Deformed relativistic Hartree Bogoliubov theory in continuum (Postprint)

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Abstract

A deformed relativistic Hartree Bogoliubov (RHB) theory in continuum is developed aiming at a proper description of exotic nuclei, particularly those with a large spatial extension. In order to give an adequate consideration of both the contribution of the continuum and the large spatial distribution in exotic nuclei, the deformed RHB equations are solved in a Woods-Saxon (WS) basis in which the radial wave functions have a proper asymptotic behavior at large distance from the nuclear center. This is crucial for the proper description of a possible halo. The formalism of deformed RHB theory in continuum is presented. A stable nucleus, 20Mg and a weakly-bound nucleus, 42Mg, are taken as examples to present numerical details and to carry out necessary numerical checks. In addition, the ground state properties of even-even magnesium isotopes are investigated. The generic conditions of the formation of a halo in weakly bound deformed systems and the shape of the halo in deformed nuclei are discussed. We show that the existence and the deformation of a possible neutron halo depend essentially on the quantum numbers of the main components of the single particle orbitals in the vicinity of the Fermi surface.

Full Text

Deformed Relativistic Hartree-Bogoliubov Theory in Continuum

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A deformed relativistic Hartree-Bogoliubov (RHB) theory in continuum is developed aiming at a proper description of exotic nuclei, particularly those with large spatial extension. In order to give adequate consideration to both the contribution of the continuum and the large spatial distribution in exotic nuclei, the deformed RHB equations are solved in a Woods-Saxon (WS) basis in which the radial wave functions have proper asymptotic behavior at large distance from the nuclear center. This is crucial for the proper description of a possible halo. The formalism of deformed RHB theory in continuum is presented. A stable nucleus, ^{20}Mg, and a weakly-bound nucleus, ^{42}Mg, are taken as examples to present numerical details and to carry out necessary numerical checks.

In addition, the ground-state properties of even-even magnesium isotopes are investigated. The generic conditions for the formation of a halo in weakly bound deformed systems and the shape of the halo in deformed nuclei are discussed. We show that the existence and deformation of a possible neutron halo depend essentially on the quantum numbers of the main components of the single-particle orbitals in the vicinity of the Fermi surface.

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Introduction

The development of radioactive ion beam facilities around the world [?, ?, ?, ?, ?, ?, ?] has greatly stimulated the study of nuclei far from the β-stability line [?, ?, ?, ?, ?, ?, ?, ?, ?]. New and exotic phenomena have been observed in nuclei close to drip lines, such as neutron or proton halos [?, ?, ?], changes of nuclear magic numbers [?], pygmy resonances [?], etc. In halo nuclei, the fact of extremely weak binding leads to many new features, e.g., the coupling between bound states and the continuum due to pairing correlations and very extended spatial density distributions. Therefore, one must properly treat the asymptotic behavior of nuclear densities at large distance r from the center and self-consistently handle discrete bound states, the continuum, and the coupling between them in order to give a proper theoretical description of the halo phenomenon [?, ?, ?]. This could be achieved by solving the non-relativistic Hartree-Fock-Bogoliubov (HFB) [?, ?] or the relativistic Hartree-Bogoliubov (RHB) [?, ?, ?] equations in coordinate (r) space, which can fully account for the mean-field effects of coupling to the continuum. The resonant-BCS (rBCS) approach presents another method to include the contribution of the resonant continuum, which has been used to study halo phenomena [?, ?].

The solution of the coupled differential equations of HFB and RHB theories is particularly simple in spherical systems with local potentials, where one-dimensional Numerov or Runge-Kutta methods [?] can be applied. This is true even for non-local problems where Finite Element Methods (FEM) [?] have been used. A different method to solve such equations is the expansion of the single-particle wave functions in an appropriate basis. The oscillator basis has been used for this purpose with great success for deformed or non-local systems in the past [?, ?, ?, ?]. The Woods-Saxon basis has been proposed in Ref. [?] as a reconciler between the harmonic oscillator basis and integration in coordinate space. Woods-Saxon wave functions have much more realistic asymptotic behavior at large r than harmonic oscillator wave functions do. A discrete set of Woods-Saxon wave functions is obtained by using box boundary conditions to discretize the continuum. It has been shown in Ref. [?] for spherical systems that the solution of the relativistic Hartree equations in a Woods-Saxon basis is almost equivalent to the solution in coordinate space. The Woods-Saxon basis has also been used in more complicated situations, e.g., for the description of exotic nuclei where both deformation and pairing must be taken into account. Recently, for spherical systems, both non-relativistic and relativistic Hartree-Fock-Bogoliubov theories with forces of finite range have been investigated in a Woods-Saxon basis [?, ?].

Over the past years, many efforts have been made to develop a deformed relativistic Hartree (RH) theory [?] and a deformed relativistic Hartree-Bogoliubov theory in continuum [?]. As a first application, halo phenomena in deformed nuclei have been investigated within the continuum RHB theory, and some brief results can be found in Ref. [?]. In this paper, we present the full version of the theoretical framework with all the details.

Spherical symmetry considerably facilitates the treatment of the continuum in non-relativistic HFB [?, ?] and relativistic RHB theory [?, ?, ?] in r-space. Since most known nuclei are deformed, interesting questions arise regarding whether deformed halos exist and what new features can be expected in deformed exotic nuclei [?, ?, ?, ?, ?, ?, ?]. Such questions can be answered by the deformed counterparts of HFB or RHB theories in coordinate space. From the experimental point of view, ^{31}Ne has been measured to be a strongly deformed halo nucleus [?], and for the well-deformed magnesium isotopes, ^{35}Mg is probably a halo nucleus too [?]. Nevertheless, for deformed nuclei, solving the HFB or RHB equations in r-space becomes much more sophisticated and numerically very time-consuming. Many efforts have been made to develop non-relativistic HFB theories either in (discretized) coordinate space or in a scaled oscillator basis with improved asymptotic behavior [?]. The HFB equations have been solved in three-dimensional coordinate space by combining the imaginary-time approach and the two-basis method [?] with a truncated basis composed of discrete localized states and discretized continuum states up to a few MeV [?]. Alternatively, the HFB equations have been solved on two-dimensional basis-spline Galerkin lattices [?, ?, ?] or on a three-dimensional Cartesian mesh [?] using the canonical-basis approach [?].

Recently, the Gaussian expansion method has been used to solve the HF and HFB equations for deformed nuclei [?], and continuum Skyrme-Hartree-Fock-Bogoliubov approaches have been developed for both spherical and deformed nuclei [?]. The deformed relativistic Hartree-Bogoliubov (RHB) theory has only been solved in the conventional harmonic oscillator basis [?, ?, ?, ?], and neither the above-mentioned approaches nor other methods that could improve the asymptotic behavior of nuclear densities at large r have been implemented in the deformed RHB theory so far.

In this paper, we present a method that allows simultaneous consideration of coupling to the continuum, deformations, and pairing correlations in a fully self-consistent way. For this purpose, we expand the deformed Dirac spinors in a basis of spherical Dirac wave functions obtained from solving the Dirac equations for potentials with spherical Woods-Saxon shape. This idea is similar to a method proposed in Ref. [?] for solving the deformed relativistic mean-field (RMF) equations in light nuclei, where the deformed Dirac spinors were expanded in terms of the self-consistent solutions of the spherical RMF equations. Compared to these early calculations, our method is simpler because it is based on Woods-Saxon wave functions. On the other hand, it is more general because it allows inclusion of pairing correlations, which play an essential role in the formation of halo structures.

The paper is organized as follows. In Sec. II, we give the formalism of the deformed RHB theory in continuum. The numerical details are presented in Sec. III, and we discuss applications and detailed results for magnesium isotopes in Sec. IV. A summary is given in Sec. V.

II. Formalism of the Deformed Relativistic Hartree-Bogoliubov Theory in Continuum

The starting point of relativistic mean-field theory is a Lagrangian density where nucleons are described as Dirac spinors that interact via the exchange of effective mesons (σ, ω, and ρ) and the photon [?, ?, ?, ?, ?, ?, ?]:

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu\partial_\mu - M)\psi + \frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - U(\sigma) - \frac{1}{4}\Omega^{\mu\nu}\Omega_{\mu\nu} + \frac{1}{2}m_\omega^2\omega^\mu\omega_\mu - g_\sigma\bar{\psi}\sigma\psi - g_\omega\bar{\psi}\gamma^\mu\omega_\mu\psi - \frac{1}{4}\vec{R}^{\mu\nu}\vec{R}_{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^\mu\vec{\rho}_\mu - g_\rho\bar{\psi}$$

where M is the nucleon mass, and m_σ, g_σ, m_ω, g_ω, m_ρ, g_ρ are the masses and coupling constants of the respective mesons.

The nonlinear self-coupling for the scalar meson is given by [?]:

$$U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4$$

The field tensors for the vector mesons and photon fields are defined as:

$$\Omega^{\mu\nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu$$

$$\vec{R}^{\mu\nu} = \partial^\mu \vec{\rho}^\nu - \partial^\nu \vec{\rho}^\mu + g_\rho (\vec{\rho}^\mu \times \vec{\rho}^\nu)$$

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$$

Pairing correlations are crucial in the description of open-shell nuclei. For exotic nuclei, the conventional BCS approach turns out to be only a poor approximation [?]. Starting from the Lagrangian density (1), a relativistic theory of pairing correlations in nuclei has been developed by Kucharek and Ring [?]. If we neglect the Fock terms as is usually done in covariant density functional theory, the Dirac Hartree-Bogoliubov (RHB) equation for the nucleons reads:

$$\int d^3 r' \begin{pmatrix} h_D(\mathbf{r}, \mathbf{r}') - \lambda & \Delta(\mathbf{r}, \mathbf{r}') \\ -\Delta^*(\mathbf{r}, \mathbf{r}') & -h_D^*(\mathbf{r}, \mathbf{r}') + \lambda \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}') \\ V_k(\mathbf{r}') \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}$$

where E_k is the quasiparticle energy, λ is the chemical potential, 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:

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

depend on the scalar field σ and on 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.

The equations of motion for the mesons and photon have as sources the various densities:

$$(-\Delta + m_\sigma^2)\sigma(\mathbf{r}) = g_\sigma \rho_s(\mathbf{r}) - \frac{\partial U(\sigma)}{\partial \sigma}$$

$$(-\Delta + m_\omega^2)\omega_0(\mathbf{r}) = g_\omega \rho_v(\mathbf{r})$$

$$(-\Delta + m_\rho^2)\rho_0(\mathbf{r}) = g_\rho \rho_3(\mathbf{r})$$

$$-\Delta A_0(\mathbf{r}) = e \rho_p(\mathbf{r})$$

where, according to the no-sea approximation, the sum over $k > 0$ runs over the quasiparticle states corresponding to single-particle energies in and above the Fermi sea.

The pairing potential reads:

$$\Delta(r_1 s_1 p_1, r_2 s_2 p_2) = \sum_{s_1', s_2'} \int d^3 r_1' d^3 r_2' V_{pp}(r_1, r_2; s_1 p_1, s_2 p_2, s_1', s_2') \kappa(r_1 s_1', r_2 s_2')$$

where $p = 1, 2$ represents the large and small components of the Dirac spinors, V_{pp} is the effective pairing interaction, and $\kappa(r_1 s_1', r_2 s_2')$ is the pairing tensor [**?**].

In the particle-particle (pp) channel, we use a density-dependent zero-range force:

$$V_{pp}(r_1, r_2) = V_0 \frac{1 - P_\sigma}{2} \delta(\mathbf{r}_1 - \mathbf{r}_2) \left(1 - \frac{\rho(\mathbf{r}_1)}{\rho_{sat}}\right)$$

where P_σ projects onto spin $S = 0$ component in the pairing field. In this case, the gap equation has the simple form:

$$\Delta(\mathbf{r}) = V_0 \left(1 - \frac{\rho(\mathbf{r})}{\rho_{sat}}\right) \kappa(\mathbf{r})$$

and we need only the local part of the pairing tensor:

$$\kappa(\mathbf{r}) = \sum_k U_k^*(\mathbf{r}) V_k(\mathbf{r})$$

Details of the calculation of the pairing interaction and pairing tensor are given in Appendices B and E, respectively.

For axially deformed nuclei with spatial reflection symmetry, we expand the potentials $S(\mathbf{r})$ and $V(\mathbf{r})$ and the densities in terms of Legendre polynomials [**?**]:

$$f(\mathbf{r}) = \sum_\lambda f_\lambda(r) P_\lambda(\cos\theta), \quad \lambda = 0, 2, 4, \cdots$$

The quasiparticle wave functions U_k and V_k are Dirac spinors. Each is expanded in terms of spherical Dirac spinors $\phi_{n\kappa m}(\mathbf{r}sp)$ with eigenvalues $\epsilon_{n\kappa}$ obtained from the solution of a Dirac equation containing spherical potentials $S^{(0)}(r)$ and $V^{(0)}(r)$ of Woods-Saxon shape [**?**, **?**]:

$$U_k(\mathbf{r}sp) = \sum_{n\kappa} u_{k,(n\kappa)}\phi_{n\kappa m}(\mathbf{r}sp), \quad V_k(\mathbf{r}sp) = \sum_{n\kappa} v_{k,(n\kappa)}\bar{\phi}_{n\kappa m}(\mathbf{r}sp)$$

The basis wave function reads:

$$\phi_{n\kappa m}(rs) = \frac{iG_{n\kappa}(r)}{r}Y^l_{jm}(\Omega, s) + \frac{F_{n\kappa}(r)}{r}Y^{\tilde{l}}_{jm}(\Omega, s)$$

where $G_{n\kappa}(r)/r$ and $F_{n\kappa}(r)/r$ are the radial wave functions for the upper and lower components. The spherical spinor $\phi_{n\kappa m}$ is characterized by the radial quantum number n, angular momentum j, and parity π. j and π are combined to the relativistic quantum number $\kappa = \pi(-1)^{j+1/2}(j + 1/2)$, which runs over positive and negative integers. Y^l_{jm} and $Y^{\tilde{l}}_{jm}$ are the spinor spherical harmonics where $l = j + \frac{1}{2}\text{sign}(\kappa)$ and $\tilde{l} = j - \frac{1}{2}\text{sign}(\kappa)$. $\bar{\phi}_{n\kappa m}(\mathbf{r}sp)$ is the time-reversal state of $\phi_{n\kappa m}(\mathbf{r}sp)$.

These states form a complete spherical and discrete basis in Dirac space (see Appendix A for details). Because of axial symmetry, the z-component m of the angular momentum j is a conserved quantum number, and the RHB Hamiltonian can be decomposed into blocks characterized by m and parity π. For each $m\pi$-block, solving the RHB equation is equivalent to the diagonalization of the matrix:

$$\begin{pmatrix} \mathcal{D} - \lambda & \Delta \\ -\Delta^* & -\mathcal{D}^* + \lambda \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = E \begin{pmatrix} u \\ v \end{pmatrix}$$

where $\mathcal{D}_{(n\kappa)(n'\kappa')} = \langle n\kappa m|h_D|n'\kappa' m\rangle$ and $\Delta_{(n\kappa)(n'\kappa')} = \langle n\kappa m|\Delta|n'\kappa' m\rangle$. Further details are given in Appendix B.

Since we use a zero-range pairing force, we must introduce a pairing cutoff in the sums of Eqs. (9) and (13) over the quasiparticle space. In the present work, a smooth cutoff is adopted where two parameters, $E^{\text{cut}}_{q.p.}$ and $\Gamma^{\text{cut}}_{q.p.}$, are introduced, and the square root of the factor:

$$s(E_k) = \sqrt{\frac{(E^{\text{cut}}_{q.p.})^2}{(E_k - E^{\text{cut}}_{q.p.})^2 + (\Gamma^{\text{cut}}_{q.p.})^2}}$$

is multiplied in the occupation component $V_k(\mathbf{r})$ of each quasiparticle state with $v^2 < 1/2$. Note that this smooth cutoff is similar to the soft cutoff proposed in Ref. [**?**].

The total energy of a nucleus is:

$$E = E_{\text{nucleon}} + E_\sigma + E_\omega + E_\rho + E_c + E_{\text{c.m.}}$$

where:

$$E_{\text{nucleon}} = \sum_k \int d^3r\, V_k^\dagger(\mathbf{r})(h_D + \frac{1}{2}\Gamma)V_k(\mathbf{r}) = \sum_k E_k v_k^2 - E_{\text{pair}}$$

$$E_\sigma = \frac{1}{2}\int d^3r [g_\sigma \sigma(\mathbf{r})\rho_s(\mathbf{r}) + U(\sigma)]$$

$$E_\omega = \frac{1}{2}\int d^3r\, g_\omega \omega(\mathbf{r})\rho_v(\mathbf{r})$$

$$E_\rho = \frac{1}{2}\int d^3r\, g_\rho \rho(\mathbf{r})\rho_3(\mathbf{r})$$

$$E_c = \frac{1}{2}\int d^3r\, A_0 \rho_Z(\mathbf{r}) + E_{\text{c.m.}}$$

For a zero-range force, the pairing field $\Delta(\mathbf{r})$ is local, and the pairing energy is calculated as:

$$E_{\text{pair}} = \int d^3r\, \kappa(\mathbf{r})\Delta(\mathbf{r})$$

The center-of-mass correction energy $E_{\text{c.m.}} = \frac{\langle \hat{P}^2 \rangle}{2Am}$ is calculated after variation with the wave functions of the self-consistent solution [**?**, **?**] or in the oscillator approximation $E_{\text{c.m.}} = \frac{3}{4}41A^{-1/3}$ MeV. Details are given in Appendix G.

The root-mean-square (rms) radius is calculated as:

$$R_{\tau,\text{rms}} \equiv \langle r^2 \rangle^{1/2} = \sqrt{\frac{\int r^2 \rho_\tau(\mathbf{r}) d^3r}{\int \rho_{\tau,v,\lambda=0}(r) d^3r}}$$

where τ represents the proton, neutron, or nucleon. The rms charge radius is calculated simply as $R_{\text{ch}} = \sqrt{R_p^2 + 0.64}$ fm^2. The intrinsic multipole moment is calculated by:

$$\beta_{\tau,2} = \sqrt{\frac{5\pi}{3}} \frac{Q_{\tau,2}}{N_\tau \langle r^2 \rangle}$$

where N_τ refers to the number of neutrons, protons, or nucleons.

III. Numerical Details and Routine Checks

A. Details on the Woods-Saxon Basis

For numerical reasons, several parameters must be introduced in the calculations, e.g., the mesh size Δr, the box size R_{box} for determining the basis wave functions by solving the spherical Dirac equations with Hamiltonian $h_D^{(0)}$, the maximal λ-value $\lambda_{\max}$ in the expansion of deformed fields and densities, and the cutoff parameters for the radial and angular quantum numbers n and κ in the expansions, $n_{\max}$ and $\kappa_{\max}$. Instead of $n_{\max}$, we introduce an energy cutoff parameter E_+^{cut} for positive-energy states in the Woods-Saxon basis, and in each κ-block, the number of negative-energy states in the Dirac sea is the same as that of positive-energy states above the Dirac gap [?].

We have investigated the dependence of our results on these parameters in spherical and deformed relativistic Hartree models [?, ?]. It is found that a box of size $R_{\mathrm{box}} = 4r_0A^{1/3}$ with $r_0 = 1.2$ fm, a step size $\Delta r = 0.1$ fm, $\lambda_{\max} = 4$, and $|\kappa_{\max}| = 15$ leads to acceptable accuracy of less than 0.1% for binding energies, rms radii, and quadrupole moments in light nuclei.

In the present work, we use a box size $R_{\mathrm{box}} = 20$ fm, a mesh size $\Delta r = 0.1$ fm, and a cutoff energy $E_+^{\mathrm{cut}} = 100$ MeV for determining the Woods-Saxon basis. In each κ-block, the number of negative-energy states in the Dirac sea equals that of positive-energy states above the Dirac gap. In Sec. III C, we investigate the convergence of our results with respect to these three parameters. To reduce computational time, we use $\lambda_{\max} = 4$ and $|\kappa_{\max}| = 10$ in this work.

The parameter sets NL3 [?] and PK1 [?] are used for the Lagrangian density. Note that the center-of-mass correction energy is calculated differently with these two parameter sets. For NL3, the empirical formula in Eq. (28) is used, while for PK1, the center-of-mass correction energy is calculated microscopically (see Appendix G).

B. Parameters for the Pairing Force

There are two parameters in the phenomenological pairing force of Eq. (11), namely V_0 and ρ_{sat}, and two additional ones in the smooth cutoff of Eq. (23). We take the empirical value 0.152 fm^{-3} for the saturation density ρ_{sat}. The pairing strength V_0 and the cutoff $E_{q.p.}^{\mathrm{cut}}$ are fixed by reproducing the proton pairing energy of the Gogny force D1S in the spherical nucleus ^{20}Mg. We first calculate the ground-state properties of ^{20}Mg using the spherical relativistic Hartree-Bogoliubov theory in a harmonic oscillator basis (SRHBHO) [?], in which the Gogny-D1S [?] force is used in the pp channel. The proton pairing energy is obtained as −9.2382 MeV. In Table I, the proton pairing energies E_p^{pair} from SRHBHO and deformed RHB calculations for ^{20}Mg are given. The deformed RHB calculation using the parameter set NL3 with $V_0 = 380$ MeV fm^3, $E_{q.p.}^{\mathrm{cut}} = 60$ MeV, and the smooth parameter $\Gamma_{q.p.}^{\mathrm{cut}} = 5.65$ MeV reproduces the proton pairing energy from the SRHBHO calculation for ^{20}Mg. These pairing parameters are used in all following calculations regardless of whether NL3 or PK1 is used for the RMF Lagrangian density.

C. Completeness of the Woods-Saxon Basis

The spherical nucleus ^{20}Mg has been investigated as the first test of the deformed RHB theory, and some results were given in Fig. 1 [Figure 1: see original paper] of Ref. [?]. A comparison was made between results obtained for ground-state properties of the spherical nucleus ^{20}Mg with the spherical RCHB code [?] based on the Runge-Kutta method in radial coordinate r and the new deformed RHB code discussed in this manuscript. We summarize this comparison in Table II. In these calculations, the parameter set NL3, a box size $R_{\text{box}} = 4r_0A^{1/3} = 13.0$ fm, and a step size $\Delta r = 0.1$ fm are used. The surface δ pairing force is used with strength $V_0 = 374$ MeV fm^3 and $\rho_{\text{sat}} = 0.152$ fm^{-3}. A sharp cutoff is applied to quasiparticle states with $E^{\text{cut}}_{q.p.} = 60$ MeV. It is shown that as the basis size increases, the total binding energy E, proton pairing energy E^{pair}_p, and rms radius R all converge to the corresponding exact values. In practical calculations, E^{cut}_+ may be chosen according to the balance between desired accuracy and computational cost. It was concluded in Ref. [?] that for light nuclei, one can safely use $E^{\text{cut}}_+ = 100$ MeV, which results in accuracies of about a hundred keV in total binding energy and proton pairing energy, and around 0.002 fm in rms radius.

Since we are also interested in drip-line nuclei, we next study the dependence of deformed RHB results on the completeness of the Woods-Saxon basis for a very neutron-rich nucleus. In this subsection, we investigate results with different values of E^{cut}_+. For calculations with a Woods-Saxon basis [?], a box size $R_{\text{box}} = 4r_0A^{1/3}$ with $r_0 = 1.2$ fm is used. In this case, R_{box} differs for different magnesium isotopes, e.g., 13.0 fm for ^{20}Mg and 16.7 fm for ^{42}Mg. In the present work, we prefer to use a fixed box size $R_{\text{box}} = 20$ fm, which is large enough for all magnesium isotopes. The mesh size for the radial wave function of each Woods-Saxon state is taken as 0.1 fm.

For ^{42}Mg, both prolate and oblate minima in the potential energy surface are searched for, and it is found that the ground state is prolate. In Fig. 1, the total binding energy E_B, quadrupole deformation β, and rms radius R are plotted as functions of E^{cut}_+ for both the prolate ground state and the oblate minimum of ^{42}Mg. Apparently, as E^{cut}_+ increases, these quantities all converge well. Similar to the case of the spherical nucleus ^{20}Mg, for light deformed nuclei, the cutoff $E^{\text{cut}}_+ = 100$ MeV results in relative accuracies of 0.5% for quadrupole deformation, 0.05% for rms radius, and 0.1% for total binding energy.

The box size $R_{\text{box}} = 20$ fm and cutoff energy $E^{\text{cut}}_+ = 100$ MeV are fixed when we investigate convergence with respect to mesh size Δr. In Fig. 2 [Figure 2: see original paper], it is shown that as the mesh size decreases, the total binding energy E_B, quadrupole deformation β, and rms radius R all converge well. The difference in binding energy between calculations with $\Delta r = 0.1$ fm and $\Delta r = 0.05$ fm is smaller than 0.025 MeV for both minima, which is about 0.008% of the total binding energy. When Δr is decreased from 0.1 fm to 0.05 fm, the relative changes in quadrupole deformation β and radius R are both smaller than 0.01%.

Figure 3 [Figure 3: see original paper] shows the same quantities as functions of box size R_{box}. The relative deviations between rms radius R at $R_{\text{box}} = 20$ fm and $R_{\text{box}} = 30$ fm are about 0.1% for the prolate ground state and 0.01% for the oblate minimum. The box size $R_{\text{box}} = 20$ fm also gives good accuracy for quadrupole deformation β and binding energy.

In conclusion, for the following calculations we fix the box size at $R_{\text{box}} = 20$ fm, mesh size at $\Delta r = 0.1$ fm, and cutoff energy for positive-energy states in the Woods-Saxon basis at $E_{+}^{\text{cut}} = 100$ MeV. In each κ-block, the number of negative-energy states in the Dirac sea equals that of positive-energy states above the Dirac gap. The cutoff parameter for λ in expansion Eq. (14) is $\lambda_{\max} = 4$, and the cutoff parameter for angular quantum number κ in expansion Eq. (17) is $|\kappa_{\max}| = 10$. With these values, we do not introduce sizable errors.

IV. Results and Discussions

In this section, we present results from the deformed RHB theory in continuum. We choose magnesium isotopes as examples. After discussing bulk properties of magnesium isotopes, we focus on the neutron-rich nucleus ^{42}Mg.

A. Bulk Properties of Magnesium Isotopes

Figure 4 [Figure 4: see original paper] shows the neutron Fermi energy λ_n and two-neutron separation energy S_{2n} of magnesium isotopes calculated with parameter sets NL3 [?] and PK1 [?]. The separation energies are compared with data from Ref. [?]. Except for different predictions of the two-neutron drip-line nucleus, the results for neutron Fermi surfaces and two-neutron separation energies are very similar for both parameter sets. The calculated two-neutron separation energies S_{2n} of magnesium isotopes agree reasonably well with available experimental values except for ^{32}Mg. The large discrepancy in ^{32}Mg is connected to shape and shell structure at $N = 20$ and will be discussed later.

Experimentally, the nucleus ^{40}Mg has been observed [?]. Theoretically, there are several predictions for the last bound nucleus in Mg isotopes: ^{44}Mg in the phenomenological finite-range droplet model [?], ^{40}Mg in a macroscopic-microscopic model [?], an RMF model with parameter set NLSH [?], and the Skyrme HFB model with parameter set SLy4 solved in a 3-dimensional Cartesian mesh [?], while ^{42}Mg is predicted by the Skyrme HFB model with SLy4 solved in a transformed harmonic oscillator basis [?] and the HFB21 mass table [?]. Therefore, the prediction of the two-neutron drip-line nucleus in Mg isotopes is both model- and parametrization-dependent. In our deformed RHB calculations with parameter set NL3, ^{46}Mg is the last nucleus with negative neutron Fermi surface and positive two-neutron separation energy. However, with parameter set PK1, ^{42}Mg is predicted to be the last nucleus within the two-neutron drip line.

The comparison of quadrupole deformation β between theory and experiment is given in Fig. 5 [Figure 5: see original paper]. The experimental values of β are extracted from measured $B(E2 : 0^+ \to 2^+)$ values and therefore only absolute values are available [?]. Generally, the ground-state quadrupole deformations β calculated with both parameter sets reproduce the data rather well. Exceptions are ^{32}Mg, which turns out to be spherical in both models, and ^{30}Mg, which is prolate and slightly less deformed than experiment for PK1 and slightly oblate for NL3. In ^{32}Mg, the gap between neutron levels $1d_{3/2}$ and $1f_{7/2}$ is almost 7 MeV, resulting in a strong closed shell at $N = 20$. Therefore, deformed RHB calculations with both parameter sets predict spherical shapes for this nucleus. This also leads to a large discrepancy from experiment for the two-neutron separation energy S_{2n} of ^{32}Mg, as seen in Fig. 4. Other mean-field models also predict spherical or almost spherical shapes for ^{32}Mg [?, ?, ?, ?, ?, ?, ?, ?]. For isotopes beyond this nucleus with $32 < A < 46$, we observe large deformations, the so-called "island of inversion" [?, ?, ?, ?], which is related to quenching of the $N = 20$ shell closure. At the mean-field level, ^{32}Mg does not belong to this island yet. In fact, going beyond mean-field and calculating the energy surface as a function of deformation parameters, one finds that this nucleus is transitional with an extended shoulder reaching to large deformations. This leads in GCM calculations with the Gogny force [?] to wavefunctions with large fluctuations in deformation space and to a large $B(E2 : 0^+ \to 2^+)$ value as observed experimentally [?]. So far it remains an open question why other GCM calculations based on Skyrme forces [?] or the relativistic point-coupling model PC-F1 [?] cannot reproduce this fact.

Up to ^{42}Mg, the deformed RHB results from parameter set NL3 are very similar to those from PK1. Therefore, in the following we focus our discussion mainly on results from PK1.

Figure 6 [Figure 6: see original paper] shows rms radii for magnesium isotopes as functions of neutron number. We display neutron radii R_n, proton radii R_p, matter radii R_t, the $r_0A^{1/3}$ curve with $r_0 = 1$ fm, and experimental matter radii [?, ?]. The proton radius is almost constant with a very slow increase with N due to neutron-proton coupling in the mean field. With increasing neutron number, the neutron radius R_n increases monotonically except at ^{32}Mg. The neutron radius of ^{32}Mg is relatively small, again due to strong shell effects at $N = 20$ in mean-field calculations. The deformed RHB results agree well with experiment for matter radii. The calculated matter radius follows roughly the $r_0A^{1/3}$ curve up to $A = 34$. From ^{36}Mg onward, the matter radius lies much higher above the $r_0A^{1/3}$ curve, which may indicate exotic structure in these nuclei.

Figure 7 [Figure 7: see original paper] shows neutron density profiles of even-even magnesium isotopes with $A \geq 28$ calculated with parameter set PK1.

$\rho_{n,\lambda=0}(r)$ represents the spherical component of the neutron density distribution (cf. Eq. 14). $\rho_n(z, r_\perp = 0)$ with $r_\perp = \sqrt{x^2 + y^2}$ refers to the density distribution along the symmetry axis z ($\theta = 0°$), and $\rho_n(z = 0, r_\perp)$ refers to that perpendicular to the symmetry axis z ($\theta = 90°$). With increasing A, the spherical component $\rho_{n,\lambda=0}(r)$ changes rapidly at ^{42}Mg. The density distribution along the symmetry axis $\rho_n(z, r_\perp = 0)$ changes abruptly from ^{32}Mg to ^{34}Mg, which can be understood by the shape change from spherical ^{32}Mg to prolate ^{34}Mg where the density is elongated along the z-axis. In the direction perpendicular to the symmetry axis, the neutron density $\rho_n(z = 0, r_\perp)$ of ^{42}Mg extends very far from the nuclear center and a long tail emerges, revealing halo formation.

By comparing $\rho_n(z, r_\perp = 0)$ and $\rho_n(z = 0, r_\perp)$ for ^{42}Mg, we find that in the tail part, the neutron density extends more along the direction perpendicular to the symmetry axis. Since this nucleus as a whole is prolate, it indicates that the neutron tail has a different shape than the core. This is similar to the decoupling of halo shape from core shape found for ^{44}Mg in Ref. [**?**]. Next we concentrate on ^{42}Mg and discuss its ground-state structure in detail.

B. Ground State of ^{42}Mg

TABLE III. Properties of ^{42}Mg at the ground state and at the oblate minimum derived from deformed RHB calculations with parameter sets NL3 and PK1. Listed are neutron and proton Fermi surfaces λ_n and λ_p, neutron, proton, and total quadrupole deformations β_n, β_p, β_t, neutron, proton, and total radii R_n, R_p, R_t, neutron and proton pairing energies E_n^{pair}, E_p^{pair}, and total binding energy E_B.

Property	NL3 (Prolate)	NL3 (Oblate)	PK1 (Prolate)	PK1 (Oblate)
λ_n (MeV)	-0.6147	-0.1753	-0.8805	-0.3989
λ_p (MeV)	-24.6731	-23.9050	-24.2695	-22.8118
β_n	0.4155	-0.3299	0.3911	-0.2426
β_p	0.4085	-0.3049	0.0000	-6.7639
β_t	0.4130	-0.3220	0.3911	-0.2426
R_n (fm)	3.3282	3.2426	3.3038	3.2381
R_p (fm)	3.2511	3.2620	3.2509	3.2595
R_t (fm)	3.2905	3.2515	3.2795	3.2475
E_n^{pair} (MeV)	-18.2511	-6.2620	-17.1509	-6.1595
E_p^{pair} (MeV)	-7.0405	-6.7639	0.0000	-6.7639
E_B (MeV)	-265.4629	-266.4505	-270.6907	-270.6993

In calculations based on parameter set PK1, the chain of Mg isotopes reaches the two-neutron drip line at ^{42}Mg. Its properties are summarized in Table III. For ^{42}Mg, we find two minima in the energy surface as a function of deformation parameter β. The lower one has a prolate shape and corresponds to the ground state of ^{42}Mg. The second minimum has an oblate shape. However, from RMF calculations allowing triaxial deformations [?], we know that the oblate minimum is not stable–it forms a saddle point in the $(\beta-\gamma)$ plane and therefore does not correspond to an isomeric state. The ground state is well deformed with a quadrupole deformation $\beta \approx 0.41$ and a very small two-neutron separation energy $S_{2n} \approx 0.22$ MeV. The density distribution of this weakly bound nucleus has a very long tail in the direction perpendicular to the symmetry axis (cf. Fig. 7), which indicates that the prolate nucleus ^{42}Mg has an oblate halo.

The density distribution in Fig. 8 [Figure 8: see original paper] is decomposed into contributions from the oblate "Halo" and the prolate "Core". Details of this decomposition will be given further below. This indicates decoupling between the deformations of the core and the halo.

Pairing correlations play a very important role in halo formation [?]. For parameter set PK1, we find in Table III that in the ground state of ^{42}Mg, the proton pairing energy vanishes while the neutron pairing energy is -6.26 MeV. For the zero-range pairing interaction in Eq. (11), only spin-singlet ($S = 0$) states and elements diagonal in quantum number p are taken into account in the pairing tensor (see Appendix F for more details concerning this assumption).

In Fig. 9 [Figure 9: see original paper], we show the components $\kappa_\lambda^{++}(r)$ from Eq. (E5) and $\kappa_\lambda^{--}(r)$ from Eq. (E6) of the pairing tensor in the ground state of ^{42}Mg for parameter set PK1. Figure 9(b) shows the main component $\kappa_\lambda^{++}(r)$ corresponding to the large components of the Dirac spinor. Comparing Figs. 9(a) and 9(b), we find that $\kappa_\lambda^{--}(r)$ is smaller than $\kappa_\lambda^{++}(r)$ by two orders of magnitude. The same sign for quadrupole ($\lambda = 2$) and spherical ($\lambda = 0$) components can be understood because the ground state of ^{42}Mg is prolate in the present calculation. The maximum of $\kappa_\lambda^{++}(r)$ appears at about 4.8 fm, indicating that pairing in nuclei is a surface effect. The hexadecapole components ($\lambda = 4$) are much smaller than the spherical components ($\lambda = 0$).

Weakly bound orbitals or those embedded in the continuum play a crucial role in nuclear halo formation [?, ?, ?]. To gain intuitive understanding of the single-particle structure, the canonical basis is constructed by the method given in Ref. [?]. The single-particle spectrum around the Fermi level for the ground state of ^{42}Mg is shown in Fig. 10 [Figure 10: see original paper]. For an axially deformed nucleus with spatial reflection symmetry, the good quantum numbers of each single-particle state include parity π and the third component of angular momentum m (labeled by the Nilsson quantum number Ω in the figures). The occupation probabilities v^2 in the canonical basis have BCS form [?] and are given by the length of horizontal lines in Fig. 10. To guide the eye, we also show by a blue dashed line the BCS formula calculated with an average gap parameter. Levels close to the threshold are labeled by number i according to their energies, and their conserved quantum numbers Ω^π and main spherical components are given on the right side. The neutron Fermi level lies within the pf shell, and most single-particle levels have negative parity. Since the chemical potential $\lambda_n \approx -175$ keV is negative, the corresponding density $\rho(\mathbf{r})$ is localized, and particles occupying levels in the continuum are bound [**?**]. Because λ_n is close to the continuum, orbitals above threshold have noticeable occupations due to pairing correlations. For instance, the occupation probability of the fifth level ($\Omega^\pi = 3/2^-$) is 31.5%. The fourth level $\Omega^\pi = 1/2^-$ is just below threshold with single-particle energy $\epsilon_{\text{can}} = -0.234$ MeV and occupation probability 53.0%. All other levels below that orbital are well bound with $\epsilon_{\text{can}} < -2$ MeV.

Similar to those of ^{44}Mg in Ref. [**?**], the single-neutron levels of ^{42}Mg can be divided into two parts: deeply bound levels ($\epsilon_{\text{can}} < -2$ MeV) corresponding to the "core", and the remaining weakly bound levels close to threshold ($\epsilon_{\text{can}} > -0.3$ MeV) and in the continuum corresponding to the "halo".

We have already seen in Fig. 8 that the core is prolate and the halo is oblate. According to Eq. (14), the density distributions of the core and halo are decomposed into spherical ($\lambda = 0$), quadrupole ($\lambda = 2$), and hexadecapole ($\lambda = 4$) components in Fig. 11 [Figure 11: see original paper]. The quadrupole component of the core is positive, consistent with the prolate shape of ^{42}Mg in its ground state. However, for the halo, the quadrupole component is mainly negative, meaning the halo has an oblate shape. This explains the decoupling between quadrupole deformations of the core and halo. We also find in Fig. 11 that the spherical component is absolutely dominant in the density distribution for both core and halo, and that the hexadecapole component in the neutron halo density distribution is also noticeable.

To study the halo formation mechanism in more detail, we show in Fig. 12 Figure 12: see original paper the main (spherical) components $\rho^i_{n,\lambda=0}(r)$ of the density distribution for weakly bound neutron orbitals i. Figure 12(b) gives the ratio of these spherical components to the spherical component of total neutron density $\rho_{n,\lambda=0}(r)$. One can clearly see that far from the center, the main contribution comes from the 4th and 5th levels. Almost 80% of the total density distribution in the tail part comes from these two levels close to the Fermi surface. Level 7 is embedded in the continuum and also contributes somewhat to the tail of the total density distribution. However, the occupation probability of this level is only 5.7%, so its contribution is very small. The occupation probability of level 6 is 7.9%, slightly larger than that of level 7, but there is almost no contribution to the tail from this level. Examining the spherical Woods-Saxon components reveals that the main component of level 6 is $1f_{7/2}$. The large centrifugal barrier of f states with $l = 3$ strongly hinders its spatial extension. For level 7, about 31.3% of the contribution comes from $2p_{1/2}$ with a small centrifugal barrier, allowing the density to extend far from the nuclear center.

As shown in Fig. 12, the halo is mainly formed by levels 4 and 5 with occupation probabilities of 53.0% and 31.5%, respectively. Considering the degeneracy of 2 for each single-particle level, the occupation number of these two orbitals is about 1.7. Decomposing the deformed wave functions of these orbitals in the spherical Woods-Saxon basis reveals that in both cases the major part comes from p waves, as indicated on the right side of Fig. 10. For level 4 ($\Omega^\pi = 1/2^-$), the probabilities of $2p_{3/2}$, $1f_{5/2}$, and $2p_{1/2}$ are 37.0%, 32.3%, and 21.2%, respectively. For level 5 ($\Omega^\pi = 3/2^-$), $2p_{3/2}$ is the dominant component with probability 78.6%. The low centrifugal barrier for p waves gives rise to halo formation.

The shape of the halo originates from the intrinsic structure of weakly bound or continuum orbitals [**?**, **?**]. As discussed, for the ground state of ^{42}Mg the halo is mainly formed by levels 4 and 5. We know that the angular distribution of $Y_{10}(\theta, \phi)$ with projection of orbital angular momentum on the symmetry axis $\Lambda = 0$ is prolate, while that of $Y_{1\pm1}(\theta, \phi)$ with $\Lambda = 1$ is oblate [**?**]. For level 4 ($\Omega^\pi = 1/2^-$), Λ could be 0 or 1 since the third component of total spin is 1/2. However, it turns out that the $\Lambda = 0$ component dominates, resulting in an oblate shape. For level 5, since the third component of total spin is 3/2, Λ can only be 1, which corresponds to an oblate shape as well. Therefore, in ^{42}Mg the halo shape is oblate and decouples from the prolate core.

V. Summary

A deformed relativistic Hartree-Bogoliubov theory in continuum has been developed to describe deformation effects in exotic nuclei allowing for halo structures. The deformed RHB equations are solved in a Woods-Saxon basis where radial wave functions have proper asymptotic behavior at large distance from the nuclear center, which is crucial for halo formation. The formalism and numerical details of the deformed RHB theory are presented. Routine checks are performed including convergence studies of deformed RHB results concerning mesh size, box size, and Woods-Saxon basis size. Results are compared for spherical nuclei with solutions of 1D continuum RHB equations in radial coordinate r based on the Runge-Kutta method.

The deformed RHB theory in continuum is applied to study the chain of magnesium isotopes with parameter sets NL3 and PK1 of the Lagrangian. Except for different predictions of the two-neutron drip-line nucleus, results for neutron Fermi surfaces and two-neutron separation energies are very similar for both parameter sets. The calculated two-neutron separation energies S_{2n} of magnesium isotopes agree reasonably well with available experimental values except for ^{32}Mg, a well-known problem connected with shape and shell structure at $N = 20$. For ^{32}Mg, the gap between neutron levels $1d_{3/2}$ and $1f_{7/2}$ is almost 7 MeV, resulting in strong shell closure at $N = 20$. Nuclear radii are also investigated; the deformed RHB results agree well with experiment for matter radii. The proton radius is almost constant with very slow increase with N due to neutron-proton coupling in the mean field. A sharp increase in neutron radius is observed at ^{42}Mg.

Detailed results are shown for the two-neutron drip-line nucleus ^{42}Mg with parameter set PK1, which is well deformed. The ground state of ^{42}Mg is prolate, yet it has an oblate neutron halo. By examining in detail the density distributions, pairing tensor, and single-particle levels in the canonical basis in the deformed nucleus ^{42}Mg, we can understand why the shape of the neutron halo decouples from that of the core. It is shown that the existence and deformation of a possible neutron halo depend essentially on the quantum numbers of the main components of single-particle orbits near the Fermi surface and the shape of their single-particle density distributions.

In stable nuclei, there are situations where valence nucleon levels are sometimes well separated from the core. However, it is a difficult question whether such shape decoupling exists for loosely bound valence orbits close to the continuum limit, because in stable nuclei even valence nucleons are well bound in the average potential.

We conclude that spherical and deformed relativistic Hartree-Bogoliubov theory in continuum is a very powerful tool providing proper description of exotic nuclei including halo phenomena, because it accounts self-consistently and microscopically for polarization effects, shape changes of individual orbitals, pairing correlations, and coupling to the continuum with proper boundary conditions.

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Appendix A: Spherical Spinors in Coordinate Space

In this work we use three different representations of wave functions. The starting point is the coordinate space representation $x = (rsp)$, where s is the spin coordinate and p describes large (upper) ($p = 1$ or $p = +$) and small (lower) ($p = 2$ or $p = -$) components. The second basis is a discrete basis of spherical Dirac spinors obtained by diagonalizing the spherical Dirac Hamiltonian with Woods-Saxon shaped fields. This basis is called the Woods-Saxon basis. In this basis the RHB equations are solved, and the solutions form a basis of quasi-particle states labeled by k. The Dirac spinors of the Woods-Saxon basis are represented in coordinate space as:

$$\phi_{n\kappa m}(\mathbf{r}sp) = i^p \frac{R_{n\kappa}(r,p)}{r} Y^{l(p)}_{\kappa m}(\Omega, s)$$

The orbital angular momenta of these components are $l(p = 1) = j + \frac{1}{2}\text{sign}(\kappa)$ and $l(p = 2) = j - \frac{1}{2}\text{sign}(\kappa)$. $R_{n\kappa}(r, 1) = G_{n\kappa}(r)$ and $R_{n\kappa}(r, 2) = F_{n\kappa}(r)$ are the radial wave functions, and $Y^l_{\kappa m}$ are the spinor spherical harmonics:

$$Y^l_{\kappa m}(\Omega, s) = \sum_{m_l, m_s} \langle l m_l, \frac{1}{2} m_s | jm \rangle Y_{l m_l}(\Omega) \chi_{\frac{1}{2} m_s}(s)$$

The time-reversal state reads:

$$\bar{\phi}_{n\kappa m}(\mathbf{r}sp) = (-1)^{p+l(p)+j-m} \phi_{n\kappa -m}(\mathbf{r}sp)$$

These basis functions are obtained from solving a Dirac equation with spherical Woods-Saxon potentials [**?**]:

$$h_D^{(0)} = \alpha \cdot \mathbf{p} + \beta(M + S^{(0)}(r)) + V^{(0)}(r)$$

on a mesh in r-space using the Runge-Kutta method. For each κ we have eigenstates with positive and negative eigenvalues $\epsilon_{n\kappa}$, and for completeness the sum over $n\kappa$ must include both positive and negative eigenvalue states [?]. This is unrelated to the no-sea approximation applied in the final quasiparticle basis where sums over k in Eq. (9) run only over solutions with positive single-particle energies.

Since the RHB equation must be solved in this basis, we evaluate matrix elements of the form:

$$\langle n\kappa m|O|n'\kappa' m\rangle = \sum_p \int dr\, R_{n\kappa}(r,p) O_{(n\kappa)(n'\kappa')}(r) R_{n'\kappa'}(r,p)$$

To simplify calculations, angular integrations are carried out analytically using angular momentum coupling techniques, and only radial integrals are calculated numerically. For local potentials we need products of basis wavefunctions $\phi_{n\kappa m}(\mathbf{r}sp)\phi^*_{n'\kappa' m}(\mathbf{r}sp)$. Following Eq. (14), they are expanded in Legendre polynomials. For the coefficient of rank λ depending only on radius r we find:

$$\phi_{n\kappa m}(\mathbf{r}sp)\phi^*_{n'\kappa' m}(\mathbf{r}sp) = \sum_\lambda \frac{1}{r^2} R_{n\kappa}(r,p) R_{n'\kappa'}(r,p) C^{\lambda m}_{(n\kappa)(n'\kappa')} P_\lambda(\cos\theta)$$

The angular matrix elements can be derived with the help of the Wigner-Eckart theorem [?]. For even values of $l + \lambda + l'$ we find:

$$C^{\lambda m}_{(n\kappa)(n'\kappa')} = (-1)^{j-m} \hat{j}\hat{j}' \begin{pmatrix} j & \lambda & j' \\ -m & 0 & m \end{pmatrix} \begin{pmatrix} j & \lambda & j' \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} \Pi^\lambda_{ll'}$$

where $\hat{j} = \sqrt{2j+1}$ and $\Pi^\lambda_{ll'}$ contains the angular integration. For odd values of $l + \lambda + l'$ these matrix elements vanish.

Appendix B: Matrix Elements of the DRHB Hamiltonian

The Dirac Hartree-Bogoliubov equations [?] read in coordinate space:

$$\int d^3r' \begin{pmatrix} h_D(\mathbf{r},\mathbf{r}') - \lambda & \Delta(\mathbf{r},\mathbf{r}') \\ -\Delta^*(\mathbf{r},\mathbf{r}') & -h_D^*(\mathbf{r},\mathbf{r}') + \lambda \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}') \\ V_k(\mathbf{r}') \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}$$

The matrix elements of the Dirac Hamiltonian h_D between Woods-Saxon basis states are:

$$\langle n\kappa m|h_D|n'\kappa' m\rangle = \epsilon_{n\kappa}\delta_{nn'}\delta_{\kappa\kappa'} + \langle n\kappa m|V(\mathbf{r})|n'\kappa' m\rangle$$

where $\epsilon_{n\kappa}$ are the eigenvalues of the spherical Woods-Saxon Hamiltonian and $V(\mathbf{r})$ is the deformed part of the potential. The matrix elements of the pairing field Δ are calculated similarly using the expansion of the pairing tensor in the Woods-Saxon basis.

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

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