Spherical Relativistic Hartree theory in a Woods-Saxon basis (Postprint)

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Abstract

The Woods-Saxon basis has been suggested to replace the widely used harmonic oscillator basis for solving the relativistic mean field (RMF) theory in order to generalize it to study exotic nuclei. As examples, relativistic Hartree theory is solved for spherical nuclei in a Woods-Saxon basis obtained by solving either the Schro¨dinger equation or the Dirac equation (labelled as SRHSWS and SRHDWS, respectively and SRHWS for both). In SRHDWS, the negative levels in the Dirac Sea must be properly included. The basis in SRHDWS could be smaller than that in SRHSWS which will simplify the deformed problem. The results from SRHWS are compared in detail with those from solving the spherical relativistic Hartree theory in the harmonic oscillator basis (SRHHO) and those in the coordinate space (SRHR). All of these approaches give identical nuclear properties such as total binding energies and root mean square radii for stable nuclei. For exotic nuclei, e.g., 72Ca, SRHWS satisfactorily reproduces the neutron density distribution from SRHR, while SRHHO fails. It is shown that the Woods-Saxon basis can be extended to more complicated situations for exotic nuclei where both deformation and pairing have to be taken into account.

Full Text

Preamble

Spherical Relativistic Hartree Theory in a Woods-Saxon Basis

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The Woods-Saxon basis has been suggested as a replacement for the widely used harmonic oscillator basis in solving relativistic mean field (RMF) theory, enabling its generalization to exotic nuclei. As examples, relativistic Hartree theory is solved for spherical nuclei in a Woods-Saxon basis obtained by solving either the Schrödinger equation or the Dirac equation (labeled as SRHSWS and SRHDWS, respectively, with SRHWS referring to both).

In SRHDWS, the negative levels in the Dirac sea must be properly included. The basis in SRHDWS could be smaller than that in SRHSWS, which simplifies the deformed problem. Results from SRHWS are compared in detail with those from solving spherical relativistic Hartree theory in the harmonic oscillator basis (SRHHO) and in coordinate space (SRHR). All approaches give identical nuclear properties such as total binding energies and root mean square radii for stable nuclei. For exotic nuclei (e.g., ^{72}Ca), SRHWS satisfactorily reproduces the neutron density distribution from SRHR, while SRHHO fails.

We show that the Woods-Saxon basis can be extended to more complicated situations for exotic nuclei where both deformation and pairing must be taken into account.

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Introduction

The existence of an average field in atomic nuclei, revealed by the exceptional role of nuclear magic numbers, provides the foundation for the nuclear shell model and various mean field approaches [**?**, **?**, **?**]. This average field is believed to be approximated most closely by a Woods-Saxon (WS) potential [**?**], either from analyzing the radial dependence of the nuclear force or by deriving it from a microscopic two-body interaction.

Since eigenfunctions for the WS potential cannot be given analytically, harmonic oscillator (HO) potentials or square wells—particularly the former—are often adopted as good approximations for stable nuclei in shell model calculations for both spherical [**?**] and deformed nuclei [**?**]. HO eigenfunctions

also frequently serve as a complete basis for solving equations in both non-relativistic and relativistic mean field approximations, such as Skyrme Hartree-Fock (SHF), Hartree-Fock-Bogoliubov (HFB), relativistic Hartree (RH), and relativistic Hartree-Bogoliubov (RHB) theories. In these approaches, solving the corresponding equations is transformed into a matrix diagonalization problem that can be easily handled.

However, due to the incorrect asymptotic properties of HO wave functions, expansion in the localized HO basis is inappropriate for describing drip-line nuclei [**?**, **?**, **?**], which display many interesting features because of their extremely weak binding: coupling between bound states and the continuum due to pairing correlations, large spatial density distributions, possible modifications of shell structure, etc. One can improve the asymptotic behavior of HO wave functions by performing a local scaling transformation [**?**], but the scaling parameter is not known beforehand, thus losing predictive power.

A proper representation for solving HFB or RHB equations for drip-line nuclei is coordinate space [**?**, **?**, **?**, **?**], where wave functions are approximated on a spatial lattice and the continuum is discretized by suitably large box boundary conditions. The HFB method solved in r-space can fully account for all mean-field effects of coupling to the continuum [**?**, **?**, **?**, **?**]. Nevertheless, for deformed nuclei, working in r-space becomes much more difficult and numerically very sophisticated [**?**], particularly when pairing correlations are included. Therefore, much effort has been directed toward more efficient solutions of HFB or RHB equations, using natural orbitals [**?**] or basis-spline Galerkin lattices [**?**], among other approaches.

A reconciler between the HO basis and r-space may be the WS basis because (i) the WS potential represents the nuclear average field more suitably than the HO potential, and (ii) there are, in principle, no localization restrictions in the WS potential. Although analytical wave functions cannot be given for the WS potential, one can easily find numerical solutions for a spherical WS potential in r-space using various effective methods for solving ordinary differential equations [**?**]. One can still use a large box boundary condition to discretize the continuum. These WS wave functions can thus be used as a complete basis for spherical or deformed systems, returning to the familiar matrix diagonalization problem.

In the present work, we restrict the application of this method to nuclei with spherical symmetry, which largely facilitates discussion of basic principles and allows presentation of illustrations for the radial dependence of all relevant physical quantities like density distributions. We combine this approach with relativistic Hartree theory [**?**], which provides a framework for describing the nuclear many-body problem as a relativistic system of baryons and mesons and, together with its extensions including deformation and/or pairing, has been successfully applied in calculations of nuclear matter and properties of finite nuclei throughout the periodic table [**?**, **?**].

The paper is organized as follows. In Sec. II, we give a brief reminder of

the formalism of relativistic Hartree theory. Numerical details for solving it in the WS basis are given in Sec. III. In Sec. IV, we present our results and compare them with those obtained in the HO basis and in r-space, and discuss contributions from negative levels in the Dirac sea. Finally, the work is summarized in Sec. V.

Throughout the paper, relativistic Hartree theories solved in r-space, in the HO basis, and in the WS basis are abbreviated as "SRHR", "SRHHO", and "SRHWS", where the first "S" represents "spherical". We use "SWS" and "DWS" to distinguish the WS basis obtained from solving the Schrödinger equation or the Dirac equation with initial WS potentials, respectively. Thus we have "SRHSWS" and "SRHDWS" theories.

II. Basic Formalism of Relativistic Hartree Theory

The starting point of relativistic Hartree theory is a Lagrangian density where nucleons are described as Dirac spinors interacting via exchange of several mesons (σ, ω, and ρ) and the photon [**?**, **?**, **?**]:

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

with summation convention used and summation over i running over all nucleons, $\gamma^\mu x_\mu = \gamma_\mu x^\mu$, M the nucleon mass, and m_σ, g_σ, m_ω, g_ω, m_ρ, g_ρ masses and coupling constants of the respective mesons. The non-linear self-coupling for scalar mesons is given by [**?**]:

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

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

$$\Omega_{\mu\nu} = \partial_\mu\omega_\nu - \partial_\nu\omega_\mu, \quad \vec{R}_{\mu\nu} = \partial_\mu\vec{\rho}_\nu - \partial_\nu\vec{\rho}_\mu - g_\rho(\vec{\rho}_\mu \times \vec{\rho}_\nu), \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu.$$

The classical variation principle yields equations of motion for nucleons, mesons, and photon. As in many applications, we study ground state properties of nuclei with time reversal symmetry, thus nucleon spinors are eigenvectors of the stationary Dirac equation:

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

and equations of motion for mesons and photon:

$$(-\Delta + \partial_\sigma U(\sigma))\sigma(r) = -g_\sigma \rho_s(r),$$

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

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

$$-\Delta A_0(r) = e\rho_p(r),$$

where ω_0 and A_0 are time-like components of the vector ω and photon fields, and ρ_0 is the 3-component of the time-like component of the isovector ρ meson. Equations (4) and (5) are coupled by the vector and scalar potentials:

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

and various densities:

$$\rho_s(r) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\psi_i(\mathbf{r}), \quad \rho_v(r) = \sum_{i=1}^{A} \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r}), \quad \rho_3(r) = \sum_{i=1}^{A} \psi_i^\dagger(\mathbf{r})\tau_3\psi_i(\mathbf{r}), \quad \rho_c(r) = \sum_{i=1}^{A} \psi_i^\dagger(\mathbf{r})\frac{1-\tau_3}{2}\psi_i(\mathbf{r}).$$

For spherical nuclei, meson fields and densities depend only on radial coordinate r. The spinor is characterized by angular momentum quantum numbers (l, j), m, parity, isospin $t = \pm 1/2$ ("+" for neutrons and "-" for protons), and radial quantum number α. The Dirac spinor has the form:

$$\psi_{\alpha\kappa m}(\mathbf{r}, s, t) = \frac{1}{r}\begin{pmatrix} iG_\kappa^\alpha(r)Y_{jm}^l(\theta,\phi) \\ -F_\kappa^\alpha(r)Y_{jm}^{\tilde{l}}(\theta,\phi) \end{pmatrix}\chi_t^\alpha(t), \quad j = l \pm \frac{1}{2},$$

with $G_\kappa^\alpha(r)/r$ and $F_\kappa^\alpha(r)/r$ the radial wave functions for upper and lower components and $Y_{jm}^l(\theta,\phi)$ the spin spherical harmonics where $\kappa = (-1)^{j+l+1/2}(j+1/2)$ and $\tilde{l} = l + (-1)^{j+l-1/2}$. The value of κ of the upper component is used to label a state both for normal levels in the Fermi sea and for negative ones in the Dirac sea. States with the same κ form a "block". The radial equation of the Dirac spinor, Eq. (4), reduces to:

$$\frac{d}{dr}G_\kappa^\alpha + \frac{\kappa}{r}G_\kappa^\alpha - (\epsilon_\alpha + M + S(r) - V(r))F_\kappa^\alpha = 0,$$

$$\frac{d}{dr}F_\kappa^\alpha - \frac{\kappa}{r}F_\kappa^\alpha + (\epsilon_\alpha - M - S(r) - V(r))G_\kappa^\alpha = 0.$$

The meson field equations become simple radial Laplace equations of the form:

$$\left(\frac{d^2}{dr^2} - m_\phi^2\right)\phi(r) = s_\phi(r),$$

where m_ϕ are meson masses for $\phi = \sigma, \omega, \rho$ and zero for photon. The source terms are:

$$s_\phi(r) = \begin{cases} -g_\sigma\rho_s(r) - g_2\sigma^2(r) - g_3\sigma^3(r), & \text{for } \sigma, \\ g_\omega\rho_v(r), & \text{for } \omega, \\ g_\rho\rho_3(r), & \text{for } \rho, \\ e\rho_c(r), & \text{for } A. \end{cases}$$

The densities can be expressed as:

$$4\pi r^2\rho_s(r) = \sum_{i=1}^{A}(|G_i(r)|^2 - |F_i(r)|^2), \quad 4\pi r^2\rho_v(r) = \sum_{i=1}^{A}(|G_i(r)|^2 + |F_i(r)|^2),$$

$$4\pi r^2\rho_3(r) = \sum_{i=1}^{A} 2t_i(|G_i(r)|^2 + |F_i(r)|^2), \quad 4\pi r^2\rho_c(r) = \sum_{i=1}^{A}\frac{1-\tau_{3i}}{2}(|G_i(r)|^2 + |F_i(r)|^2).$$

These coupled equations have been solved in r-space [**?**] and in the HO basis [**?**] with the no-sea and mean-field approximations. Here we briefly depict the procedure for solving these coupled equations. With estimated meson and photon fields, the scalar and vector potentials are calculated and the radial Dirac equation is solved. The resulting nucleon wave functions are used to calculate source terms for each radial Laplace equation for mesons and photon. New meson and photon fields are obtained by solving these Laplace equations. This procedure is iterated until a demanded accuracy is achieved. Laplace equations are usually solved using the Green's function method [**?**, **?**], though in Ref. [**?**] Laplace equations for mesons are solved in the HO basis. SRHR, SRHHO, and SRHWS differ mainly in how the Dirac equation is solved. In the following, we present the numerical solution of the Dirac equation in the WS basis.

III. Solving the Dirac Equation in a Woods-Saxon Basis and Numerical Details

A. Woods-Saxon basis from solving a Schrödinger equation (the SWS basis)

For the Schrödinger equation with a spherical Woods-Saxon potential:

$$V_{\mathrm{WS}}(r)=\begin{cases}\frac{V_0}{1+e^{(r-R_0)/a_0}}, & r<R_{\max},\\ \infty, & r\geq R_{\max},\end{cases}$$

where $R_{\max}$ is introduced for practical reasons to define the box boundary, the eigenfunction can be written as $\phi_{nlml}(\mathbf{r})=R_{nl}(r)Y_{lml}(\theta,\phi)$. Its radial Schrödinger equation is:

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2}+\frac{l(l+1)}{2mr^2}+V_{\mathrm{WS}}(r)\right]R_{nl}(r)=E_{nl}R_{nl}(r).$$

Equation (14) is solved on a discretized radial mesh with mesh size Δr. $R_{\max}$ (Δr) should be chosen large (small) enough to ensure final results do not depend on it. The radial wave functions thus obtained form a complete basis $\{R_{nl}(r);n=0,1,\cdots;l=0,1,\cdots,n\}$, in terms of which the radial parts of upper and lower components of the Dirac spinor in Eq. (9) are expanded respectively as:

$$G^{\alpha}_{\kappa}(r)=\sum_{n=0}^{n_{\max}}g_{\alpha n\kappa}R_{nl}(r),\quad F^{\alpha}_{\kappa}(r)=\sum_{\tilde{n}=0}^{\tilde{n}_{\max}}f_{\alpha\tilde{n}\kappa}R_{\tilde{n}\tilde{l}}(r).$$

The radial Dirac equation, Eq. (9), is transformed into the WS basis as:

$$\sum_{n=0}^{n_{\max}}A_{mn}g_{\alpha n\kappa}+\sum_{\tilde{n}=0}^{\tilde{n}_{\max}}B_{m\tilde{n}}f_{\alpha\tilde{n}\kappa}=\epsilon_{\alpha}g_{\alpha m\kappa},$$

$$\sum_{n=0}^{n_{\max}}C_{\tilde{m}n}g_{\alpha n\kappa}+\sum_{\tilde{n}=0}^{\tilde{n}_{\max}}D_{\tilde{m}\tilde{n}}f_{\alpha\tilde{n}\kappa}=\epsilon_{\alpha}f_{\alpha\tilde{m}\kappa},$$

where matrix elements are calculated as:

$$A_{mn}=\int_0^{R_{\max}}r^2drR_{ml}(r)(V(r)+S(r)+M)R_{nl}(r),$$

$$B_{m\tilde{n}}=\int_0^{R_{\max}}r^2drR_{ml}(r)\frac{\kappa-1}{r}R_{\tilde{n}\tilde{l}}(r),$$

$$C_{\tilde{m}n}=\int_0^{R_{\max}}r^2drR_{\tilde{m}\tilde{l}}(r)\frac{\kappa+1}{r}R_{nl}(r),$$

$$D_{\tilde{m}\tilde{n}} = \int_0^{R_{\max}} r^2 dr R_{\tilde{m}\tilde{l}}(r)(V(r) - S(r) - M)R_{\tilde{n}\tilde{l}}(r).$$

In practical calculations, an energy cutoff E_{cut} (relative to nucleon mass M) determines the cutoff of radial quantum number $n_{\max}$ for each block. In expansion of the corresponding lower component, we take $\tilde{n}_{\max} = n_{\max} + \Delta n$ with $\Delta n \geq 1$ to avoid spurious states [**?**].

The following Woods-Saxon parameters from Ref. [**?**] are used:

$$V_0 = (-51 \pm 33(N-Z)/A) \text{ MeV}, \quad R_0 = 1.27A^{1/3} \text{ fm}, \quad a_0 = 0.67 \text{ fm},$$

where "+" is for neutrons and "-" for protons. As expected, dependence of final results on the initial WS potential is almost negligible. For example, a 50% variation in V_0 gives differences in total binding energies of less than 0.1% and in charge radii of less than 0.5% for ^{16}O, ^{48}Ca, and ^{208}Pb. This also holds for the other two WS potential parameters, R_0 and a_0.

B. Woods-Saxon basis from solving a Dirac equation (the DWS basis)

The radial Dirac equation, Eq. (9), may be solved in r-space [**?**] with Woods-Saxon-like potentials for $V_0(r) \pm S_0(r)$ [**?**] within a spherical box of size $R_{\max}$, together with spherical spinors that give a complete WS basis $\psi^0_{n\kappa m}(\mathbf{r}, s, t)$ with $n = 0, 1, \cdots$, $\kappa = \pm 1, \pm 2, \cdots$, and $m = -j_\kappa, \cdots, j_\kappa$. The spinor takes the form of Eq. (8). We note that states both in the Fermi sea and in the Dirac sea should be included in the basis for completeness. The nucleon wave function, Eq. (8), can be expanded in this basis as:

$$\psi_{\alpha\kappa m}(\mathbf{r}, s, t) = \sum_{n=0}^{n_{\max}} c_{\alpha n} \psi^0_{n\kappa m}(\mathbf{r}, s, t),$$

where $n_{\max} = n^+_{\max} + n^-_{\max} + 1$ and the summation runs over normal levels in the Fermi sea for $0 \leq n \leq n^+_{\max}$ and over negative levels in the Dirac sea for $n^+_{\max} + 1 \leq n \leq n_{\max}$. Negative states are obtained with the same method as positive ones [**?**].

In this WS basis, the Dirac equation, Eq. (4), becomes:

$$\sum_{n=1}^{n_{\max}} c_{\alpha m} \epsilon^0_n \delta_{mn} + \sum_{n=1}^{n_{\max}} c_{\alpha n} H'_{mn} = \epsilon_\alpha c_{\alpha m}, \quad m = 1, \cdots, n_{\max},$$

where:

$$H'_{mn} = \int_0^{R_{\max}} dr \left[G^0_m(r)(\Delta V(r) + \Delta S(r)) G^0_n(r) + F^0_m(r)(\Delta V(r) - \Delta S(r)) F^0_n(r) \right],$$

with $\Delta V(r) = V(r) - V_0(r)$ and $\Delta S(r) = S(r) - S_0(r)$. Angular, spin, and isospin quantum numbers are omitted for brevity.

It should be mentioned that Eq. (9) can be solved directly in r-space with the same method used to generate the DWS basis. Our aim is to test the validity of an efficient solution not only for the spherical RH model but also for its extension to include deformation and/or pairing correlation. In fact, if only the SRH theory is concerned, this procedure is just a replacement of direct solution in r-space by diagonalization of a matrix with some complication introduced by the fact that contributions from states in the Dirac sea must be included.

An energy cutoff $E_{\rm cut}$ (relative to nucleon mass M) and cutoff of radial quantum numbers $n^+_{\max}$ are applied to normal levels according to practical convenience. For the initial Woods-Saxon potentials $V_0(r) \pm S_0(r)$, we follow Ref. [**?**].

C. Comparison with the r-space method

To check the validity of solving the Dirac equation in the WS basis and provide numerical experience for future applications, we compare results for ^{16}O and ^{208}Pb from solving the Dirac equation in the WS basis with those from solving the same equation in coordinate space. The latter is the most accurate method for solving the Dirac equation for realistic nuclei and is used as a standard here. Scalar and vector potentials in the Dirac equation are provided by very accurate SRHR calculations with parameter set NL3 for the Lagrangian, mesh size $\Delta r = 0.05$ fm, box size $R_{\max} = 30$ fm for ^{16}O and $R_{\max} = 35$ fm for ^{208}Pb. Then with these $S(r)$ and $V(r)$, the Dirac equation is solved in coordinate space and in the WS basis also using parameter set NL3.

Comparing results only from solving the Dirac equation avoids errors from other numerical procedures, such as iteration errors and errors from solving Laplace equations. For the same reason, we compare not the binding energy (which contains meson contributions) but the average single-particle energy $E_{\rm sp}/A$, where $E_{\rm sp} = \sum_i \epsilon_i$ with ϵ_i the single-particle energy summed over all occupied states for both neutrons and protons. We also compare the rms radius $\langle r^2 \rangle^{1/2}$ and $\langle r^4 \rangle^{1/4}$, where the latter reflects nucleon densities in the tail more than the rms radius.

Table I presents the dependence of results for the Dirac equation in the SWS basis on mesh size Δr. As Δr decreases, results in the SWS basis approach the standard r-space results, with $\Delta r = 0.1$ fm giving sufficient accuracy. The dependence on box size $R_{\max}$ and basis size determined by $E_{\rm cut}$ is investigated in Figs. 1 and 2, where deviations of average single-particle energy $E_{\rm sp}/A$, rms

radius $\langle r^2\rangle^{1/2}$, and $\langle r^4\rangle^{1/4}$ from standards are plotted versus $E_{\rm cut}$ for different $R_{\rm max}$.

If $R_{\rm max}$ is not large enough, it is difficult to approach standard results. For example, when $R_{\rm max} = 3r_0A^{1/3} = 9.4$ fm and $E_{\rm cut} = 300$ MeV for ^{16}O (corresponding to $N_{\rm max} \sim 20$), results appear to converge but the discrepancy in average single-particle energy from the standard remains 0.1 keV. Therefore, one must use a sufficiently large box with size $R_{\rm max}$ around $4r_0A^{1/3}$ for light nuclei and $3r_0A^{1/3}$ for heavy ones. Interestingly, convergence does not depend on $N_{\rm max}$ but only on $E_{\rm cut}$. For ^{16}O (^{208}Pb), results converge to standards at ~ 300 (400) MeV. From Figs. 1 and 2, the radius $\langle r^4\rangle^{1/4}$ also converges very well, implying that nucleon densities can be calculated accurately even at large r.

Similar investigations for the DWS basis yield similar conclusions. For instance, deviations of $E_{\rm sp}/A$, $\langle r^2\rangle^{1/2}$, and $\langle r^4\rangle^{1/4}$ from standards are plotted versus $E_{\rm cut}$ for different $R_{\rm max}$ in Figs. 3 and 4.

In expanding the nucleon wave function, Eq. (21), one must consider not only levels in the Fermi sea but also those in the Dirac sea because they form a complete basis together. The question arises: how many levels in the Dirac sea must be included? In calculations for Figs. 3 and 4, we used $n^-_{\rm max} = n^+_{\rm max}$ with $n^+_{\rm max}$ determined by $E_{\rm cut}$.

Table III shows the dependence of average single-particle energy, rms radius $\langle r^2\rangle^{1/2}$, and $\langle r^4\rangle^{1/4}$ on maximum principal quantum number $\tilde{N}_{\rm max} = 2n^-_{\rm max}+l$—a cutoff on principal quantum number of levels in the Dirac sea—for ^{16}O and ^{208}Pb. A merit of solving the Dirac equation in the DWS basis is that the number of negative states included can be much smaller than that of positive states. For ^{16}O, $R_{\rm max} = 4r_0A^{1/3}$ and $E_{\rm cut} = 300$ MeV for positive states correspond to $N^+_{\rm max} \sim 28$, but for negative states, $\tilde{N}_{\rm max} = 10$ gives very accurate results (e.g., discrepancy in $E_{\rm sp}/A$ from standard is smaller than 0.1 keV). This significantly simplifies the deformed problem by decreasing matrix dimension compared to solving the Dirac equation in the SWS basis.

These investigations are somewhat academic. In practical applications, accuracy around keV in single-particle energy or 10^{-4} fm in radius is unnecessary. Therefore, in following calculations we use $R_{\rm max} = 20$ fm, $\Delta r = 0.1$ fm, and $E_{\rm cut} = 60 - 80$ MeV for heavy and light nuclei, which give reasonable accuracy for both binding energy and radius. This set of cutoffs corresponds approximately to $N_{\rm max} = 2n_{\rm max} + l \sim 25$, where l is the orbital angular momentum of the relevant state.

IV. Results and Discussions

We present results of SRHWS. Since our main aim is to demonstrate virtues of SRHWS compared to SRHHO and SRHR, we do not include pairing correlations and restrict our study to doubly magic or magic nuclei only. Unless specified,

parameter set NLSH is used for the Lagrangian, $R_{\max} = 20$ fm and $\Delta r = 0.1$ fm throughout this section. Other parameter sets for the Lagrangian do not change conclusions here. In SRHDWS, the number of normal levels in the Fermi sea and negative ones in the Dirac sea are the same for convenience (i.e., $n^+_{\max} = n^-_{\max}$). For SRHHO, $\hbar\omega_0 = 41A^{-1/3}$ is used and cutoffs of expansion for fermions and bosons are the same (i.e., $N_F = N_B \equiv N_{\max}$).

A. Bulk properties of stable nuclei from different SRH theories

Table IV presents binding energy per nucleon (E/A) and neutron, proton, and charge radii (r_n, r_p, and r_c) of typical spherical nuclei calculated with available codes including SRHR, SRHSWS, SRHDWS, and SRHHO. Available data [**?**, **?**] are included for comparison. Approximately the same $N_{\max}$ is used in SRHHO as in SRHWS, determined by E_{cut}.

Generally, for each studied nucleus, the four approaches give almost identical results with accuracy within 0.1%, with few exceptions where differences are still less than 0.3%. They are in excellent agreement with available data. With the same spatial lattice parameters $R_{\max}$ and Δr, SRHWS should reproduce SRHR results when E_{cut} (or $N_{\max}$) is large enough, as justified in Table IV. One finds exactly coincident results between SRHSWS and SRHR for most studied nuclei. Remaining differences and those between SRHDWS and SRHR could be diminished by increasing E_{cut}.

Figures 5, 6, and 7 compare neutron density distributions between SRHR, SRHSWS, SRHDWS, and SRHHO for ^{16}O, ^{48}Ca, and ^{208}Pb as examples. Calculation details are the same as in Table IV. For these stable nuclei, all SRH methods are valid and calculations agree excellently from central to outer regions. Tiny differences in the central region do not affect physical observables like binding energy or nuclear radius, as seen in Table IV, and could be decreased by increasing E_{cut} or $N_{\max}$.

These discussions clearly show that SRHWS is equivalent to SRHR and SRHHO for stable nuclei. Thus, Woods-Saxon basis provides another possibility to solve (non-)relativistic mean field theories.

B. Neutron density distributions for ^{72}Ca in different SRH theories

As discussed in the introduction, one merit of SRHR over SRHHO is its proper description of exotic nuclei. Here we demonstrate equivalence between SRHWS and SRHR when reasonably large E_{cut} is applied.

To examine results for unstable nuclei near the neutron drip line, we study neutron density distribution for ^{72}Ca, predicted to be the last bound calcium isotope [**?**, **?**, **?**, **?**]. Since it is not doubly magic, some uncertainty may exist due to lack of pairing correlations. However, as stressed at the beginning of this section, our main aim is to show virtue of SRHWS compared to SRHHO, and pairing is unlikely to change our conclusion qualitatively.

For stable nuclei, $R_{\max} \sim 20$ fm is large enough. For drip-line nuclei, Table V presents dependence of results on $R_{\max}$ for ^{72}Ca. For both SRHR and SRHWS, $\Delta r = 0.1$ fm and $R_{\max} = 20, 25, 30$, and 35 fm are adopted. Energy cutoff $E_{\text{cut}} = 75$ MeV is used for SRHWS. In SRHR and SRHWS calculations, neutron rms radius r_n and Fermi energy λ_n of ^{72}Ca converge around $R_{\max} = 35$ fm, while binding energy per nucleon E/A and proton rms radius r_p show independence from box size. These SRHWS parameters correspond to cutoffs in principal quantum number $N_{\max} = 25, 31, 37$, and 43 used in SRHHO calculations for fair comparison. Similar to SRHR and SRHWS, E/A and r_p depend little on $N_{\max}$ in SRHHO. However, neutron rms radius r_n increases steadily with $N_{\max}$, showing much slower convergence. Since SRHHO is based on a complete basis, it can reach convergence of r_n if $N_{\max}$ is large enough. For the same $N_{\max}$ (or equivalent $R_{\max}$), a difference of $\Delta r_n \approx 0.2$ fm exists between SRHHO and SRHWS (SRHR). From slow convergence of r_n with $N_{\max}$ ($\Delta N_{\max} = 6$ gives $\Delta r_n \approx 0.02$ fm), we estimate a lower limit of $N_{\max} \approx 90$ is needed for SRHHO to give $r_n = 4.8$ fm as in SRHR or SRHWS.

We compare neutron density distribution of ^{72}Ca from different SRH approaches in Figs. 8 and 9. With the same box size, density distributions from SRHR are almost identical to those from SRHWS, indicating equivalence between SRHWS and SRHR. For brevity, only $\rho_n(r)$ from SRHR with $R_{\max} = 35$ fm is displayed, which covers the curve for $\rho_n(r)$ from SRHSWS with $R_{\max} = 35$ fm in Fig. 8. In contrast, $\rho_n(r)$ from SRHHO even with $N_{\max} = 43$ fails to reproduce SRHR results due to the localization property of the HO potential. Additionally, with the same $N_{\max}$, spatial extension of $\rho_n(r)$ from SRHWS is always larger than that from SRHHO. The variational tendency of $\rho_n(r) \sim r$ also explains different convergence behaviors of r_n in SRHWS and SRHHO given in Table V. With increasing $R_{\max}$, $\rho_n(r)$ in SRHWS has correct asymptotic behavior while that in SRHHO decays too quickly.

This result is very encouraging, showing that even the long tail (or halo) behavior in neutron density distribution for nuclei near the drip line can be described by SRHSWS as well as SRHR, if pairing correlations are incorporated properly.

C. Contribution from negative levels in the SRHDWS theory

In expanding the nucleon wave function, Eq. (21), one must consider not only levels in the Fermi sea but also those in the Dirac sea because they form a complete basis together. We study effects of negative levels and present results for ^{16}O in Table VI. Without negative levels included, the nucleus is overbound and its size is smaller. Moreover, calculated nuclear properties depend strongly on initial potentials when negative levels are omitted.

The contribution from negative levels depends on the initial Woods-Saxon potentials used to generate the DWS basis, as do the cutoffs $N_{\max}$ or E_{cut} for convergence. If initial Woods-Saxon potentials are exactly identical to converged potentials, the matrix in Eq. (22) is diagonal and negative states do not

contribute due to the no-sea approximation. Positive states can also be chosen minimally (e.g., $1s_{1/2}$, $1p_{3/2}$, and $1p_{1/2}$ are sufficient for ^{16}O). From the column corresponding to $V_0 = 72$ MeV in Table VI, the initial nuclear potential for the Dirac equation proposed in Ref. [**?**] is a good choice for SRHDWS, as negative states contribute only $\sim 1.25\%$ to both E/A and $r_{\rm rms}$. Changing initial potentials (e.g., varying V_0 by 25%) yields much larger contributions from negative states, as shown in Table VI.

To assess contribution of negative levels in the Dirac sea to wave functions, values of $\sum_n |c^-_{\alpha n}|^2$ in expansion Eq. (21) are given in Table VII for occupied states of ^{16}O. The nucleon wave function is normalized to one. A small component from negative states in wave functions, about 10^{-4}-10^{-5}, contributes to physical observables such as E/A and $r_{\rm rms}$ by 1%-10%, as seen in Table VI. When initial Woods-Saxon potentials differ more from converged ones, contribution from negative levels becomes more important.

V. Summary

We have solved spherical relativistic Hartree theory in the Woods-Saxon basis (SRHWS). The Woods-Saxon basis is obtained by solving either the Schrödinger equation (SRHSWS) or the Dirac equation (SRHDWS). Formalism and numerical details for both cases are presented. The WS basis in SRHDWS theory could be much smaller than in SRHSWS theory, which greatly facilitates solving the deformed problem.

Results from SRHWS are compared with those from solving spherical relativistic Hartree theory in the harmonic oscillator basis (SRHHO) and in coordinate space (SRHR). For stable nuclei, all approaches give identical results for properties such as total binding energies, neutron/proton/charge rms radii, and neutron density distributions.

For neutron drip-line nuclei (e.g., ^{72}Ca) with very small neutron Fermi energy $\lambda_n \sim 0.2$ MeV, both SRHR and SRHWS easily approach convergence by increasing box size while SRHHO does not. Furthermore, SRHWS satisfactorily reproduces neutron density distributions from SRHR, but SRHHO fails with similar cutoffs.

In SRHDWS calculations, negative levels in the Dirac sea must be included in the basis for expanding nucleon wave functions. We studied effects and contributions of negative states in detail. Without negative levels, calculated nuclear properties depend strongly on initial potentials. A small component from negative states in wave functions, about 10^{-4}-10^{-5}, contributes to physical observables such as E/A and $r_{\rm rms}$ by 1%-10%. When initial potentials differ more from converged ones, contribution from negative levels becomes more important.

We conclude that the Woods-Saxon basis provides a reconciler between the harmonic oscillator basis and coordinate space that may be used to describe exotic nuclei both properly and efficiently. Extension of spherical relativistic Hartree

theory in the Woods-Saxon basis to deformed cases with pairing included is in progress.

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