Odd-A Systems in Deformed Relativistic Hartree-Bogoliubov Theory in the Continuum (Postprint)

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Abstract

In order to describe the exotic nuclear structure in unstable odd-A or odd-odd nuclei, the deformed relativistic Hartree Bogoliubov theory in continuum has been extended to incorporate the blocking effect due to the odd nucleon. For a microscopic and self-consistent description of pairing correlations, continuum, deformation, blocking effects, and the extended spatial density distribution in exotic nuclei, the deformed relativistic Hartree Bogoliubov equations are solved in a Woods-Saxon basis in which the radial wave functions have a proper asymptotic behavior at large r. The formalism and numerical details are provided. The code is checked by comparing the results with those of spherical relativistic continuum Hartree Bogoliubov theory in the nucleus 19O. The prolate deformed nucleus 15C is studied by examining the neutron levels and density distributions.

Full Text

Preamble

Odd Systems in Deformed Relativistic Hartree-Bogoliubov Theory in Continuum

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Abstract. To describe exotic nuclear structures in unstable odd-A or odd-odd nuclei, the deformed relativistic Hartree-Bogoliubov theory in continuum has been extended to incorporate the blocking effect due to odd nucleons. For a microscopic and self-consistent description of pairing correlations, continuum effects, deformation, blocking, and extended spatial density distributions in exotic nuclei, the deformed relativistic Hartree-Bogoliubov equations are solved in a Woods-Saxon basis that ensures proper asymptotic behavior of radial wave functions at large r. The formalism and numerical details are presented, and the code is validated by comparing results for the spherical nucleus ^{19}O with those from spherical relativistic continuum Hartree-Bogoliubov theory. The prolate-deformed nucleus ^{15}C is investigated through examination of neutron levels and density distributions.

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Introduction

Nuclear halo represents one of the most fascinating phenomena discovered in exotic nuclei, exhibiting many novel features such as greatly extended spatial density distributions, dilute pure neutron matter, Borromean properties, and coupling between bound states and the continuum [?]. Previously, several relativistic Hartree-Bogoliubov theories with and without the Fock term have been developed for self-consistent description of spherical halo nuclei [?, ?, ?, ?, ?, ?]. To investigate halo phenomena in deformed nuclei microscopically and self-consistently, a deformed relativistic Hartree-Bogoliubov (RHB) theory in continuum was developed for even-even nuclei [?, ?, ?]. Within this model, a decoupling in shape between the core and halo has been predicted in certain deformed nuclei near the neutron drip line, such as ^{42,44}Mg [?, ?].

To describe exotic nuclear structures in unstable odd-A or odd-odd nuclei, the blocking effect of one or several nucleons must be taken into account. In this Letter, the deformed relativistic Hartree-Bogoliubov theory in continuum [?, ?, ?] is extended to incorporate the blocking effect due to an odd nucleon. This enables microscopic and self-consistent treatment of pairing correlations, continuum effects, deformation, blocking, and extended spatial density distributions in exotic odd-A or odd-odd nuclei.

Theoretical Framework

To treat pairing correlations, we adopt the quasi-particle concept, representing the ground state of an even-even nucleus $|\Phi_0\rangle$ as a vacuum with respect to quasi-particles [?]:

$$\beta_k|\Phi_0\rangle = 0, \quad \text{for all } k = 1, \dots, N,$$

where N is the dimension of the quasi-particle space and the quasi-particle operators $\beta_k^\dagger, \beta_k$ are obtained through Bogoliubov transformation from the particle operators $c_l^\dagger, c_l$:

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = W^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \quad W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}.$$

The coefficient matrix W is unitary, which guarantees that the quasi-particle operators satisfy the same anticommutation rules as the particle operators [?]. Starting from the bare vacuum $|0\rangle$, the ground state of a system with an even number of particles $|\Phi_0\rangle$ can be constructed as:

$$|\Phi_0\rangle = \prod_{k=1}^{N} \beta_k|0\rangle.$$

For an odd system, the corresponding ground state can be constructed as a one-quasi-particle state $|\Phi_1\rangle$:

$$|\Phi_1\rangle = \beta_1^\dagger|\Phi_0\rangle = \beta_1^\dagger \prod_{k=1}^{N} \beta_k|0\rangle,$$

where $\beta_1^\dagger$ corresponds to the quasi-particle state with the lowest quasi-particle energy. In other words, the one-quasi-particle state $|\Phi_1\rangle$ is the vacuum with respect to the set of quasi-particle operators $(\beta_1', \dots, \beta_N')$ with $\beta_1' = \beta_1^\dagger$, $\beta_2' = \beta_2$, ..., $\beta_N' = \beta_N$, and the exchange of operators $\beta_1^\dagger \leftrightarrow \beta_1$ forms a new set of quasi-particle operators $(\beta_1', \dots, \beta_N', \beta_1'^\dagger, \dots, \beta_N'^\dagger)$. This corresponds to exchanging the columns $(U_{l1}, V_{l1}) \leftrightarrow (V_{l1}^*, U_{l1}^*)$ in the matrix W. Thus, the blocking effect in an odd system can be realized by exchanging the creator $\beta_1^\dagger$ with the corresponding annihilator β_1 in the quasi-particle space. Accordingly, the blocking effect in multi-quasi-particle configurations can be treated similarly.

The covariant density functional theory has been successfully applied to describe nuclear structure across the entire periodic table [?, ?, ?, ?, ?]. The relativistic Hartree-Bogoliubov equations [?, ?, ?] for nucleons read:

$$\begin{pmatrix} h_D - \lambda & -\Delta^* \\ \Delta & -h_D + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix},$$

where E_k is the quasi-particle energy, λ is the chemical potential that ensures the proper average particle number, and h_D is the Dirac Hamiltonian:

$$h_D(\mathbf{r}, \mathbf{r}') = \alpha \cdot \mathbf{p} + V(\mathbf{r}) + \beta[M + S(\mathbf{r})].$$

The scalar and vector potentials $S(\mathbf{r})$ and $V(\mathbf{r})$ are given by:

$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r}), \quad V(\mathbf{r}) = g_\omega \omega_0(\mathbf{r}) + g_\rho \tau_3 \rho_0(\mathbf{r}) + e\frac{1-\tau_3}{2} A_0(\mathbf{r}),$$

which depend on the scalar field σ as well as the time-like components ω_0, ρ_0, and A_0 of the isoscalar vector field ω, the 3-component of the isovector field ρ, and the photon field A.

For a fully paired, axially symmetric deformed system with time-reversal symmetry, the projection of total angular momentum on the symmetry axis Ω is conserved, and each single-particle state has a twofold degeneracy. The RHB equation can be reduced to half-dimension $M = N/2$ and decomposed into degenerate blocks with quantum numbers $+\Omega$ or $-\Omega$. The corresponding density and pairing tensors have dimension M:

$$\rho_{M\times M} = V^* V^T, \quad \kappa_{M\times M} = V^* U^T,$$

where V and U are the coefficients in the corresponding subspace.

For an odd system with the k_b-th level blocked in the $+\Omega$ subspace, time-reversal symmetry is violated and currents appear in the system. These currents maintain axial symmetry, i.e., Ω remains a good quantum number, but the quasiparticle energies are no longer degenerate between the two subspaces because the $+\Omega$ subspace contains the odd particle while the corresponding $-\Omega$ subspace contains an empty level. Therefore, in principle, one must diagonalize the RHB equation twice—once for the $+\Omega$ subspace and once for the $-\Omega$ subspace. Using the equal-filling approximation commonly employed [?, ?], we neglect currents and statistically average over the two configurations of a particle in the $+\Omega$ space and a particle in the $-\Omega$ space. The corresponding currents cancel each other, yielding fields with time-reversal symmetry at each iteration step. In practice, we average the density matrix ρ and symmetrize the pairing tensor κ in the two subspaces, replacing the two densities by:

$$\rho' = \rho_{M\times M} - V^*_{k_b} V^T_{k_b} + U^*_{k_b} U^T_{k_b},$$

$$\kappa' = \kappa_{M\times M} - V^*_{k_b} U^T_{k_b} + U^*_{k_b} V^T_{k_b},$$

where V_{k_b} and U_{k_b} are column vectors in matrices V and U corresponding to the blocked level. Note that these equations are equivalent to those given in Refs. [?, ?] when time-reversal symmetry is considered and the dimension of the densities is $M = N/2$.

Applications and Results

In the following applications, we employ the density functional PK1 [?] and a zero-range density-dependent pairing force [?, ?]. The deformed RHB equations are solved in a spherical Dirac Woods-Saxon basis [?], with deformed potentials and densities expanded in terms of Legendre polynomials $P_\lambda(\cos\theta)$ (for details see Refs. [?, ?, ?]).

To verify the accuracy of the deformed code with blocking, we investigate the spherical nucleus ^{19}O and compare results from the deformed RHB code (allowing only spherical components of the fields, i.e., $\lambda = 0$) with those from spherical relativistic continuum Hartree-Bogoliubov (RCHB) theory [?]. Ground-state properties from both calculations are listed in Table I, showing excellent agreement. For instance, the difference in total binding energies is approximately 0.02 MeV, corresponding to an accuracy of about 0.01%.

[TABLE I]

To examine the details of the deformed RHB calculation, Fig. 1 displays neutron single-particle levels in the canonical basis for ^{19}O, compared with spherical RCHB results. Each level's length is proportional to its occupation probability. In the spherical RCHB calculation, the blocked orbital is $1d_{5/2}$. The deformed RHB code enforces a spherical solution by retaining only the $\lambda = 0$ component in the Legendre expansion, making the three sublevels of the $1d_{5/2}$ orbital with $\Omega^\pi = 1/2^+, 3/2^+$, and $5/2^+$ degenerate. The results in Fig. 1 were obtained with the $\Omega^\pi = 1/2^+$ level blocked in the deformed RHB code, though blocking any of these three levels yields identical results. Excellent agreement is evident between the deformed RHB and RCHB calculations.

[Figure 1: see original paper]

After validating the code for the spherical case, we now apply deformed RHB theory to an exotic deformed nucleus with an odd number of particles. The deformed halo candidate ^{15}C [?] is studied using the PK1 parameter set [?]. Unlike the spherical even-even nucleus ^{14}C, the deformed RHB theory predicts a deformation $\beta = 0.25$ for the odd-A nucleus ^{15}C. The neutron root-mean-square radii are 2.56 fm for ^{14}C and 2.79 fm for ^{15}C.

The deformed RHB calculations yield axially symmetric density distributions for ^{15}C. Figure 2 plots neutron densities along the symmetry axis $\rho_n(r_z, r_\perp = 0)$ and perpendicular to it $\rho_n(r_z = 0, r_\perp)$ as dashed and dashed-dotted lines, respectively, with the spherical density for ^{14}C shown as a solid line for reference. Notably, the neutron densities perpendicular to the symmetry axis are nearly identical for ^{14}C and ^{15}C (at least for $r_\perp < 6$ fm). Along the symmetry axis, however, the neutron density of ^{15}C extends much further than that of ^{14}C, partly because ^{15}C is prolate and the weakly bound $1/2^+$ level is occupied.

[Figure 2: see original paper]

Single-particle levels of ^{15}C in the canonical basis are shown in Fig. 3. Being a deformed nucleus, the $1p_{3/2}$ orbit splits into two levels with $\Omega^\pi = 1/2^-$ and $\Omega^\pi = 3/2^-$. One neutron occupies the $\Omega^\pi = 1/2^+$ level near the threshold, with occupation probability $v^2 = 0.5$, indicating averaging over the two configurations with $\Omega^\pi = \pm 1/2^+$. Due to deformation, this level mixes spherical orbits $1d_{5/2}$ (62%) and $2s_{1/2}$ (36%). The weakly bound nature and relatively large s-wave component of this level cause the neutron density of ^{15}C to extend further along the symmetry axis.

[Figure 3: see original paper]

Summary

In summary, to describe odd-A or odd-odd exotic nuclei, the blocking effect due to an odd nucleon has been incorporated into deformed relativistic Hartree-Bogoliubov (RHB) theory in continuum. The formalism is briefly presented, and numerical validation is performed by comparing deformed RHB results for the spherical nucleus ^{19}O with spherical RCHB calculations. As a first application, the deformed nucleus ^{15}C is studied through examination of neutron levels, deformation, and density distributions along and perpendicular to the symmetry axis. The neutron density of ^{15}C extends much further along the symmetry axis because ^{15}C is prolate and the weakly bound valence level with $\Omega^\pi = 1/2^+$ has a relatively large s-wave component.

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