Halo Phenomena in Deformed Nuclei and Post-Shape-Decoupling Imprint

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Date: 2023-09-04T00:00:00+00:00

Abstract

With the rapid development of radioactive nuclear beam physics, many exotic nuclear structure phenomena have been discovered or predicted in nuclei far from the β-stability line, including deformed halos and shape decoupling in deformed halo nuclei. The study of these exotic nuclear phenomena represents an important frontier in current nuclear physics. Covariant density functional theory is one of the most successful theoretical models for describing nuclear structure properties. This paper reviews the results and progress of research on deformed halo nuclei based on covariant density functional theory. The deformed relativistic Hartree-Bogoliubov theory, which incorporates continuum effects, has achieved a microscopic self-consistent description of deformed halo nuclei and predicted the deformed halo in magnesium-44 as well as the shape decoupling phenomenon between the core and the halo. Subsequently, this theory has also been applied to investigate deformed halo phenomena in nuclei along the boron and carbon isotopic chains. Angular momentum projection calculations based on this theory demonstrate that halo phenomena and shape decoupling persist in the low-lying rotational excited states of deformed halo nuclei.

Full Text

Preamble

Vol. 46, No. 8

August 2023

Nuclear Techniques www.hjs.sinap.ac.cn Vol. 46, No. 8 August 2023 ChinaXiv Partner Journal

Deformed Halo Nuclei and Shape Decoupling Effects

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Abstract

With the rapid development of radioactive-ion-beam facilities worldwide, many exotic nuclear phenomena have been observed or predicted in nuclei far from the β-stability line, including deformed halos and shape decoupling in deformed halo nuclei. The study of these exotic phenomena represents an important frontier in current nuclear physics research. Covariant density functional theory (CDFT) is one of the most successful theoretical models for describing nuclear structure properties. This paper reviews results and progress on deformed halo nuclei based on CDFT. The deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc), which incorporates continuum effects, has achieved a microscopic and self-consistent description of deformed halo nuclei and predicted the deformed halo and shape decoupling between core and halo in ^{44}Mg. Subsequently, this theory has been applied to study deformed halo phenomena in boron and carbon isotopic chains. Angular momentum projection calculations based on this theory demonstrate that halo phenomena and shape decoupling persist in the low-lying rotational excited states of deformed halo nuclei.

Keywords: Covariant density functional theory, Deformed halo nuclei, Shape decoupling effects, Rotational excitation

1. Introduction

The rapid development of radioactive-ion-beam physics worldwide has led to the discovery of numerous exotic nuclear phenomena in nuclei far from the β-stability line, including cluster structures, neutron and proton halos, neutron skins, the disappearance of traditional magic numbers, and the emergence of new magic numbers. The study of halo phenomena represents a frontier area in nuclear physics. In 1985, scientists first observed nuclear halo structure in ^{11}Li, initiating an intensive research effort in exotic nuclei. Since then, approximately twenty halo nuclei have been discovered in laboratories, with more recent discoveries including ^{31}Ne, ^{37}Mg, ^{17,19}B, and ^{29}F. Numerous studies have combined experimental results with theoretical descriptions to elucidate halo formation mechanisms. For instance, through one-neutron removal reactions and shell model calculations, Nakamura et al. revealed that ^{31}Ne is deformed and possesses a p-wave halo structure, marking the first experimentally confirmed deformed halo nucleus. While experimental-theoretical collaborations have explained the properties of several halo nuclei, the properties and formation mechanisms of most halo nuclei remain to be explored.

The earliest discovered halo nucleus, ^{11}Li, is spherical, but most open-shell nuclei are deformed. Many halo nuclei (including ^{17},^{19}B, ^{22}C, ^{29}F, ^{31},^{34},^{36}Ne, and ^{37},^{42},^{44}Mg) have been confirmed or predicted to be deformed. Particularly for halo nuclei near the island of inversion around N = 20, such as ^{29},^{31}F and ^{31}Ne, their properties are intimately connected to shell evolution, deformation effects, continuum contributions, and the coupling among these factors, necessitating further in-depth investigation. Additionally, excited states have been observed in some drip-line nuclei and halo nuclei, making the study of low-lying excitation spectra in weakly bound nuclei, including halo nuclei, another frontier in theoretical and experimental nuclear physics.

Theoretical approaches for studying halo structure include halo effective field theory, antisymmetrized molecular dynamics, few-body models, Gamow shell model, ab initio calculations, and density functional theory (DFT). Each model has distinct advantages. DFT, based on an intrinsic frame of reference and employing global effective nucleon-nucleon interactions, can microscopically and self-consistently investigate halo formation mechanisms while incorporating deformation effects. However, studying excitation spectra requires introducing symmetry restoration methods. DFT is one of the most successful theories for describing nuclear properties. As early as 1996, Meng and Ring used the relativistic continuum Hartree-Bogoliubov (RCHB) theory within the DFT framework to microscopically explain the two-neutron halo structure in ^{11}Li. The RCHB theory also predicted giant halo phenomena in calcium and zirconium isotopic chains. Spherical halos have been studied based on DFT in numerous works, while the microscopic and self-consistent description of deformed halo nuclei was realized through the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc). Subsequently, non-relativistic DFT has also been employed to investigate deformed halo properties. The DRHBc theory further predicted that in deformed halo nuclei, the halo and core can have different shapes—a phenomenon termed "shape decoupling."

Most DFT-based studies of deformed halo nuclei have focused on ground-state properties, with few exploring excited states, particularly rotational excitations. Within the DFT framework, nuclear spectroscopy must account for spontaneous symmetry breaking from the laboratory to intrinsic frame, including U(1) and SO(3) symmetries. Particle number projection and angular momentum projection are typically used to restore the broken U(1) and SO(3) symmetries. Additionally, as quantum many-body systems, fluctuations in collective degrees of freedom near the ground state must be treated with generator coordinate methods. Beyond-mean-field methods based on relativistic or non-relativistic mean-field models have been widely applied to study low-lying excitation spectra. These methods have also been used to investigate excitation spectra of nuclei with axial symmetry, triaxial deformation, octupole deformation, and more complex shapes. However, these models are solved in a harmonic oscillator basis, which cannot properly describe the asymptotic behavior of wave functions far from the core and are therefore unsuitable for halo nuclei. Recently, angular momentum projection has been implemented based on DRHBc theory, achieving a microscopic and self-consistent description of rotational excitations in deformed halo nuclei. This model can self-consistently provide properties of both ground and low-lying excited states in deformed halo nuclei. This paper summarizes research on deformed halo nuclei based on DRHBc theory over the past decade.

2. DRHBc Theory and Angular Momentum Projection DRHBc Theory

The DRHBc theory is based on meson-exchange or point-coupling nucleon-nucleon effective interactions, neglecting exchange terms (Hartree approximation) and treating continuum contributions induced by pairing correlations through Bogoliubov transformation. The system's quasiparticle wave functions are obtained from the Dirac-Hartree-Bogoliubov (DHB) equations. For halo nuclei, whose valence nucleon wave functions can extend far from the core, proper treatment of this asymptotic behavior is essential. For spherical halo nuclei, the DHB equations can be solved directly in one-dimensional coordinate space using shooting methods, finite element methods, or Lagrange-mesh methods. However, for axially deformed nuclei, direct numerical solution of the DHB equations in coordinate space is challenging. Basis expansion methods are typically employed, with complete bases including harmonic oscillator basis, Dirac Woods-Saxon (DWS) basis, or transformed harmonic oscillator basis. The DRHBc theory uses the DWS basis to solve the deformed DHB equations. Compared to the harmonic oscillator basis, the DWS basis advantageously preserves the asymptotic behavior of weakly bound orbital wave functions. In the DWS basis, quasiparticle wave functions and corresponding energies are obtained by diagonalizing the DHB matrix for the deformed system. Using these quasiparticle wave functions, ground-state properties including energy, radius, and density distributions can be calculated for comparison with experiments or for predicting properties of exotic nuclei.

The DRHBc theory can only provide ground-state properties in the intrinsic frame and cannot study excited states because the SO(3) symmetry of the laboratory frame is spontaneously broken in the intrinsic frame for deformed nuclei. Restoring the broken SO(3) symmetry is necessary to describe excited states. Within the DFT framework, angular momentum projection is typically employed to restore SO(3) symmetry. To study excited-state properties of weakly bound nuclei such as halo nuclei, we have implemented angular momentum projection in a variation-after-projection scheme based on DRHBc theory. Notably, while nearly all previous beyond-mean-field calculations in DFT have been based on the harmonic oscillator basis, we have realized beyond-mean-field calculations using the DWS basis. As isolated systems, nuclei have good quantum numbers for angular momentum. However, due to spontaneous symmetry breaking, the mean-field wave function in the intrinsic frame is a superposition of components with different angular momenta. Through angular momentum projection, states with definite angular momentum (good quantum numbers) can be projected out, yielding the ground state and low-lying excitation spectra.

3. Deformed Halo Structure and Rotational Excitations of Deformed Halo Nuclei

This section presents the DRHBc theory description of halo nuclei in boron, carbon, and magnesium isotopic chains and beyond-mean-field studies of excited states in deformed halo nuclei. Numerical conditions may vary slightly when studying nuclei in different mass regions with DRHBc theory. In most calculations, a density-dependent zero-range pairing force is employed with a quasiparticle energy cutoff of 60 MeV. The pairing strength is typically determined by fitting experimental pairing gaps or nuclear mass odd-even differences. When numerically solving DWS basis wave functions, the radial coordinate is truncated at 20 fm with a step size of 0.1 fm. The angular momentum cutoff for the single-particle DWS basis is 21/2 . The energy cutoff for single-particle DWS basis states in the Fermi sea is 100 MeV, with the number of DWS basis wave functions in the Dirac sea matching that in the Fermi sea. These numerical conditions have been verified to provide appropriate precision for calculations of light-mass nuclear properties.

3.1 Deformed Halos in Magnesium Isotopic Chain

A significant application of DRHBc theory is the study of deformed halo structure in the magnesium isotopic chain. Using the NL3 effective interaction, DRHBc predicts that ^{46}Mg is the neutron drip-line nucleus in this chain and that ^{44}Mg is a deformed halo nucleus. ^{44}Mg has a very small two-neutron separation energy of only 0.44 MeV and a quadrupole deformation parameter β_2 of 0.32, indicating a prolate ground-state shape. Figure 1: see original paper shows the two-dimensional proton and neutron density distributions of ^{44}Mg, with the z-axis as the symmetry axis and red dots indicating circular contours. As a weakly bound, extremely neutron-rich nucleus, ^{44}Mg exhibits neutron densities that extend much further in space than proton densities.

In mean-field models, analyzing the orbital composition of valence neutrons can reveal the configuration and formation mechanism of halo nuclei. [Figure 2: see original paper] displays the neutron single-particle level diagram of ^{44}Mg in the canonical basis near the neutron Fermi level (λ). Each level is labeled by the z-component of angular momentum Ω and parity π, with line lengths proportional to neutron occupation numbers, where n denotes the level order. On the right side of the figure, the main spherical DWS basis components for some levels are shown. Dashed lines represent occupation numbers obtained using the BCS formula with average pairing gaps. Below the neutron Fermi level, valence neutrons occupy weakly bound $3/2^-$ and $1/2^-$ levels, with partial occupation also present in continuum levels above the Fermi surface. Typically, halo formation arises from low orbital angular momentum (s- or p-wave) wave functions that are weakly bound or in the continuum. In the valence nucleon wave functions of ^{44}Mg, levels n=3, 4, and 6 contain p-wave contributions with approximately two nucleons occupying p-wave orbitals, leading to the halo structure in this nucleus.

Based on the neutron level structure, the contribution to neutron pair density can be divided into two parts: neutrons in levels 1 and 2 and lower-energy levels form the neutron core, while neutrons occupying level 3 and higher-energy levels form the neutron halo. Accordingly, the total neutron density can also be separated into neutron core and neutron halo components. The two-dimensional density distributions of these two parts are shown in Figure 1: see original paper and (c). The neutron core exhibits a prolate shape, while the neutron halo displays an oblate shape. Therefore, in deformed halo nuclei, the halo and core can have different deformations—a phenomenon termed "shape decoupling." The shapes of the core and halo originate from properties of the intrinsic wave function. For the neutron halo in ^{44}Mg, the spatial angular distribution of p-wave orbitals includes contributions from spherical harmonics Y_{10}( ) and $Y_1 \pm_1$( ), where the former yields a prolate shape and the latter an oblate shape. In the valence nucleon wave function of ^{44}Mg, the $Y_1 \pm_1$( ) component is larger, resulting in an oblate neutron halo.

In DRHBc descriptions of magnesium isotopes, ^{42}Mg is also a deformed two-neutron halo nucleus, with its halo structure arising from p-wave components in weakly bound valence nucleon orbitals. However, the heaviest magnesium isotope observed experimentally to date is ^{40}Mg, so the deformed halos in ^{42,44}Mg await experimental verification. Whether ^{40}Mg contains deformed halo structure remains an open question, with DRHBc theory predicting that ^{40}Mg is not a deformed halo nucleus. In the magnesium isotopic chain, a one-neutron halo has been experimentally observed in ^{37}Mg. DRHBc studies incorporating odd-nucleon blocking effects and contributions from odd-time fields indicate that ^{37}Mg is a deformed one-neutron halo nucleus.

3.2 Deformed Halo Structure in Boron and Carbon Isotopic Chains

Experimental observations in boron and carbon isotopic chains have indicated neutron halos in ^{17}B, ^{19}B, ^{15}C, ^{19}C, and ^{22}C, yet questions regarding halo formation mechanisms, properties, and the existence of deformed halos remain unresolved. This section briefly presents the DRHBc theory description of these halo nuclei. compares DRHBc calculations of deformation values, neutron separation energies, nuclear matter radii, and experimental results for these nuclei, showing good agreement between theory and experiment.

In the boron isotopic chain, DRHBc theory predicts deformed halos in both ^{17}B and ^{19}B, with halo neutrons partially occupying s-orbitals. Experimental neutron removal reactions indicate that the s-wave component constitutes only 9(2)% of the two valence neutrons in ^{17}B, representing the smallest low angular momentum orbital fraction observed in a halo nucleus to date. Based on the deformed halo mechanism, DRHBc calculations show this nucleus is deformed with an s-wave fraction of 14%, yielding neutron separation energies and radii in reasonable agreement with experiment. In 2020, Coulomb breakup reaction measurements of the B(E1) excitation spectrum of ^{19}B indicated a neutron halo, though its structure and formation mechanism require further exploration. Assuming a two-neutron separation energy of 0.5 MeV, three-body model calculations suggest ^{19}B is a two-neutron halo nucleus caused by s-waves with a fraction of 35%. DRHBc theory calculations indicate ^{19}B is a deformed two-neutron halo nucleus with an s-wave fraction consistent with three-body model predictions. Both two-neutron halo nuclei ^{17,19}B exhibit shape decoupling: a prolate neutron core and an oblate neutron halo.

DRHBc theory predicts deformed halo structures in the ground states of ^{15,22}C in the carbon isotopic chain. The ^{15}C ground state is prolate with an s-wave one-neutron halo, where the neutron core is nearly spherical while the neutron halo is prolate, demonstrating that shape decoupling also exists in one-neutron halo nuclei. Recent time-dependent density functional calculations indicate that the deformed halo structure of ^{15}C enhances sub-barrier fusion cross sections in ^{15}C+^{232}Th reactions. For ^{22}C, current experimental data are limited to radius measurements and momentum distributions of the core in breakup reactions, with no B(E1) transition results available. DRHBc calculations reveal multiple exotic phenomena in ^{22}C, including deformed halos ("shrunken halos"), shell structure changes caused by single-particle level inversion, and shape decoupling, explaining puzzles related to its two-neutron separation energy, radius, and configuration. For ^{19}C, DRHBc calculations yield an oblate ground state without a neutron halo, with spin-parity $3/2^+$, inconsistent with the experimental value of $1/2^+$. However, in DRHBc calculations, the prolate isomeric state of ^{19}C (denoted ^{19}C*) has spin-parity $1/2^+$ and possesses a one-neutron halo structure.

Beyond predicting and exploring ground-state properties of deformed halos, DRHBc theory has been applied to study particle numbers beyond classical forbidden regions to characterize halo structure, explore bound nuclei beyond the drip line, and investigate shape coexistence and bubble structures in heavy nuclei. Mass is one of the most fundamental nuclear properties, and high-precision nuclear mass tables incorporating both deformation and continuum effects are currently being constructed based on DRHBc theory.

3.3 Rotational Excitations of Deformed Halo Nuclei

Do deformed halo nuclei have excited states? If so, what are their excitation modes and properties? These are hot topics in deformed halo research. The above discussions have focused only on ground-state properties. By developing angular momentum projection methods based on DRHBc theory, we can explore rotational excitation properties of deformed halo nuclei. Using the intrinsic wave function of deformed ^{44}Mg obtained from DRHBc theory, excited-state wave functions can be obtained through angular momentum projection, enabling investigation of excited-state properties. Calculations show that the excitation spectrum obtained from the deformed ^{44}Mg ground-state wave function follows the pattern of nuclear rotational excitation, with excitation energies showing a linear relationship with the square of angular momentum. Solving for the expectation value of the one-body density operator in projected wave functions yields density distributions for excited states. For the one-body density operator, the division into neutron core and halo introduced in the intrinsic frame can still be applied to projected excited states. [Figure 3: see original paper] shows the density distributions of neutron halo, neutron core, and total neutrons for 0^+, 2^+, and 4^+ states. For the 0^+ state, the nuclear density distribution is spherical, so both neutron halo and core densities are spherical. In the 2^+ and 4^+ states, the halo structure persists, and the shape decoupling between core and halo is maintained. Fundamentally, single-particle configurations change little during nuclear rotational excitation, causing intrinsic properties in the intrinsic frame to be preserved in rotational excited states. Therefore, the deformed halo structure and shape decoupling present in the intrinsic frame remain intact in low-lying rotational excited states—a prediction awaiting experimental verification.

4. Summary and Outlook

This paper has summarized the description of deformed halo nuclei based on covariant density functional theory. The DRHBc theory provides structures and properties of deformed halo nuclei in the intrinsic frame through self-consistent inclusion of deformation and continuum effects. Using DRHBc theory: (1) it predicted p-wave deformed halos in ^{42,44}Mg, a conclusion awaiting experimental verification; (2) it explained halo phenomena observed in boron isotopes ^{17,19}B based on the deformed halo mechanism; (3) it explained halo structures in ^{15,22}C, particularly revealing that halo properties in ^{22}C are closely related to shell structure and deformation effects. Additionally, shape decoupling between halo and core exists in all these halo nuclei. Beyond-mean-field methods developed based on DRHBc theory can be used to explore excited-state properties of deformed halos. Angular momentum projection calculations demonstrate that halo structures present in the intrinsic frame persist in rotational excited states.

Halo nuclear properties are related to nuclear shape density. Currently, DRHBc theory can study reflection-symmetric axially deformed and triaxially deformed nuclei but has not yet considered reflection-asymmetric deformation. Therefore, extending DRHBc theory to include reflection-asymmetric deformation is necessary. Since hyperons do not obey the Pauli exclusion principle for nucleons, they can be used as "probes" to investigate nuclear properties, such as exploring hyperon effects on deformed halo nuclei. Current beyond-mean-field calculations based on DRHBc theory include only angular momentum projection. Incorporating particle number projection to account for particle number fluctuations and using generator coordinate methods to treat fluctuations in collective degrees of freedom to achieve a microscopic and self-consistent description from ground to excited states in deformed halo nuclei represents a primary goal for future work.

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Author Contributions

SUN Xiangxiang was responsible for drafting, revising, and compiling the manuscript; ZHOU Shangui was responsible for the article framework, overall direction, and final version revision.

Note: Figure translations are in progress. See original paper for figures.