ?]. Consequently, theoretical frameworks that properly treat both pairing and continuum states are essential for describing the properties of exotic nuclei and understanding how continuum-energy states interfere with bound many-body systems and how large neutron excess affects nuclear structure.

It is well known that the BCS approximation for pairing correlations, which works well for stable nuclei, cannot provide correct wave functions near the drip lines (see e.g., [?]). By incorporating pairing correlations through the Bogoliubov transformation, relativistic and non-relativistic mean-field approaches have been extensively employed to describe and predict halo phenomena in exotic nuclei.

Previous studies using the relativistic continuum Hartree-Bogoliubov (RCHB) or non-relativistic Hartree-Fock-Bogoliubov (HFB) method have predicted halo structures in Ne [?, ?], Na [?, ?], Ca [?], and Zr [?] isotopes near the neutron drip line. More comprehensive details can be found in recent review papers, e.g., [?]. Since more than two particles occupy weakly bound or positive-energy states in Ca and Zr isotopes near the neutron drip line, the halo phenomena in these cases are termed "giant halo" [?, ?].

Systematic surveys of proton-magic nuclei from O to Pb have shown that the halo signature in Zr is the clearest [?], while no evidence for halo is found in Ni, Sn, and Pb isotopic chains [?]. In non-relativistic HFB approaches, Skyrme calculations with the SLy4 parameter set predict halo in Sn and Ni [?], and it has been suggested that pairing gaps can reduce halo formation at the neutron drip line [?, ?, ?].

To compare with halos predicted in relativistic approaches [?, ?, ?], it is necessary to investigate Ca and Zr isotopes using non-relativistic approaches—a crucial study that remains missing in the literature. Therefore, this paper is dedicated to investigating neutron-rich even-Ca isotopes up to the neutron drip line, presenting and comparing results from both relativistic and non-relativistic mean-field approaches that incorporate pairing correlations via the Bogoliubov transformation.

The numerical details for both calculations are explained in Sec. II, followed by an examination of the neutron-number dependence of energy and rms radii in Sec. III. Single-particle properties are discussed in Sec. IV to understand the halo structure, and a brief summary is provided in Sec. V.

II. Method of Calculation

Detailed formulations of the RCHB and HFB methods can be found in Refs. [?, ?] and [?, ?], respectively. Both calculations employ coordinate-space representation with a box size of 20 fm, assuming spherical symmetry and using a mesh size of 0.1 fm. Quasiparticle states are obtained up to 120 MeV (corresponding to 165–190 radial wave functions in Ca), and all these states are used for calculating potentials. The maximum angular momentum of quasiparticles is j = 13/2 for Skyrme HFB calculations.

The parameter sets NL-SH [?] and PK1 [?] are used for RCHB calculations, while SkM* [?] and SLy4 [?] are employed for Skyrme HFB calculations. For the pairing channel, a surface-type delta interaction [?, ?] is adopted with density parameters = 0.152 fm^{3} for RCHB and = 0.160 fm^{3} for Skyrme HFB calculations.

The strength of the pairing interaction in mean-field calculations is normally determined to reproduce pairing gaps obtained from odd-even mass differences (see e.g., Ref. [?]). However, for nuclei near the neutron drip line where experimental data are scarce, the pairing energy from Gogny interaction calculations in the pairing channel is used to fix the strength of the surface-type delta pairing interaction. The pairing strength V is -325 MeV · fm^3 in RCHB calculations, and -365 MeV · fm^3 (-330 MeV · fm^3) in SLy4 (SkM*) Skyrme HFB calculations. The average pairing energy from PK1 and NL-SH calculations (-8.2 MeV at Ca) is used to determine V for Skyrme HFB calculations. We verified that when j = 13/2 is used in Skyrme HFB calculations, the rms radii do not change with the re-adjusted V determined from the pairing energy.

III. Neutron-Number Dependence of the Halo Structure

Figures 1 and 2 show the binding energy per nucleon B/A and the two-neutron separation energy S for even-Ca isotopes from RCHB calculations with NL-SH and PK1 and Skyrme HFB calculations with SkM* and SLy4, respectively. The most important differences between these calculations concern the location of the two-neutron drip line and the presence of a shell gap at N = 40. RCHB calculations predict the two-neutron drip line at N = 50 (PK1) or N = 52 (NL-

SH), while Skyrme HFB calculations predict N = 46 (SLy4) or N = 58 (SkM*). Both RCHB and SLy4 calculations exhibit a clear shell gap at N = 40 (Fig. 2), whereas the SkM* calculation shows no such gap. Although the SkM* calculation displays a small additional downward trend in S at N = 50, it is too weak to be considered a shell gap. Consequently, no new shell gap is predicted for N > 40 in any of the calculations.

The two RCHB calculations yield similar results for both B/A and S , while the two Skyrme HFB calculations differ by 0.1–0.2 MeV in B/A. The S values from SLy4 are close to those from SkM* for 34 N 40 and then coincide with PK1 results for 42 N 48. Experimental data are currently available up to N = 32 [**?**]. The RCHB calculations reproduce well the measured B/A values at N = 30 (8.550 MeV) and N = 32 (8.396 ± 0.013 MeV), as well as S at N = 32 (9.081 ± 0.699 MeV). For S at N = 30, the SLy4 calculation gives a value very close to the experimental one (11.499 ± 0.008 MeV).

Figure 3 shows the systematic behavior of neutron and proton rms radii ($\bar{r}$ and $\bar{r}$) for even-Ca isotopes from N = 30 to the two-neutron drip lines. An increase in the curvature of $\bar{r}$ indicates halo formation. (For discussions on defining halo criteria or halo size, see Refs. [**?**, **?**, **?**] and references therein.) For Ca isotopes, the number of nucleons in the positive-energy region N is 0.6–2.2 for ^{2} ^{2}Ca, with an average of 1.7 in the NL-SH calculation [**?**], while the corresponding value in the SkM* calculation is always smaller than 0.5 (average 0.27). Since more than two nucleons occupy weakly bound or positive-energy orbits in these nuclei and halo phenomena appear in neighboring nuclei with incremental neutrons, the halo in Ca isotopes is referred to as giant halo, following Refs. [**?**, **?**]. The SkM* calculation shows halo formation from N = 52, while RCHB calculations exhibit a gradual development of giant halo. The onset of halo in SkM* corresponds to the extra lowering of S . The SLy4 calculation does not produce halo because the particle-stable region ends at N = 46.

The large difference between $\bar{r}$ and $\bar{r}$ shown in Fig. 3 is identified as neutron skin in regions without halo. Figure 4 displays $\bar{r}$ - $\bar{r}$, where differences between parameter sets are evident: the SLy4 curve runs parallel to that of SkM*, while PK1 shows larger curvature than other parameter sets for N 50. An important aspect of halo is how $\bar{r}$ changes when two neutrons are added, making it worthwhile to examine the difference $\bar{r}$ (N) - $\bar{r}$ (N - 2) (Fig. 5). Without halo, two additional neutrons increase $\bar{r}$ by 0.05 fm, whereas this increase rises to 0.11 fm in halo nuclei. In all figures (3–5), clear differences in $\bar{r}$ appear between RCHB and Skyrme HFB calculations. It should be noted that $\bar{r}$ is not constant, reflecting the self-consistency of neutron-proton interactions.

IV. Single-Particle Structure

To understand the halo phenomena and the different predictions between RCHB and Skyrme HFB calculations, we examine Ca as a representative case. Figure 6 [Figure 6: see original paper] shows the neutron single-particle levels in

RCHB calculations with NL-SH and PK1 and Skyrme HFB calculations with SkM* and SLy4—the diagonal elements of the mean-field Hamiltonian in the canonical basis.

The level ordering is essentially the same across all calculations, with RCHB spectra for PK1 and NL-SH being quite similar. However, the 1s / level in SkM* is noticeably higher than in other parameter sets. From left to right, shell gaps become less apparent. Shell gaps at N = 2, 8, 20, 28, and 40 are clearly visible in RCHB spectra, while those at N = 28 and 40 are absent in the SkM* calculation (see also Fig. 2).

It has been pointed out [?] that the neutron 3s / level plays an important role in giant halo formation. Figure 7 [Figure 7: see original paper] compares the rms radii of each single-particle orbit (canonical basis) $\bar{r}$ in RCHB calculations with NL-SH and PK1 and Skyrme HFB calculations with SkM* and SLy4. The $\bar{r}$ versus curves are quite similar except for the 1s / level and the region around = 0, indicating similar potential walls except at the bottom. A magnification around = 0 is displayed in Fig. 7b. The most significant difference appears in the 3s / orbit: $\bar{r}$ / from PK1 is more than 2 fm larger than that from SkM*. These differences are more clearly illustrated in Fig. 8 [Figure 8: see original paper], which shows $\bar{r}$ as circle radii.

Table I presents , $\bar{r}$, occupation probability v^2, and $v^2 \bar{r}$ for the neutron 3s / orbit, along with $\bar{r}$ for Ca. Both $\bar{r}$ / and v^2 / contribute to making $\bar{r}$ largest in PK1. Since the orbit' s contribution to $\bar{r}$ is given by $2v^2$ / $\bar{r}$ /, Table I shows that 54% (0.082 fm) of the difference $\bar{r}$ (PK1) - $\bar{r}$ (SkM*) = 0.153 fm originates from the neutron 3s / orbit. It is also noteworthy that higher energy does not necessarily imply a larger spatial distribution.

The difference in the neutron 3s / orbit is further demonstrated in Fig. 9 [Figure 9: see original paper], which shows the squared radial wave functions. The PK1 tail has a significantly longer distribution than the others, with correspondingly smaller amplitude in the inner region. The number and locations of nodes are identical across all four calculations. Neutron density distributions show appreciable differences (Fig. 10 [Figure 10: see original paper]) consistent with the behavior in Fig. 9.

Figure 11 [Figure 11: see original paper] depicts central potentials—the sum of scalar and vector potentials in RCHB calculations, and the sum of t and t terms in the particle-hole potential in Skyrme HFB calculations (see Eq. (A.5a) of Ref. [?]). A significant difference is that the SkM* calculation has shallower potential depth than other calculations, as anticipated from Fig. 6, along with slight differences in the tail region (see inset of Fig. 11). Notably, RCHB calculations have longer tails than Skyrme HFB calculations, with PK1 showing the longest tail. Figure 12 [Figure 12: see original paper] displays the pairing potential $\tilde{}$ (r), where (r) is the total nuclear density and $\tilde{}$ (r) is the neutron pairing density [?]. For RCHB calculations, the S = 1 component of the pairing interaction is explicitly removed. Again, the PK1 curve has the longest tail, explaining the large $\bar{r}$ / in PK1 in terms of the tails of both central and pairing potentials.

Finally, we emphasize the importance of pairing correlations. When the surface-type pairing interaction strength was adjusted to reproduce neutron pairing gaps of 1.0-1.9 MeV for ^{2}, , , Ca obtained from experimental odd-even mass differences [?], the pairing energy in SkM* calculations became -(35-39) MeV for 40 N 50, completely washing out the kink in $\bar{r}$ at N = 50 (circles in Fig. 13 [Figure 13: see original paper]). This pairing energy is more than three times larger than RCHB values of 8-9 MeV. In contrast, a volume-type pairing interaction V (r - r) can simultaneously reproduce both the RCHB pairing energy and experimental pairing gaps, preserving the kink in $\bar{r}$ (triangles in Fig. 13). Therefore, the kink is strongly influenced by the pairing interaction (see also Refs. [?, ?]).

V. Conclusion

In this paper, we have investigated and compared giant halo and halo phenomena in neutron-rich even-Ca isotopes using RCHB and Skyrme HFB calculations. With two parameter sets for each approach, we find that although halo phenomena exist for Ca isotopes near the neutron drip line in both calculations, the halo in Skyrme HFB calculations begins at more neutron-rich nuclei than in RCHB calculations, and RCHB calculations systematically yield larger neutron rms radii for N 40. The former difference arises from variations in shell structure, while the latter can be partially explained by the neutron 3s / orbit, which accounts for 50% of the difference in neutron rms radii among the four calculations at Ca.

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