Relativistic Hartree-Fock model for axially deformed nuclei postprint

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Abstract

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Preamble

Relativistic Hartree-Fock model for axially deformed nuclei

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In this work, we establish an axially deformed relativistic Hartree-Fock (RHF) model with density-dependent meson-nucleon couplings, in which the integro-differential Dirac equations are solved by expanding the Dirac spinor on the spherical Dirac Woods-Saxon basis. Using the RHF Lagrangians PKOi (i = 1, 2, 3), the reliability of the method is illustrated by taking the light nucleus ^{20}Ne, medium-heavy ^{56}Fe, and heavy Pb isotopes as examples. As a preliminary application, a systematic study of ^{20}Ne shows that PKO1 and PKO3, which contain the π-pseudovector (π-PV) coupling, improve the description of the binding energy of ^{20}Ne compared to PKO2 and the selected RMF Lagrangian. Moreover, it is found that the tensor force components carried by the π-PV coupling can have substantial effects in determining the shape evolution of the nucleus.

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Introduction

Over the past decades, worldwide developments of radioactive-ion-beam (RIB) facilities and advanced detectors [1–5] have greatly enriched the field of nuclear physics, extending it from traditional stable nuclei to exotic nuclei far from the stability line in the nuclear chart [6–10]. Meanwhile, many novel nuclear phenomena have been observed when approaching the drip lines, such as the quenching of traditional magic shells and the emergence of new ones [11–19], dilute matter distributions—halo phenomena [20–22], etc. These interesting phenomena not only provide abundant new opportunities for nuclear physics but also challenge our understanding of nuclear systems from both theoretical and experimental perspectives.

On the other hand, it is well known that most nuclei in the nuclear chart are deformed, except for a few near magic numbers. In the early 1950s, much evidence, such as the relationship between nuclear quadrupole moments and shell structure [23–27] and rotational-like spectra [28, 29], indicated that nuclei can have shapes deviating from spherical. It is worth mentioning that some consequences of nuclear deformation were even discussed by Bohr and Kalckar in 1937 [30]. Recently, intensive attention has been paid to the evolution of nuclear shape due to notable progress in laser spectroscopy at RIB facilities [31, 32]. Coupled with deformation effects, more and more novel nuclear phenomena have been discovered during the exploration of the nuclear chart boundaries, such as the island of inversion [33–36], shape coexistence [37–39], and superdeformed and hyperdeformed configurations [40, 41]. In fact, intensive efforts have been devoted to understanding these rich phenomena, which are potentially related to deformation.

As one of the typical representatives, the relativistic mean field (RMF) theory, founded on the meson exchange diagram of nuclear force [42] and also referred to as covariant density functional theory (CDFT) in recent years, provides an efficient and predictive tool for exploring nuclear structure properties across almost the entire nuclear chart [43–49]. With a renormalized relativistic mean field, i.e., the so-called σ-ω model [50], the RMF theory provides an appropriate saturation mechanism for nuclear matter. Afterwards, intensive attempts have been devoted to modeling nuclear in-medium effects [51], either via nonlinear self-couplings of meson fields [52–54] or density dependencies of meson-nucleon coupling strengths [55–58], and the accuracy and reliability in describing various nuclear phenomena have been greatly improved with proposed effective nuclear interactions. With the covariant representation of strong scalar and vector potentials of the order of several hundred MeV, the RMF theory provides simple and efficient descriptions of nuclear structure properties, such as the natural interpretation of strong spin-orbit couplings [59, 60] and the origin of pseudospin symmetry [61, 62].

Extending to nuclei with deformation away from spherical symmetry, large efforts have been devoted to solving the partial differential Dirac equations for nucleons in the relativistic framework, for instance by expanding Dirac spinors on analytic harmonic oscillator (HO) [63–65] or numerical Dirac Woods-Saxon (DWS) [66, 67] bases. For the former, the Dirac spinor and the relativistic mean field containing only the Hartree terms of meson-nucleon couplings are expanded in terms of fermionic and bosonic harmonic oscillators, respectively, which works well for exploring the structure properties of axially deformed nuclei [44]. However, when extrapolating to regions far from stability, namely exotic nuclei, it encounters serious difficulties in providing appropriate asymptotic behaviors of wave functions due to the limitation of the HO potential, particularly for halo nuclei. Although such defects may be overcome by considering a large number of oscillator shells [68], this strongly increases numerical cost and violates the simplicity of the HO basis. Another alternative is to employ local-scaling point transformations to modify the unphysical asymptotic properties, namely the transformed HO basis [69–71].

With the rapid development of computational technology, it becomes possible to expand wave functions numerically on the complete set made of solutions to the Dirac equation with a Dirac Woods-Saxon potential [72], namely the DWS basis [66]. Compared to the HO potential, the Woods-Saxon potential [73] decreases smoothly to zero at large distances, which is essential for providing appropriate asymptotic behaviors of density distributions, particularly for exotic nuclei. Practically, the extension of RMF theory—relativistic continuum Hartree-Bogoliubov (RCHB) theory [74]—has achieved great success in describing not only spherical exotic nuclei [47] but also axially deformed ones with the help of the DWS basis [75–77]. As a typical example, a novel mechanism—the decoupling between the deformations of the core and the halo in ^{44}Mg—has been predicted by axially deformed RCHB theory [75].

Note that the Fock terms, an inseparable part of the meson exchange diagram of nuclear force, are dropped in the RMF theory for simplicity. Thus, due to the limitation of the Hartree approach, the important degrees of freedom associated with π and -tensor couplings cannot be taken into account by the RMF approach. In particular, the important ingredient—the tensor force, which plays a significant role in nuclear shell evolutions [78, 79], symmetry energy [80], and excitations [81–85]—is also missing in the RMF scheme. Over the past decade, density-dependent relativistic Hartree-Fock (DDRHF) theory [67, 86] with proposed relativistic Hartree-Fock (RHF) Lagrangians PKOi (i = 1,2,3) [78, 86] and PKA1 [87] has achieved comparable accuracy to the conventional RMF model in describing nuclear structure properties. Meanwhile, with the inclusion of Fock terms, significant improvements have been obtained in the self-consistent description of nuclear shell evolutions [78, 79, 88, 89], tensor force [80, 90, 91], spin and isospin excitations [92–96], effective masses [86], symmetry energy [97–99], new magicity [89, 100, 101], and novel phenomena [101–103]. Thus, it would be quite valuable to investigate the effects of Fock terms, particularly the π- and -tensor couplings, in describing structure properties of deformed nuclei.

In fact, some attempts have already been made to extend RHF theory to describe deformed nuclei. In 2011, the relativistic Hartree-Fock-Bogoliubov (RHFB) model for axially deformed nuclei was established by expanding Dirac spinors and the RHF mean field on deformed fermionic and bosonic HO bases, respectively [104]. However, due to numerical complexity induced by Fock terms, the calculations are quite time-consuming, especially for rearrangement terms arising from density dependencies of meson-nucleon coupling strengths, and applications have been limited to light deformed nuclei. On the other hand, it is not quite suitable for exploring light exotic nuclei due to the limitations of the HO basis. In this work, inspired by successes achieved with DDRHF theory, the axially deformed relativistic Hartree-Fock model is developed by expanding Dirac spinors on the numerical DWS basis. As a preliminary application, the role played by π-pseudovector coupling in nuclear shape evolution is clarified by taking ^{20}Ne as an example. Note that pairing correlations are still restricted to the BCS scheme in this work, which works well for describing nuclei near the stability line but is less reliable for unstable ones, particularly in exploring halo structures in exotic nuclei [105]. Moreover, for nuclei with super/hyperdeformation, the validity of expansion on the spherical DWS basis should be tested more carefully, which is not the focus of the current work.

The paper is organized as follows. In Sec. II, we present the general formalism of the axially deformed RHF model based on the DWS basis. In Sec. III, results and discussions are presented, including space truncation, convergence checks, and the description of ^{20}Ne by PKOi, in which the role of π-pseudovector coupling is analyzed. Finally, a summary is given in Sec. IV.

II. General Formalism

In this section, we briefly recall the general formalism of relativistic Hartree-Fock (RHF) theory and the RHF energy functional for an axially deformed nucleus with the spherical Dirac Woods-Saxon (DWS) basis. To give readers a complete impression, some details related to density-dependent meson-nucleon coupling strengths, pairing correlations, DWS potentials, etc., are also introduced. Meanwhile, the numerical difficulties in previous RHF calculations of deformed nuclei are emphasized to provide readers with an overall understanding of the status.

A. RHF Energy Functional

Based on the meson-exchange diagram of nuclear force, the Lagrangian density for nuclear systems—the starting point of the theory—can be constructed by considering the degrees of freedom associated with the Dirac field (nucleon) and meson fields: isoscalar mesons including the σ meson (σ) and ω meson ($\omega^{\frown}$), isovector mesons including the meson ($^{\frown}$) and π meson (π), and the photon field (A$^{\frown}$). Among the selected degrees of freedom, isoscalar mesons account for strong attractions and repulsions between nucleons, isovector mesons for isospin-related aspects of nuclear force, and the photon field for electromagnetic interactions between protons [51]. Therefore, the Lagrangian density for nuclear systems can be expressed as

$$\mathcal{L} = \mathcal{L}_M + \mathcal{L}_\sigma + \mathcal{L}_\omega + \mathcal{L}_\rho + \mathcal{L}_\pi + \mathcal{L}_A + \mathcal{L}_I,$$

where the Lagrangians of the free fields $\mathcal{L}_\phi$ ($\phi =$, σ, ω^ , ^ , π, and A^) read as

$$\mathcal{L}_\sigma = +\frac{1}{2}\partial^\mu\sigma\partial_\mu\sigma - \frac{1}{2}m_\sigma^2\sigma^2,$$

$$\mathcal{L}_M = \bar{\psi}(i\gamma^\mu\partial_\mu - M)\psi,$$

$$\mathcal{L}_\omega = -\frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega_\mu\omega^\mu,$$

$$\mathcal{L}_\rho = -\frac{1}{4}\mathbf{R}_{\mu\nu}\cdot\mathbf{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\rho_\mu\cdot\rho^\mu,$$

$$\mathcal{L}_\pi = +\frac{1}{2}\partial^\mu\pi\cdot\partial_\mu\pi - \frac{1}{2}m_\pi^2\pi\cdot\pi,$$

$$\mathcal{L}_A = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu},$$

with the field tensors $\Omega_{\mu\nu} \equiv \partial_\mu\omega_\nu - \partial_\nu\omega_\mu$, $\mathbf{R}_{\mu\nu} \equiv \partial_\mu\rho_\nu - \partial_\nu\rho_\mu$, and $F^{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu$. Considering Lorentz scalar (σ-S), vector (ω-V, -V, and A-V), tensor (-T), and pseudovector (π-PV) couplings, the Lagrangian density $\mathcal{L}_I$ describing the interaction between nucleons and mesons (photon) reads as

$$\mathcal{L}_I = \bar{\psi}\left[-g_\sigma\sigma - g_\omega\gamma^\mu\omega_\mu - g_\rho\gamma^\mu\tau\cdot\rho_\mu - e\gamma^\mu\frac{1-\tau_3}{2}A_\mu - \frac{f_\rho}{2m}\sigma^{\mu\nu}\partial_\nu\rho_\mu\cdot\tau - \frac{f_\pi}{m}\gamma_5\gamma^\mu\partial_\mu\pi\cdot\tau\right]\psi.$$

In the Lagrangian densities, M and m_ϕ are the masses of the nucleon and mesons, and g_ϕ ($\phi = \sigma$, ω^ , ^) and $f_{\phi'}$ (ϕ' = ^ , π) represent the coupling strengths of various meson-nucleon couplings. In this paper, we use arrows to denote isovector quantities and bold types for space vectors.

Following the standard variational procedure, one can derive the Dirac equations for nucleons, Klein-Gordon equations for mesons, and the Proca equation for photons from the Lagrangian density $\mathcal{L}$ as

$$(-i\gamma^\mu\partial_\mu + M + \Sigma)\psi(x) = 0,$$

$$(\Box + m_\sigma^2)\,\sigma = -g_\sigma\bar{\psi}\psi,$$

$$(\Box + m_\omega^2)\,\omega^\mu = +g_\omega\bar{\psi}\gamma^\mu\psi,$$

$$(\Box + m_\rho^2)\,\rho^\mu = +g_\rho\bar{\psi}\gamma^\mu\tau\psi - \partial_\nu\left(\frac{f_\rho}{2m}\bar{\psi}\sigma^{\nu\mu}\tau\psi\right),$$

$$(\Box + m_\pi^2)\,\pi = +\partial_\nu\left(\frac{f_\pi}{m}\bar{\psi}\gamma_5\gamma^\nu\tau\psi\right),$$

$$\partial_\nu F^{\nu\mu} = e\bar{\psi}\frac{1-\tau_3}{2}\gamma^\mu\psi,$$

where the square box $\Box \equiv \partial_\mu\partial^\mu$. In the Dirac equation (9), the self-energy Σ can be obtained following the variational principle.

From the Lagrangian density (1), one can also obtain the Hamiltonian via Legendre transformation. After neglecting the time component of the four-momentum carried by mesons and photons, and substituting the relevant equations, the Hamiltonian can be derived as

$$H = T + \sum_\phi V_\phi,$$

where the kinetic energy (T) and potential energy (V_ϕ) terms read as

$$T = \int d^3x\,\bar{\psi}(\mathbf{x})\left[-i\gamma\cdot\nabla + M\right]\psi(\mathbf{x}),$$

$$V_\phi = \frac{1}{2}\int d^3x\,d^3x'\,\bar{\psi}(\mathbf{x})\bar{\psi}(\mathbf{x}')\Gamma_\phi D_\phi\psi(\mathbf{x}')\psi(\mathbf{x}).$$

In the potential energy terms V_ϕ, ϕ represents various two-body interaction channels: σ-scalar (σ-S), ω-vector (ω-V), -vector (-V), -tensor (-T), -vector-tensor (-VT), π-pseudovector (π-PV), and photon-vector (A-V) couplings. The interaction vertices $\Gamma_\phi(\mathbf{x},\mathbf{x}')$ have the following forms:

$$\Gamma_{\sigma\text{-S}} \equiv -g_\sigma(\mathbf{x})g_\sigma(\mathbf{x}'),$$

$$\Gamma_{\omega\text{-V}} \equiv (g_\omega \gamma^\mu)_{\mathbf{x}} \cdot (g_\omega \gamma_\mu)_{\mathbf{x}'},$$

$$\Gamma_{\rho\text{-V}} \equiv (g_\rho \gamma^\mu \tau)_{\mathbf{x}} \cdot (g_\rho \gamma_\mu \tau)_{\mathbf{x}'},$$

$$\Gamma_{\rho\text{-T}} \equiv \left(\frac{f_\rho}{2m} \sigma^{\nu k} \tau \partial_k\right)_{\mathbf{x}} \cdot \left(\frac{f_\rho}{2m} \sigma_{\nu k} \tau \partial^k\right)_{\mathbf{x}'},$$

$$\Gamma_{\rho\text{-VT}} \equiv (g_\rho \gamma^\nu \tau)_{\mathbf{x}} \cdot \left(\frac{f_\rho}{2m} \sigma_{\nu k} \tau \partial^k\right)_{\mathbf{x}'} + \left(\frac{f_\rho}{2m} \sigma^{\nu k} \tau \partial_k\right)_{\mathbf{x}} \cdot (g_\rho \gamma_\nu \tau)_{\mathbf{x}'},$$

$$\Gamma_{\pi\text{-PV}} \equiv \left(\frac{f_\pi}{m} \tau \gamma_5 \gamma^\mu \partial_\mu\right)_{\mathbf{x}} \cdot \left(\frac{f_\pi}{m} \tau \gamma_5 \gamma^\nu \partial_\nu\right)_{\mathbf{x}'},$$

$$\Gamma_{A\text{-V}} \equiv \left(e \gamma^\mu \frac{1-\tau_3}{2}\right)_{\mathbf{x}} \cdot \left(e \gamma_\mu \frac{1-\tau_3}{2}\right)_{\mathbf{x}'}.$$

After neglecting retardation effects (ignoring the time component of the four-momentum carried by mesons and photons), the propagators $D_\phi(\mathbf{x}, \mathbf{x}')$ in the potential terms V_ϕ read as

$$D_\phi(\mathbf{x}, \mathbf{x}') = \frac{e^{-m_\phi |\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}.$$

To obtain the energy functional, we restrict ourselves to the mean-field approach. In this framework, the nucleon field operator ψ in the Hamiltonian (16) can be quantized as

$$\psi(\mathbf{x}) = \sum_i \psi_i(\mathbf{x}) e^{-i\varepsilon_i t} c_i,$$

where the annihilation operators c_i are defined by the positive-energy solutions of the Dirac equation (9), ε_i is the single-particle energy ($\varepsilon_i > 0$), and $\psi_i(\mathbf{x})$ is the Dirac spinor of state i. It should be noted that in quantizing the nucleon spinor ψ [i.e., in Eq. (20)], contributions from negative-energy states are neglected—the no-sea approximation—consistent with the mean-field approach commonly used in studying ground-state properties of nuclei [43, 44, 47, 106]. With the no-sea approximation, the energy functional E can be deduced from the expectation value of the Hamiltonian with respect to the Hartree-Fock ground state $|\Phi_0\rangle$ as

$$E = \langle \Phi_0 | H | \Phi_0 \rangle = \langle \Phi_0 | T | \Phi_0 \rangle + \sum_\phi \langle \Phi_0 | V_\phi | \Phi_0 \rangle,$$

where A is the mass number of the nucleus and $|0\rangle$ is the vacuum state.

In the two-body interaction part V_ϕ, the expectation value leads to two types of contributions: direct Hartree terms and exchange Fock terms. Considering only the Hartree terms leads to the relativistic mean field (RMF) theory, while including both Hartree and Fock terms corresponds to the relativistic Hartree-Fock (RHF) theory.

With the obtained energy functional, the variational operation $\delta[E - \sum_i \varepsilon_i \langle\psi_i|\psi_i\rangle] = 0$ leads to the integro-differential Dirac equation

$$\int d^3x'\, h(\mathbf{x}, \mathbf{x}')\psi_i(\mathbf{x}') = \varepsilon_i \psi_i(\mathbf{x}),$$

where ε_i is the single-particle energy of state i, and the single-particle Hamiltonian h contains three parts: the kinetic term h_{kin}, local mean-field contributions h_D, and nonlocal contributions from Fock terms h_E:

$$h_{\text{kin}} = [\alpha \cdot \mathbf{p} + \gamma^0 M]\, \delta(\mathbf{x} - \mathbf{x}'),$$

$$h_D = [\Sigma_T(\mathbf{x})\gamma_5 + \Sigma_0(\mathbf{x}) + \gamma^0 \Sigma_S(\mathbf{x})]\, \delta(\mathbf{x} - \mathbf{x}'),$$

$$h_E = \begin{pmatrix} Y_G(\mathbf{x}, \mathbf{x}') & Y_F(\mathbf{x}, \mathbf{x}') \\ X_G(\mathbf{x}, \mathbf{x}') & X_F(\mathbf{x}, \mathbf{x}') \end{pmatrix}.$$

In the above expressions, h_D contains the local scalar self-energy Σ_S, the time component of the vector self-energy Σ_0, and the tensor self-energy Σ_T, while h_E contains nonlocal mean fields X_G, X_F, Y_G, and Y_F contributed by Fock terms. When considering density dependencies in meson-nucleon coupling strengths—taking g_ϕ ($\phi = \sigma, \omega\hat{}\,, \hat{}\,$) and $f_{\phi'}$ (ϕ' $= \hat{}\,, \pi$) as functions of nucleon density $\rho_b = \bar{\psi}\gamma^0\psi$—the variation (23) may lead to an additional contribution to the self-energy Σ_0, i.e., rearrangement terms Σ_R [58, 67, 86, 87].

B. Numerical Difficulties in RHF Descriptions of Axially Deformed Nuclei

In this work, we restrict ourselves to axial symmetry, focusing on axially deformed nuclei. At the mean-field level, nucleons are considered as point-like particles moving in an axially symmetric mean field. Consistent with axial symmetry and reflection symmetry with respect to the $z = 0$ plane, the complete set of good quantum numbers is denoted as $(\nu\pi m)$, where ν is the principal quantum number, π represents parity, and m is the projection of total angular momentum on the symmetric z axis. For simplicity, we use index i to denote the quantum number set $(\nu\pi, m \gtrless 0)$. The Dirac spinor of the nucleon in Eq. (20) therefore has the following form in cylindrical coordinates (ϱ, z, ϕ):

$$\psi_{\nu\pi m}(\varrho,z,\phi)=\begin{pmatrix} f_{\nu\pi}^{(1)}(\varrho,z)e^{i(m-1/2)\phi}\\ f_{\nu\pi}^{(2)}(\varrho,z)e^{i(m+1/2)\phi}\\ g_{\nu\pi}^{(1)}(\varrho,z)e^{i(m-1/2)\phi}\\ g_{\nu\pi}^{(2)}(\varrho,z)e^{i(m+1/2)\phi}\end{pmatrix}.$$

In practice, it is not straightforward to solve the integro-differential equation (24), particularly for axially deformed nuclei. Within the RMF approach, the Dirac equation (24) reduces to a partial differential equation for axially deformed nuclei, which can be solved by expanding the Dirac spinor on a deformed oscillator basis, with local mean fields also calculated via expansion in a deformed harmonic oscillator basis [65]. In Ref. [104], a similar attempt was made to solve the integro-differential Dirac equation for axially deformed nuclei, with both local and nonlocal mean fields calculated via expansion on axially deformed oscillator bases. However, calculations of nonlocal mean fields are too time-consuming, particularly when dealing with rearrangement terms generated by density dependence of coupling strengths [104], which largely limits extensive studies of heavy nuclei.

In cylindrical coordinate space (ϱ,z,ϕ), the meson propagators D_ϕ can be decomposed as

$$D_\phi(\mathbf{x},\mathbf{x}')=\frac{1}{\pi}\sum_\mu e^{i\mu(\phi-\phi')}\int_0^\infty dk\,a_\phi(k)\times J_\mu(k\varrho)J_\mu(k\varrho')e^{-a_\phi(k)|z-z'|},$$

where $a_\phi(k)=\sqrt{k^2+m_\phi^2}$. A similar decomposition can be obtained for the photon propagator D_A if we set $m_\phi=0$ [107]. As an alternative, one can solve the Dirac equation (24) by expanding the Dirac spinor on some selected basis, such as the oscillator basis [65, 104]. Then, the RHF mean fields can be calculated directly in cylindrical coordinate space with the obtained wave functions.

In principle, such a procedure should be valid for RHF calculations of axially deformed nuclei. However, in the expansion (29), the exponential term $\exp[-a_\phi(k)|z-z'|]$ induces singularities, i.e., rather sharp peaks appear at $z=z'$. This introduces additional algorithmic difficulty for integration over the z coordinate. Moreover, the Bessel functions J_μ result in oscillating and slowly decaying integral terms in Eq. (29), making precise numerical calculation of the integration over k rather difficult.

In contrast to cylindrical space, the propagator in spherical coordinate space (r,ϑ,ϕ) can be expressed as [106, 108]

$$D_\phi(\mathbf{x},\mathbf{x}')=\sum_{\lambda_y\mu_y}(-1)^{\mu_y}R_\phi^{\lambda_y}(r,r')Y_{\lambda_y\mu_y}(\Omega)Y_{\lambda_y-\mu_y}(\Omega'),$$

where $\Omega = (\vartheta, \phi)$, the index λ_y denotes expansion terms of the Yukawa propagator, and $R_\phi^{\lambda_y}$ contains modified Bessel functions I and K as

$$R_\phi^{\lambda_y}(r, r') = \frac{m_\phi}{2\lambda_y + 1} \frac{r_<^{\lambda_y}}{r_>^{\lambda_y+1}} I_{\lambda_y+1/2}(m_\phi r_<) K_{\lambda_y+1/2}(m_\phi r_>),$$

with $r_< = \min(r, r')$ and $r_> = \max(r, r')$.

Comparing the expressions in cylindrical and spherical geometries, it is clear that the integration in Eq. (29) corresponds to the infinite sum over λ_y in Eq. (30) for a given μ_y. Apparently, it is not an easy task to overcome the oscillating integration over k in Eq. (29).

Due to these algorithmic difficulties, in this work we consider expanding the Dirac spinor in a spherical Dirac Woods-Saxon (DWS) basis [66, 67]. Compared to the oscillator basis, the DWS basis has the advantage of providing appropriate asymptotic behaviors of wave functions, enabling reliable descriptions of exotic nuclei. On the other hand, it becomes similar to dealing with the energy functional (21) as in the spherical case [106], and the cutoff of the DWS basis in expanding the Dirac spinor (28) automatically truncates the infinite sum over λ_y in the propagator expansion (30), naturally avoiding divergence.

C. RHF Energy Functional for Axially Deformed Nuclei with the DWS Basis

Restricted to spherical symmetry, the complete set of good quantum numbers contains the principal quantum number n, angular momentum j and its projection m, and parity $\pi = (-1)^l$ (where l is the orbital angular momentum). For convenience, the quantum number κ is often used to denote angular momentum j and parity π, i.e., $\kappa = j + 1/2$ for $j = l - 1/2$ and $\kappa = -(j + 1/2)$ for $j = l + 1/2$, with $\pi = (-1)^\kappa \text{sign}(\kappa)$ [108]. The Dirac spinor in the DWS basis has the following form:

$$\psi_{am}(\mathbf{x}) = \begin{pmatrix} G_a(r)\Omega_{\kappa m}(\vartheta, \phi) \\ iF_a(r)\Omega_{-\kappa m}(\vartheta, \phi) \end{pmatrix},$$

where index a represents the set of quantum numbers $(n\kappa) = (njl)$, and $\Omega_{\kappa m}$ (also referred to as Ω_{ljm}) is the spherical spinor [108]. Here, we use l_u and l_d to denote the orbital angular momenta of the upper and lower components of the Dirac spinor ψ_{am}, respectively, with $l_u + l_d = 2j$. Note that if quantity κ denotes (jl_u), then $-\kappa$ corresponds to (jl_d). Considering both positive and negative energy states in the spherical DWS basis, the expansion of the spinor (28) can be expressed as

$$\psi_{\nu\pi m}(\mathbf{x}) = \sum_a C_{a,i} \psi_{am}(\mathbf{x}) = \sum_\kappa \psi_{\nu\kappa m}(\mathbf{x}),$$

where the expansion coefficient $C_{a,i}$ [i represents $(\nu\pi m)$] is restricted to be real, and $\psi_{\nu\kappa m}$ reads as

$$\psi_{\nu\kappa m} = \sum_n C_{n\kappa,i}\psi_{n\kappa m} = \begin{pmatrix} G_i^\kappa \Omega_{\kappa m} \\ iF_i^\kappa \Omega_{-\kappa m} \end{pmatrix},$$

with $G_i^\kappa = \sum_n C_{n\kappa,i} G_{n\kappa}$ and $F_i^\kappa = \sum_n C_{n\kappa,i} F_{n\kappa}$.

In the present work, we focus on the RHF Lagrangians PKOi (i = 1, 2, 3) [78, 86]. Note that PKO2 contains σ-S, ω-V, -V, and A-V couplings, while PKO1 and PKO3 additionally include π-PV coupling. Thus, the RHF energy functional can be expressed as

$$E = E_{\text{kin}} + \sum_\phi \left(E_\phi^D + E_\phi^E\right),$$

where $E_{\text{kin}} = \langle\Phi_0|T|\Phi_0\rangle$, and E_ϕ^D and E_ϕ^E are the Hartree and Fock terms of the two-body potential energies $E_\phi = \langle\Phi_0|V_\phi|\Phi_0\rangle$ with $\phi = \sigma$-S, ω-V, -V, π-PV, and A-V.

With the expansion (34), the kinetic energy functional E_{kin} can be derived as

$$E_{\text{kin}} = \sum_i v_i^2 \int dr \sum_\kappa \left\{\left[\frac{dG_i^\kappa}{dr} G_i^\kappa - M F_i^\kappa F_i^\kappa\right] - \left[\frac{dF_i^\kappa}{dr} F_i^\kappa - M G_i^\kappa G_i^\kappa\right]\right\},$$

where $v_i^2 (\in [0,2])$ denotes the occupation of orbit i.

For PKOi, only the local self-energies Σ_S and Σ_0 remain in h_D (26), and the relevant scalar and baryon densities, i.e., ρ_s and ρ_b, can be deduced as

$$\rho_s(\mathbf{x}) = \sum_i \bar{\psi}_i(\mathbf{x})\psi_i(\mathbf{x}) = \sum_{\lambda_d} \rho^s_{\lambda_d}(r) P_{\lambda_d}(\cos\vartheta),$$

$$\rho_b(\mathbf{x}) = \sum_i \bar{\psi}_i(\mathbf{x})\gamma^0\psi_i(\mathbf{x}) = \sum_{\lambda_d} \rho^b_{\lambda_d}(r) P_{\lambda_d}(\cos\vartheta),$$

where P_{λ_d} is the Legendre polynomial, λ_d must be even integers starting from 0 due to parity conservation, and the cutoff of λ_d is naturally determined by truncation of the DWS basis in expansion (34). The expansion term ρ_{λ_d} can be derived as

$$\rho_{\lambda_d}(r) = \sum_{\kappa\kappa'} \sum_{m>0} (-1)^{m+1/2} D^{\kappa m,\kappa' m}_{\lambda_d 0} \left[G_i^\kappa(r) G_i^{\kappa'}(r) \pm F_i^\kappa(r) F_i^{\kappa'}(r)\right],$$

where the $\pm$ in brackets corresponds to baryonic and scalar densities, respectively, and for the symbol D see Eq. (A4) for details.

With the density expansion (38), the Hartree terms of the energy functional E_ϕ^D can be expressed as

$$E^D_{\sigma\text{-S}} = \int r^2 dr \sum_{\lambda_d} \Sigma^{S,\sigma\text{-S}}_{\lambda_d}(r)\rho^s_{\lambda_d}(r),$$

$$E^D_{\omega\text{-V}} = \int r^2 dr \sum_{\lambda_d} \Sigma^{0,\omega\text{-V}}_{\lambda_d}(r)\rho^b_{\lambda_d}(r),$$

where the expansion terms of self-energies are given in Eq. (A9). For the other two vector couplings (-V and A-V), expressions can be obtained similarly to the ω-V case, with details found in Appendix A 2.

For contributions from Fock terms to the energy functional (21), namely E^E_ϕ, they can be expressed in a unified form as

$$E^E_\phi = \int dr\, dr' \sum_{\kappa_1\kappa_2} \begin{pmatrix} G^{\kappa_1}_i & F^{\kappa_1}_i \end{pmatrix} \begin{pmatrix} Y^{\kappa_1,\kappa_2;\phi}_G & Y^{\kappa_1,\kappa_2;\phi}_F \\ X^{\kappa_1,\kappa_2;\phi}_G & X^{\kappa_1,\kappa_2;\phi}_F \end{pmatrix}_{\pi m} \begin{pmatrix} G^{\kappa_2}_i \\ F^{\kappa_2}_i \end{pmatrix}_{r'},$$

where ϕ represents the σ-S coupling, time and space components of vector (ω-V, -V, and A-V) couplings, and the π-PV coupling. Here, we introduce R to denote nonlocal density terms, which appear as source terms in the nonlocal self-energies Y_G, Y_F, X_G, and X_F:

$$R^G_{\kappa\kappa',\pi m}(r,r') = \sum_i G_{\nu\pi m,\kappa}(r)G_{\nu\pi m,\kappa'}(r'),$$

$$R^F_{\kappa\kappa',\pi m}(r,r') = \sum_i G_{\nu\pi m,\kappa}(r)F_{\nu\pi m,\kappa'}(r'),$$

$$R^G_{\kappa\kappa',\pi m}(r,r') = \sum_i F_{\nu\pi m,\kappa}(r)G_{\nu\pi m,\kappa'}(r'),$$

$$R^F_{\kappa\kappa',\pi m}(r,r') = \sum_i F_{\nu\pi m,\kappa}(r)F_{\nu\pi m,\kappa'}(r').$$

For details of the nonlocal self-energies Y_G, Y_F, X_G, and X_F in Eq. (41), readers are referred to Appendix D.

D. Density-Dependent Meson-Nucleon Couplings

In the current RHF approach, namely DDRHF theory, nuclear in-medium effects are introduced phenomenologically by taking coupling strengths as functions of density ρ_b [86, 87]:

$$g_\phi(\rho_b) = g_\phi(\rho_0) f_\phi(\xi), \quad \text{for } \phi = \sigma\text{-S}, \omega\text{-V},$$

$$g_{\phi'}(\rho_b) = g_{\phi'}(0) e^{-a_{\phi'}\xi}, \quad \text{for } g_{\phi'} = g_\rho, f_\rho, f_\pi,$$

where $\xi = \rho_b/\rho_0$, ρ_0 is the saturation density, and

$$f_\phi(\xi) = a_\phi \frac{1 + b_\phi(\xi + d_\phi)^2}{1 + c_\phi(\xi + d_\phi)^2}.$$

The parameters a, b, c, d in expressions (46) are determined through parametrization referring to properties of nuclear matter and selected finite nuclei [78, 86, 87].

Under axial symmetry, the coupling constant g_ϕ can be expressed in terms of Legendre polynomials as

$$g_\phi(\rho_b) = \sum_{\lambda_p} g^\phi_{\lambda_p}(\rho_b) P_{\lambda_p}(\cos\vartheta),$$

where λ_p must be even integers due to parity conservation and its cutoff is determined by convergence requirements. The expansion term $g^\phi_{\lambda_p}$ is calculated by

$$g^\phi_{\lambda_p}(\rho_b) = \int_{-1}^{1} d(\cos\vartheta) P_{\lambda_p}(\cos\vartheta) g_\phi(\rho_b).$$

Because of density dependence in g_ϕ, one must include rearrangement terms Σ_R to preserve energy-momentum conservation [58]. The variation of coupling constants g_ϕ can be expressed as

$$\delta g_\phi(\rho_b) = \sum_{\lambda_p} P_{\lambda_p}(\cos\vartheta) \sum_{\lambda_d} \frac{\partial g^\phi_{\lambda_p}}{\partial \rho^b_{\lambda_d}} \delta\rho^b_{\lambda_d},$$

where the fraction term $\partial\rho^b_{\lambda_d}/\partial C_{a,i}$ can be deduced easily from the expression of ρ_{λ_d} (39), and the term $\partial g^\phi_{\lambda_p}/\partial\rho^b_{\lambda_d}$ is derived as

$$\frac{\partial g^{\phi}_{\lambda_p}}{\partial \rho^b_{\lambda_d}} = \left(\frac{C^{\lambda_d 0}_{\lambda_p 0}}{2\lambda_d+1}\right)^2 \int_{-1}^{1} dt P_{\lambda_p}(t)\frac{\partial g_\phi}{\partial \rho_b},$$

where $\partial g_\phi/\partial\rho_b$ is determined by the density-dependent form (46), and $\hat{L} = \sqrt{2L+1}$. Note that both $g^{\phi}_{\lambda_p}$ and $\partial g^{\phi}_{\lambda_p}/\partial\rho^b_{\lambda_d}$ are calculated numerically, with integration evaluated using Gaussian quadrature.

Due to density dependencies in coupling strengths, rearrangement terms appearing in the self-energy $\Sigma^0_{\lambda_d}$ can be simply expressed as

$$\Sigma^{R,0}_{\lambda_d} = \sum_\phi \left[\Sigma^{R,\phi}_{D,\lambda_d} + \Sigma^{R,\phi}_{E,\lambda_d}\right],$$

where detailed contributions from Hartree and Fock terms are given in Appendices A 2 and A 3, respectively.

E. Eigenvalue Equations: Dirac Equations with the Spherical DWS Basis

Since the Dirac spinors (28) are expanded on the spherical DWS basis, the total energy of an axially deformed nucleus is expressed as a functional of the coefficient set $\{C_{a,i}\}$. The variation (23) is therefore performed with respect to $C_{a,i}$, leading to a series of eigenvalue equations

$$\sum_{a'} H^{\pi m}_{aa'}\tilde{C}_{a',i} = \varepsilon_i \tilde{C}_{a,i}.$$

Note that the expansion of the Dirac spinor [see Eq. (34)] contains $N = (N_F + N_D) \times K_m$ terms, where N_F, N_D, and K_m will be introduced in the following context. Therefore, $H^{\pi m} = (H^{\pi m}_{aa'})$ is an $N \times N$ square matrix, and $\tilde{C}_i = (C_{a,i})$ is a column matrix with N terms. The eigenvalue (single-particle energy ε_i) and eigenvector $\tilde{C}_i$ can be determined by diagonalizing $H^{\pi m}$.

Similar to the single-particle Hamiltonian in the integro-differential Dirac equation (24), the matrix $H^{\pi m}$ in Eq. (52) consists of three parts: kinetic $H_{\rm kin}$, local H_D, and nonlocal H_E terms.

F. Pairing Correlations: BCS Method with Gogny Force

For open-shell nuclei, pairing correlations play an important role in determining ground-state properties, particularly for nuclei close to the drip line [47, 74, 109–112]. For deformed nuclei, pairing correlations also play an essential role in shape evolution since the single-particle structure changes significantly with deformation. In this work, pairing correlations are treated within the BCS scheme.

For even-even nuclei, the BCS ground state can be expressed as

$$|\mathrm{BCS}\rangle = \prod_{m>0} (u_i + v_i c_i^\dagger c_{\bar{i}}^\dagger)|-\rangle,$$

where $v_i^2 (\in [0,1])$ represents the occupation probability of state i, $u_i^2 = 1 - v_i^2$, and $\bar{i}$ denotes the time-reversal partner of i. From variation with respect to v_i, $\delta\langle\mathrm{BCS}|(H - \lambda\hat{N})|\mathrm{BCS}\rangle = 0$, with $H = H_{\mathrm{kin}} + H_D + H_E$, the gap equations can be derived as

$$\Delta_i = -\sum_{i'>0} \frac{V_{ii'}^{pp} \Delta_{i'}}{\sqrt{(\varepsilon_{i'} - \lambda)^2 + \Delta_{i'}^2}},$$

where the subscript (πm) is omitted. With the spherical DWS basis, the kinetic term can be expressed as

$$H_{\mathrm{kin},aa'}^{\pi m} = \int dr \left\{ \left[\frac{dF_{a'}}{dr} F_{a'} - M G_{a'} F_{a'} \right] - \left[\frac{dG_{a'}}{dr} G_{a'} - M F_{a'} G_{a'} \right] \right\},$$

where $a = (n\kappa)$ and $a' = (n'\kappa')$, and for H_{kin}, $\kappa = \kappa'$. For the local H_D containing Hartree mean fields and rearrangement terms, it can be expressed as

$$H_{D,aa'}^{\pi m} = \sum_{\lambda_d} (-1)^{m+1/2} D_{\lambda_d 0}^{\kappa m,\kappa' m} \begin{pmatrix} G_a & F_a \end{pmatrix} \left(\gamma^0 \Sigma_{\lambda_d}^{S,\sigma\text{-S}} + \Sigma_{\lambda_d}^{0,\phi'} + \Sigma_{\lambda_d}^{R,\phi'} \right) \begin{pmatrix} G_{a'} \\ F_{a'} \end{pmatrix},$$

where ϕ' represents vector channels (ω-V, -V, and A-V couplings). For the nonlocal term, it can be expressed using nonlocal mean fields Y_G, Y_F, X_G, and X_F from the energy functional (41):

$$H_{E,aa'}^{\pi m} = \int dr\, dr' \sum_{\kappa\kappa'} \begin{pmatrix} G_a & F_a \end{pmatrix} \begin{pmatrix} Y_G^{\kappa\kappa',\phi} & Y_F^{\kappa\kappa',\phi} \\ X_G^{\kappa\kappa',\phi} & X_F^{\kappa\kappa',\phi} \end{pmatrix}_{\pi m} (r, r') \begin{pmatrix} G_{a'} \\ F_{a'} \end{pmatrix}_{r'}.$$

In this work, we focus on the RHF Lagrangians PKOi (i = 1, 2, 3), and ϕ represents σ-S, ω-V, -V, π-PV, and A-V couplings.

G. Dirac Woods-Saxon Potentials and Deformation Parameters

In calculating nuclear structure within CDFT, self-consistent iterations generally start from an initial potential. In this work, we take local Dirac Woods-Saxon potentials [72] as the initial potentials, which are also used to determine the spherical DWS basis. The only difference is that in the initial DWS potential we need to consider deformation effects, i.e., choose appropriate initial deformation parameters β_0. With underlying iteration, the calculation converges to a local minimum of the energy functional near β_0.

In the Dirac equation, local self-energies consist of vector and scalar terms, i.e., $\Sigma_0 + \gamma^0\Sigma_S$, also referred to as $\Sigma^\pm = \Sigma_0 \pm \Sigma_S$ for convenience. As an initial approximation, the local self-energy Σ_T and nonlocal terms in the Dirac equation (24) are set to zero, and the Woods-Saxon type local $\Sigma^\pm$ can be expressed as

$$\Sigma^+_{n,p}(r) = V_0 \frac{1 - a_0(N-Z)\tau_3/A}{1+\exp[(r-R^+_{\tau_3})/a_{\tau_3}]},$$

$$\Sigma^-_{n,p}(r) = V_0 \frac{1 - a_0(N-Z)\tau_3/A}{1+\exp[(r-R^-_{\tau_3})/a_{\tau_3}]} + V^{\mathrm{Coul}}_{\tau_3},$$

where the isospin projection operator τ_3 is defined with the convention $\tau_3|n\rangle = |n\rangle$ and $\tau_3|p\rangle = -|p\rangle$, and $R^\pm_{\tau_3} = r^{0,\pm}_{\tau_3} A^{1/3}$ represent empirical radii of neutrons or protons for a nucleus with mass number A, and $V^{\mathrm{Coul}}_{\tau_3}$ represents the Coulomb potential between protons ($\tau_3 = -1$). The parameters in the Dirac Woods-Saxon potential, used in this work to provide the spherical DWS basis and initial potential, are given in Table I.

[TABLE I]

In the Dirac Woods-Saxon potentials (71), the Coulomb potential between protons is evaluated by assuming a uniformly distributed charge:

$$V_c(r) = \frac{\alpha Z}{2R_c}\left(3 - \frac{r^2}{R_c^2}\right) \quad \text{when } r < R_c,$$

$$V_c(r) = \frac{\alpha Z}{r} \quad \text{when } r \geq R_c,$$

where $R_c = R_{\tau_3=-1}$ and α is the fine-structure constant.

Unlike determining the spherical DWS basis, one must account for deformation effects in the initial DWS potentials (71). If restricted to spherical symmetry, a nucleus can be divided into spherical shells with equal density at various radial distances. Extending to an axially deformed nucleus, surfaces of equal density become ellipsoidal, described as

$$R(\vartheta, \phi) = R_0 \left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\vartheta, \phi)\right],$$

where R_0 corresponds to the radius of a spherical nucleus with equal volume. Considering axial symmetry and reflection symmetry with respect to the $z = 0$ plane, $R(\vartheta, \phi)$ can be further reduced to

$$R(\vartheta; \beta) = R_0 \left[1 + \sqrt{\frac{5}{16\pi}}\beta\left(3\cos^2\vartheta - 1\right)\right],$$

where β describes nuclear deformation deviating from spherical shape, with positive and negative values corresponding to prolate and oblate shapes, respectively. In the DWS potentials (71), the empirical radii $R^{\pm}_{\tau_3}$ are replaced by $R^{\pm}_{\tau_3}(\vartheta, \beta)$, leading to $\Sigma^{\pm}_{\tau_3}(r, \vartheta; \beta)$:

$$R^{\pm}_{\tau_3}(\vartheta; \beta) = R^{0,\pm}_{\tau_3} A^{1/3} \left[1 + \sqrt{\frac{5}{16\pi}}\beta\left(3\cos^2\vartheta - 1\right)\right]^{\mp 2/3} \left[1 + \delta\left(3\cos^2\vartheta - 1\right)\right]^{-1/3},$$

where $\delta = 3\sqrt{5/16\pi}\beta$, and the values of $r^{0,\pm}_{\tau_3}$ are given in Table I.

For the initial DWS potentials $\Sigma^{\pm}_{\tau_3}(r, \vartheta; \beta)$, similar expansion terms as for local self-energies in the Hartree energy functional (40) can be determined by

$$\Sigma^{\pm}_{\tau_3, \lambda_d}(r) = \int_0^{\pi} \Sigma^{\pm}_{\tau_3}(r, \vartheta) P_\lambda(\cos\vartheta) \sin\vartheta d\vartheta,$$

where the integration can be evaluated using Gauss-Legendre quadrature. The initial matrix in the eigenvalue equation (52) is then obtained by replacing the expansion terms $\Sigma^0_{\lambda_d} \pm \Sigma^S_{\lambda_d}$ in H_D (55) with $\Sigma^{\pm}_{\tau_3, \lambda_d}$, since the kinetic part H_{kin} depends only on the DWS basis and the nonlocal part H_E is set to zero.

With the density expansion (38), it is straightforward to deduce the intrinsic multipole moment Q_{λ_d} for a deformed nucleus:

$$Q_{\lambda_d} = \sqrt{\frac{8\pi}{2\lambda_d + 1}} \int dr\, r^{\lambda_d + 2} \rho^b_{\lambda_d}(r),$$

and with the obtained quadrupole moment Q_2, the quadrupole deformation β can be evaluated approximately by

$$\beta = \sqrt{\frac{5}{16\pi}}\frac{Q_2}{AR_0^2},$$

where $R_0 = 1.2A^{1/3}$.

III. Results and Discussions

As the first attempt at RHF calculations with the DWS basis for an axially deformed nucleus, we first introduce space truncation in this section. As a convergence check of space truncations, we show test calculations for light ^{20}Ne, medium-heavy ^{56}Fe, and heavy Pb isotopes. Furthermore, we concentrate on structure properties of ^{20}Ne described by the RHF Lagrangians PKOi, compared to calculations with the RMF Lagrangian DD-ME2 [114] and available experimental data.

A. Space Truncations

Within DDRHF theory, calculations for axially deformed nuclei in this work are performed by expanding Dirac spinors on a spherical DWS basis (34). Related to this, two additional expansions must be considered carefully: the decomposition of propagators (30) in spherical coordinates (r, ϑ, ϕ) and the expansion of coupling strengths in terms of Legendre functions (47). Thus, one needs to handle truncations related to $(n\kappa)$ in (34), λ_y in (30), and λ_p in (47).

In fact, these three truncations are not independent of each other. For a given λ_p in (47), the propagator expansion λ_y is automatically truncated by the cutoff on $(n\kappa)$ in the spherical DWS basis. Eventually, two independent truncations remain: the cutoffs on $(n\kappa)$ in expanding Dirac spinors (34) and λ_p in expanding density-dependent coupling strengths (47).

For the Dirac spinor $\psi_{\nu\pi m}$ with axial symmetry, where parity π and angular momentum projection m are good quantum numbers, expansions (34) are carried out with respect to principal quantum number n and κ quantity on the spherical DWS basis $\{\psi_{n\kappa m}\}$. For completeness, both positive and negative energy states of the spherical DWS basis must be taken into account. This should not be confused with the no-sea approximation adopted in the mean-field approach, which corresponds to neglecting the Dirac sea in calculating densities or currents. Note that in expanding Dirac spinors (34)-(35), the sum over principal quantum number n is carried out beforehand. Thus, for all included κ blocks, the numbers of positive and negative energy states can be simply fixed as the same N_F and N_D values, respectively. One just needs to consider sufficiently large N_F and N_D values, which does not bring additional computational cost since the complicated nonlocal self-energies are independent of principal quantum numbers ν or n (see Appendix for details).

In general, the Dirac equation with spherical DWS potentials is solved in a spherical box of size R_m. To maintain numerical accuracy, the N_F value must be modified with respect to R_m. In most cases, it is accurate enough to set $R_m = 20$ fm, with N_F and N_D chosen as 28 and 10, respectively, and this accuracy has been verified in RHFB calculations [67]. For the κ cutoff, we use K_m to denote the number of κ blocks included in expansion (34) of the Dirac spinor $\psi_{\nu\pi m}$ (28). In total, the number of expansion terms in Eq. (34) is then $K_m \times (N_F + N_D)$.

For open-shell nuclei, one needs to truncate the configuration space when evaluating pairing effects. Practically, such truncation corresponds to maximum values of m and ν for each m orbit. In this work, the finite-range Gogny force D1S is introduced as the pairing force, allowing calculations to converge smoothly with respect to truncation. Thus, one can consider ν and m values as large as possible. For the former, increasing ν does not increase numerical burden in calculating Fock terms, which dominate computational cost. However, for the maximum m value $m_{\max}$, computational cost increases significantly when enlarging $m_{\max}$.

To unify cutoffs and reduce numerical complexity, we set the maximum m value as $m_{\max}$ and the number of κ blocks considered in expanding the Dirac spinor $\psi_{\nu\pi m_{\max}}$ as $K_{m_{\max}}$, giving the maximum absolute κ value as $k_{\max} = m_{\max} + K_{m_{\max}} - 1/2$. Hence, for an arbitrary Dirac spinor $\psi_{\nu\pi m}$, the κ quantities in expansion (34) include $|\kappa| = m+1/2, m+3/2, \cdots, k_{\max}$ and $\text{sign}(\kappa) = \pi\times(-1)^{|\kappa|}$, with $\pi = \pm 1$ for positive and negative parities, respectively.

For a given nucleus, the $m_{\max}$ value is usually determined by convergence requirements of BCS pairing. Practically, both $m_{\max}$ and $k_{\max}$ (or $K_{m_{\max}}$) values are decided through careful convergence checks. For instance, in cases of large deformation, some orbits containing components with large κ values may intrude even across well-known major shells. Thus, one needs to enlarge $m_{\max}$ and $K_{m_{\max}}$ values, which can remarkably increase computational cost.

For density-dependent coupling strengths (47), the λ_p value must be an even integer starting from 0 due to axial symmetry and parity conservation. In general, it is accurate enough to have four terms $\lambda_p = 0, 2, 4, 6$ for most nuclei. Thus, with fixed truncation in expanding Dirac spinors, the cutoff on λ_y in decomposing propagators (30) is automatically determined as $\lambda_y^{\max} = 2k_{\max} + \lambda_p^{\max}$.

B. Convergence Check

First, we take the light nucleus ^{20}Ne as an example for convergence checks. Figure 2 [Figure 2: see original paper] shows binding energy [plot (a)] and quadrupole deformation β [plot (b)] as functions of m-cutoff $m_{\max}$, with $K_{m_{\max}}$ fixed as 3. In Fig. 2(a), binding energies converge when $m_{\max} \geq 9/2$, as does the deformation parameter β shown in Fig. 2(b). It is also shown that with different initial deformations β_0, calculations converge to the nearby local minimum. One may notice that with $m_{\max} = 3/2$, calculations with $\beta_0 = 0$ and 0.5 give the same binding energy. For ^{20}Ne with spherical symmetry, the last occupied orbits are $d_{5/2}$, which exceed $m_{\max} = 3/2$. Thus, calculations with $\beta_0 = 0$ cannot converge to spherical shape. Considering convergence of binding energy and deformation, it is precise enough to choose $m_{\max} = 11/2$ and $K_{m_{\max}} = 3$ for ^{20}Ne.

[Figure 1: see original paper] (Color online) Binding energy E_B (MeV) (a) and quadrupole deformation β (b) of ^{20}Ne calculated by PKOi and DD-ME2 with respect to $m_{\max}$, in which $K_{m_{\max}}$ is fixed as 3. The open symbols denote calculations with initial deformation $\beta_0 = 0$ and filled ones for $\beta_0 = 0.5$.

Here, we only show convergence checks with respect to $m_{\max}$. For expansion of density-dependent coupling strength, $\lambda_p^{\max}$ has been checked for nuclei across a wide range of mass numbers, and it is sufficient to choose $\lambda_p^{\max} = 6$ for most nuclei. For the $K_{m_{\max}}$ value, it is accurate enough to fix $K_{m_{\max}} = 3$ with an appropriate $m_{\max}$ value that is generally decided by the configuration space of pairing correlations. For economical reasons, one can carefully choose an appropriate combination of $m_{\max}$ and $K_{m_{\max}}$ values.

We further check convergence for medium-heavy nuclei, taking ^{56}Fe as an example. Table II shows binding energy E_B (MeV), total, neutron, and proton quadrupole deformations β, β_n, and β_p with respect to m-cutoff $m_{\max}$, with $K_{m_{\max}}$ set as 3 and $\beta_0 = 0.3$.

[TABLE II]

It is seen that for both PKO1 and PKO2, calculations converge after $m_{\max} \geq 11/2$. Even for $m_{\max} < 11/2$, results are rather close to converged ones. This is similar to calculations of ^{20}Ne with $\beta_0 = 0.0$, which converge quickly when $m_{\max} \geq 5/2$. This is because with small deformation or spherical shape, contributions from high κ blocks contribute little to expansion of the Dirac spinor $\psi_{\nu\pi m}$, whereas with large deformation (e.g., calculations of ^{20}Ne with $\beta_0 = 0.5$ in Fig. 1), components with large κ values may have substantial contributions.

For heavy nuclei, we take even Pb isotopes from ^{182}Pb to ^{214}Pb as examples for convergence checks. Table III shows binding energies calculated by PKOi and DD-ME2, with experimental values [115] and results from spherical code (Sph.) given as references. For deformed (Def.) code calculations, $m_{\max}$ is set as 15/2 and $K_{m_{\max}} = 3$. Note that in both Sph. and Def. calculations, pairing correlations are treated with the BCS method using the Gogny force D1S as the pairing force. For all selected isotopes, Def. calculations with $\beta_0 = 0$ give spherical shape. It can be seen that deviations between Def. and Sph. calculations are rather tiny (dozens of keV), particularly for doubly magic ^{208}Pb, illustrating the accuracy of the Def. code for heavy nuclei. For open-shell Pb isotopes, accuracies are as perfect as for doubly magic ^{208}Pb, with relative deviations usually less than 0.01%. Similar accuracy can be obtained for matter radii, though these are not shown for simplicity.

As a further example of convergence checks, we choose the heavier nucleus ^{220}Rn, which has a reported experimental quadrupole deformation of $\beta = 0.1269$ [117].

It is worthwhile to note that for heavy nuclei, truncations of expansions (34) and (47) must be tested carefully. Here, we take five terms $\lambda_p = 0, 2, 4, 6, 8$ in expanding density-dependent coupling strengths (47) for ^{220}Rn. Using PKO1 and DD-ME2, convergence tests with respect to $m_{\max}$ are shown in Table IV, including binding energy E_B, matter and charge radii r and $r_{\rm ch}$, and quadrupole deformations (β, β_n, β_p). As shown in Table IV, both RHF (PKO1) and RMF (DD-ME2) calculations show appropriate convergence with respect to $m_{\max}$, illustrating the reliability of expansion on the DWS basis. Moreover, both RHF and RMF Lagrangians provide reasonable descriptions of bulk properties of ^{220}Rn, referring to available data.

C. Description of ^{20}Ne

After careful convergence checks, we performed systematic calculations for ^{20}Ne, a typically deformed nucleus. First, we show constrained calculations with respect to quadrupole deformation β for ^{20}Ne in Fig. 2, where space truncations are set as $m_{\max} = 11/2$ and $K_{m_{\max}} = 3$, and filled circles denote local minima. For comparison, we employed RHF Lagrangians PKOi and the RMF Lagrangian DD-ME2 [114].

[Figure 2: see original paper] (Color online) Binding energy E_B (MeV) as a function of deformation β for ^{20}Ne. Results are calculated by PKOi and DD-ME2 with $m_{\max} = 11/2$ and $K_{m_{\max}} = 3$. Filled circles denote local minima.

For ^{20}Ne as shown in Fig. 2, RHF Lagrangians PKO1 and PKO3, which contain π-PV coupling, present rather similar results. In contrast, RHF Lagrangian PKO2 and RMF Lagrangian DD-ME2 give systematically less bound results. Referring to the experimental binding energy of ^{20}Ne, it can be seen that PKO1 and PKO3 show nice agreement, while results from PKO2 and DD-ME2 are less bound with deviations of   5 MeV. It should be mentioned that there exists some discrepancy between our results and those in Ref. [104] (Figs. 1 and 9 therein). For the RMF Lagrangian DD-ME2, our results coincide with calculations using the code developed from Ref. [65], while showing about 1.5 MeV less binding than the RHF Lagrangian in Ref. [104]. For PKO2, calculations in Ref. [104] (Fig. 1 therein) only present nearly converged results for ^{20}Ne, showing similar deviation from our calculations as DD-ME2. The possible reason might be that stronger pairing effects are obtained by the general Bogoliubov method [104] than by the BCS method [118].

Local minima extracted from Fig. 2 are summarized in Table V. Within the range $\beta \in (-1.0, 1.0)$, three local minima exist in PKO1 and PKO3 results: a stable and strongly deformed prolate, a soft oblate, and a high-lying largely deformed oblate. For the former two prolate and oblate shapes, PKO2 and DD-ME2 present rather similar deformations, while the largely deformed oblate is not supported.

From Table V and Fig. 2, selected effective Lagrangians give similar binding energies at oblate minima [$\beta \sim (-0.1, -0.2)$] of ^{20}Ne, particularly for RHF

Lagrangians PKOi. When approaching prolate minima—the ground state of ^{20}Ne—deviations between PKO2 and PKO1 (PKO3) become more notable. Eventually, PKO1 and PKO3, which contain π-PV coupling, show much better agreement with experimental binding energy data for ^{20}Ne [115].

To understand deviations between PKO2 and PKO1 (PKO3), we show evolution of neutron (left panel) and proton (right panel) single-particle energies with respect to quadrupole deformation $\beta \in [0, 0.6)$ in Fig. 3 [Figure 3: see original paper], where notation $\nu[m]^{\pi}$ is introduced to denote orbits. It can be seen that both neutron and proton single-particle energies show similar systematic evolutions with respect to β. Following shape evolution, both neutron and proton spherical shells $N/Z = 8$ are continuously reduced and eventually deformed shells $N/Z = 10$ emerge at large β values. In general, orbits branched from the same degenerate spherical orbit nlj ($j > 3/2$) deviate from each other with respect to deformation β. As seen from PKO2 results (dotted lines), orbits $2[1/2]^{+}$ and $1[1/2]^{-}$ with smallest m values, branched from spherical $1d_{5/2}$ and $1p_{3/2}$ states respectively, become more bound, while those $1[5/2]^{+}$ and $1[3/2]^{-}$ with largest m values become less bound, along shape evolution from spherical to prolate. This reflects typical deformation effects.

However, compared to results from PKO3 which contains π-PV coupling [78], the situation can be notably different. As shown in Fig. 3, PKO3 (solid lines) and PKO2 (dotted lines) present different systematics on shape evolution of valence orbits branched from degenerate spherical $1d_{5/2}$. To understand effects of π-PV coupling, Fig. 4 [Figure 4: see original paper] shows splittings between valence neutron orbits $2[1/2]^{+}$ and $1[3/2]^{+}$, namely $\Delta E = E_{1[3/2]^{+}} - E_{2[1/2]^{+}}$ (MeV), with respect to quadrupole deformation β, with the inset showing effective neutron pairing gap Δ_n (MeV) as functions of β. It can be seen that following shape evolution from spherical to prolate, PKO3 (solid line) presents notably larger splittings ΔE than PKO2 (dotted line), and enhancements from PKO2 to PKO3 are almost fully due to contributions from π-PV coupling (grid pattern).

[Figure 3: see original paper] (Color online) Evolution of neutron (left panel) and proton (right panel) single-particle energies given by PKO2 (dotted lines) and PKO3 (solid lines) for ^{20}Ne with respect to deformation $\beta \in [0, 0.6)$, where filled and open circles denote Fermi energies E_F given by PKO3 and PKO2, respectively.

[Figure 4: see original paper] (Color online) Splittings (MeV) between neutron valence orbits $2[1/2]^{+}$ and $1[3/2]^{+}$ given by PKO3 (solid line) and PKO2 (dotted line), namely $\Delta E = E_{1[3/2]^{+}} - E_{2[1/2]^{+}}$, with respect to deformation $\beta \in [0, 0.6)$ for ^{20}Ne, where the grid pattern denotes contributions from π-PV coupling in PKO3. The inset shows neutron pairing gaps Δ_n (MeV) as functions of β given by PKO3 and PKO2.

Qualitatively, such enhancement can be understood from the nature of the tensor force carried by π-PV coupling in PKO3 [78, 90], which leads to repulsive/attractive couplings between components with same/opposite signs [119]. As a supplement, we show in Fig. 5 [Figure 5: see original paper] proportions (in percentage) of main expansion components [see Eq. (29)] as functions of deformation β for neutron orbit $2[1/2]^+$, namely components $1d_{5/2}$ ($\kappa = -3$), $1d_{3/2}$ ($\kappa = 2$), and $2s_{1/2}$ ($\kappa = -1$). For both PKO2 (dotted lines) and PKO3 (solid lines), the negative component $1d_{5/2}$ dominates expansion of the Dirac spinor (more than 60%). In fact, for two other neutron orbits $1[3/2]^+$ and $1[5/2]^+$, which are not shown for simplicity, the negative component $1d_{5/2}$ plays a comprehensively dominant role (more than 90%). Similar situations are found for proton orbits.

If looking at core configurations of both neutron and proton ($N, Z = 8$), only one orbit $2[1/2]^-$ can be dominated by positive components $1p_{1/2}$ ($\kappa = 1$), while the other three ($1[1/2]^+$, $1[1/2]^-$, and $1[3/2]^-$) contain mainly negative components, indicating the core exhibits negative components overall. Thus, tensor force components carried by π-PV coupling in PKO3 present additional repulsive interactions between the core and valence orbits $2[1/2]^+$, $1[3/2]^+$, and $1[5/2]^+$.

However, for orbit $2[1/2]^+$, proportions of positive component $1d_{3/2}$ ($\kappa = 2$) are notable and are largely enhanced from PKO2 to PKO3 following shape evolution. In contrast to negative component $1d_{5/2}$, tensor couplings between positive component $1d_{3/2}$ and the core (which behaves like negative components) are attractive, tending to make ^{20}Ne more bound. Comparing to orbits $1[3/2]^+$ and $1[5/2]^+$, repulsive tensor couplings between orbit $2[1/2]^+$ and the core are notably reduced by enhanced proportions of positive component $1d_{3/2}$. This explains well the enhanced splittings ΔE from PKO2 to PKO3 in Fig. 4, as well as the more bound ground state given by PKO3 than PKO2 in Fig. 2.

On the other hand, via π-PV coupling, the core of ^{20}Ne can also be polarized differently by valence nucleons in PKO2 and PKO3 calculations, manifested as notably different compositions of valence orbit $2[1/2]^+$ in Fig. 5 [Figure 5: see original paper]. It is thus expected that mean fields described by PKO2 and PKO3 can be notably different. As direct evidence, not only do PKO2 and PKO3 present different compositions of valence orbit $2[1/2]^+$, they also give distinctively different systematics on shape evolutions of orbits $1[3/2]^+$ and $1[5/2]^+$ (see Fig. 3). Coincidentally, some similarity can be found between shape evolutions of orbits $1[3/2]^+$ and $1[5/2]^+$ and those of $2s_{1/2}$ and $1d_{3/2}$ proportions for orbit $2[1/2]^+$ (see Figs. 3 and 5). To some extent, such similarity might illustrate the consistent relation between systematics of orbits $1[3/2]^+$ and $1[5/2]^+$ and core polarization by valence nucleons occupying orbit $2[1/2]^+$. It should be noted that shape evolution of orbits $1[3/2]^+$ and $1[5/2]^+$ cannot be attributed directly to the role of tensor force, since both orbits are similarly dominated by negative component $1d_{5/2}$. Moreover, pairing correlations may not play a substantial role in interpreting systematic differences between PKO2 and PKO3, since both show similar pairing effects, as seen in the inset of Fig. 4.

IV. Summary

In this paper, the axially deformed relativistic Hartree-Fock (RHF) model is established by utilizing the spherical Dirac Woods-Saxon (DWS) basis that can properly describe asymptotic behaviors of wave functions. The formalism of the axially deformed RHF model based on the spherical DWS basis is presented in detail, along with relevant space truncations. Taking light ^{20}Ne, medium-heavy ^{56}Fe, and heavy Pb isotopes as examples, the reliability of the expansions is illustrated, and the accuracy of the deformed RHF code is verified.

The axially deformed RHF model based on the spherical DWS basis is applied preliminarily to study structure properties of ^{20}Ne, a typically deformed nucleus, using RHF effective Lagrangians PKOi and RMF Lagrangian DD-ME2. It is found that RHF Lagrangians PKO1 and PKO3, which contain π-pseudovector coupling, improve the description of the binding energy of ^{20}Ne. Furthermore, discussions on systematics of shape evolution of single-particle energies indicate that the π-PV coupling, mainly the tensor force component, may have notable effects in determining nuclear shape evolution and core polarization. Thus, as perspectives, it is valuable to investigate effects of Fock terms, especially π-PV and -T couplings, in determining structure properties of deformed nuclei, which deserves further systematic investigation with existing RHF Lagrangians PKOi and PKA1.

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Appendix A: Energy Functionals and Self-Energies in Various Coupling Channels

1. Compounded Symbols

In energy functionals, it is more convenient to express expansion of coupling strengths as

$$g_\phi(\rho_b) = \sum_{\lambda_p} g^{\phi}_{\lambda_p}(r) Y_{\lambda_p 0}(\vartheta, \phi),$$

where g_ϕ corresponds to g_σ, g_ω, g_ρ, and f_π. In practice, we perform integrations with respect to angle variables $\Omega = (\vartheta, \phi)$ since wave function expansions $\psi_{\nu\pi m}$ are carried on the spherical DWS basis $\psi_{n\kappa m}$. Such integration contains harmonic functions from propagator expansions (30), coupling strength expansions (A1), and couplings between spherical spinors:

$$\int d\Omega Y_{\lambda_d\mu_d}(\Omega) Y_{\lambda_y -\mu_y}(\Omega) Y_{\lambda_p 0}(\Omega) = \sqrt{\frac{(2\lambda_d+1)(2\lambda_y+1)}{4\pi(2\lambda_p+1)}} C^{\lambda_p 0}_{\lambda_d 0 \lambda_y 0} C^{\lambda_p 0}_{\lambda_d \mu_d \lambda_y -\mu_y},$$

where $\mu = \mu_d = \mu_y$, and (λ_d, μ_d), (λ_y, μ_y), and λ_p denote terms from couplings between spinors, propagator expansions, and coupling strengths, respectively. As an abbreviation, we introduce symbol Θ to denote the above integration:

$$\Theta^{\lambda_d\lambda_p}_{\lambda_y\mu} \equiv (-1)^{\mu} \sqrt{\frac{(2\lambda_d+1)(2\lambda_y+1)}{4\pi(2\lambda_p+1)}} C^{\lambda_p 0}_{\lambda_d 0 \lambda_y 0} C^{\lambda_p 0}_{\lambda_d \mu \lambda_y -\mu}.$$

For couplings between spherical spinors, we introduce symbols D ($\bar{D}$) and Q ($\bar{Q}$) as

$$D^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda\mu} \equiv (-1)^{j_1-m_1} \hat{j}_1 \hat{j}_2 \hat{\lambda}^{-1} C^{\lambda\mu}_{j_1 -m_1 j_2 m_2},$$

$$\bar{D}^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda\bar{\mu}} = (-1)^{\kappa_1} D^{\kappa_1 -m_1;\kappa_2 m_2}_{\lambda\bar{\mu}},$$

$$Q^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda\mu\sigma} \equiv (-1)^{j_1+l_1-1/2} \sqrt{3} \hat{j}_1 \hat{j}_2 \sum_{l_1 l_2} C^{\lambda 0}_{l_1 0 l_2 0} C^{l_1 l_2 \lambda}_{j_1 j_2 J} C^{\lambda\mu}_{j_1 -m_1 j_2 m_2} C^{10}_{j_1 \sigma j_2 -\sigma},$$

$$\bar{Q}^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda\bar{\mu}\sigma} = (-1)^{\kappa_1} Q^{\kappa_1 -m_1;\kappa_2 m_2}_{\lambda\bar{\mu}\sigma}.$$

In symbols D and $\bar{D}$, $\mu = m_2 - m_1$ and $\bar{\mu} = m_2 + m_1$, while for Q and $\bar{Q}$, $\mu + \sigma = m_2 - m_1$ and $\bar{\mu} + \sigma = m_2 + m_1$. With these symbols, couplings of spherical spinors can be simply expressed as

$$\Omega^{\dagger}_{\kappa_1 m_1}\Omega_{\kappa_2 m_2} = (-1)^{m_1+1/2}\sum_{\lambda_d\mu_d} D^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda_d\mu_d} Y_{\lambda_d\mu_d},$$

$$\Omega^{\dagger}_{\kappa_1 m_1}\sigma\cdot\mathbf{e}_{\sigma}\Omega_{\kappa_2 m_2} = (-1)^{m_1-1/2}\sum_{\lambda_d\mu_d} Q^{\kappa_1 m_1;\kappa_2 m_2}_{\lambda_d\mu_d\sigma} Y_{\lambda_d\mu_d} e_{\sigma},$$

where $\mathbf{e}_{\sigma}$ is the covariant spherical basis vector with $\sigma = -1, 0, +1$. Note that quantity κ denotes the combination of quantum numbers (j, l).

2. Energy Functionals and Self-Energies from Hartree Terms

For σ-S coupling and time component of ω-V coupling, self-energies from Hartree terms can be expressed as

$$\Sigma^{S,\sigma}_{\lambda_d}(r) = -2\pi\sum_{\lambda'_d}\int r'^2 dr' R^{\lambda_d}_{\sigma}(r,r')\sum_{\lambda_p} g^{\sigma}_{\lambda_p}(r')\rho^{s}_{\lambda'_d}(r'),$$

$$\Sigma^{0,\omega}_{\lambda_d}(r) = +2\pi\sum_{\lambda'_d}\int r'^2 dr' R^{\lambda_d}_{\omega}(r,r')\sum_{\lambda_p} g^{\omega}_{\lambda_p}(r')\rho^{b}_{\lambda'_d}(r').$$

Thus, relevant energy functionals read as

$$E^{D}_{\sigma\text{-S}} = +\int r^2 dr\sum_{\lambda_d}\rho^{s}_{\lambda_d}(r)\Sigma^{S,\sigma}_{\lambda_d}(r),$$

$$E^{D}_{\omega\text{-V}} = +\int r^2 dr\sum_{\lambda_d}\rho^{b}_{\lambda_d}(r)\Sigma^{0,\omega}_{\lambda_d}(r).$$

For time component of -V coupling, these expressions can be obtained by replacing $g^{\omega}_{\lambda_p}$ with $g^{\rho}_{\lambda_p}$ and $\rho^{b}_{\lambda_d}$ with $\rho^{b,n}_{\lambda_d} - \rho^{b,p}_{\lambda_d}$. For Coulomb field (A-V coupling), these expressions can be derived by setting $\lambda_p = 0$ and replacing nucleon density ρ_b with proton density ρ_p. For space components of vector couplings, as well as π-PV couplings, contributions are zero.

Since coupling strengths g_{σ}, g_{ω}, and g_{ρ} are density-dependent, variations of energy functionals (A10) may lead to additional rearrangement terms:

$$\Sigma^{R,\sigma}_{D,\lambda_d}(r) = -2\pi\sum_{\lambda'_d}\int r'^2 dr' R^{\lambda_d}_{\sigma}(r,r')\sum_{\lambda_p}\frac{\partial g^{\sigma}_{\lambda_p}}{\partial\rho^{b}_{\lambda'_d}}\rho^{s}_{\lambda'_d}(r'),$$

$$\Sigma_{D,\lambda_d}^{R,\omega}(r) = +2\pi \sum_{\lambda'_d} \int r'^2 dr' R_\omega^{\lambda_d}(r,r') \sum_{\lambda_p} \frac{\partial g_{\lambda_p}^\omega}{\partial \rho_{\lambda'_d}^b} \rho_{\lambda'_d}^b(r').$$

3. Energy Functionals and Self-Energies from Fock Terms

Fock term expressions are much more complicated than Hartree terms. Note that in deriving both Hartree and Fock terms, we set angular momentum projection m to be positive for convenience. Thus, we need to revise expansion of spinor $\psi_{\nu\pi m}$. In principle, one can set the time-conjugation partner as $\psi_{\nu\pi -m} \equiv \hat{P}_t \psi_{\nu\pi m}$, with $\hat{P}_t$ being the time-reversal operator, and expansion of $\psi_{\nu\pi -m}$ reads as

$$\psi_{\nu\pi -m} = \sum_\kappa (-1)^{j+l_u-m} \psi_{\nu\kappa -m},$$

where by definition $\psi_{\nu\kappa m}$ and $\psi_{\nu\kappa -m}$ share radial components G_i^κ and F_i^κ. For Hartree terms, this does not bring additional complexity, while for Fock terms one must carefully treat couplings between orbits m and $-m'$ $(m, m' > 0)$. It can be found that partner $(-m, -m')$ gives identical contributions to (m, m'), and partners $(m, -m')$ and $(-m, m')$ provide identical contributions.

To express Fock term contributions compactly, we introduce symbol $\tilde{D}$ for σ-S coupling and time components of vector couplings:

$$\tilde{D}_{\lambda_p\lambda'}^{\kappa_1\kappa_2 m;\kappa'_1\kappa'_2 m'} = \sum_{\lambda_d\lambda'_d} \left[D_{\lambda_d\mu}^{\kappa_1 m;\kappa'_1 m'} D_{\lambda'_d\mu}^{\kappa'_2 m';\kappa_2 m} \Theta_{\lambda_y\mu}^{\lambda_d\lambda_p} + \bar{D}_{\lambda_d\bar{\mu}}^{\kappa_1 m;\kappa'_1 m'} \bar{D}_{\lambda'_d\bar{\mu}}^{\kappa'_2 m';\kappa_2 m} \Theta_{\lambda_y\bar{\mu}}^{\lambda_d\lambda_p} \right],$$

with similar definitions for other sign combinations (++), (+-), (-+), and (–). Thus, nonlocal self-energies of σ-S coupling can be expressed as

$$Y_G^{\kappa_1,\kappa_2;\sigma} = + \sum_{\pi' m'} \delta_{\tau\tau'} \sum_{\kappa'_1\kappa'_2} R_{\kappa'_1\kappa'_2,\pi' m'}^G(r,r') \sum_{\lambda_p\lambda'} g_{\lambda_p}^\sigma(r) g_{\lambda'}^\sigma(r') \tilde{D}_{\lambda_p\lambda'}^{\kappa_1\kappa_2 m;\kappa'_1\kappa'_2 m'},$$

$$Y_F^{\kappa_1,\kappa_2;\sigma} = - \sum_{\pi' m'} \delta_{\tau\tau'} \sum_{\kappa'_1\kappa'_2} R_{\kappa'_1\kappa'_2,\pi' m'}^F(r,r') \sum_{\lambda_p\lambda'} g_{\lambda_p}^\sigma(r) g_{\lambda'}^\sigma(r') \tilde{D}_{\lambda_p\lambda'}^{\kappa_1\kappa_2 m;\kappa'_1\kappa'_2 m'},$$

$$X_G^{\kappa_1,\kappa_2;\sigma} = - \sum_{\pi' m'} \delta_{\tau\tau'} \sum_{\kappa'_1\kappa'_2} R_{\kappa'_1\kappa'_2,\pi' m'}^G(r,r') \sum_{\lambda_p\lambda'} g_{\lambda_p}^\sigma(r) g_{\lambda'}^\sigma(r') \tilde{D}_{\lambda_p\lambda'}^{\kappa_1\kappa_2 m;\kappa'_1\kappa'_2 m'},$$

$$X_F^{\kappa_1,\kappa_2;\sigma} = +\sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^F_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^\sigma_{\lambda_p}(r) g^\sigma_{\lambda'}(r') \tilde{D}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'},$$

where the sum over ν' has been absorbed into nonlocal densities R, and factor $\delta_{\tau\tau'}$ indicates that orbits πm and $\pi' m'$ should be both neutron or proton. In terms of nonlocal self-energies, the energy functional of σ-S coupling reads as

$$E^E_{\sigma\text{-S}} = \int dr\, dr' \sum_{\kappa_1\kappa_2} \begin{pmatrix} G_i^{\kappa_1} & F_i^{\kappa_1} \end{pmatrix} \begin{pmatrix} Y_G^{\kappa_1,\kappa_2;\sigma} & Y_F^{\kappa_1,\kappa_2;\sigma} \\ X_G^{\kappa_1,\kappa_2;\sigma} & X_F^{\kappa_1,\kappa_2;\sigma} \end{pmatrix}_{\pi m} \begin{pmatrix} G_i^{\kappa_2} \\ F_i^{\kappa_2} \end{pmatrix}_{r'}.$$

For rearrangement terms, contributions to self-energy $\Sigma^0_{\lambda_d}$ can be similarly expressed as

$$\Sigma^{R,\sigma}_{E,\lambda_d} = \int dr' \sum_{\kappa_1\kappa_2} \begin{pmatrix} G_i^{\kappa_1} & F_i^{\kappa_1} \end{pmatrix} \begin{pmatrix} P_G^{\kappa_1,\kappa_2;\sigma} & Q_G^{\kappa_1,\kappa_2;\sigma} \\ P_F^{\kappa_1,\kappa_2;\sigma} & Q_F^{\kappa_1,\kappa_2;\sigma} \end{pmatrix}_{\pi m,\lambda_d} \begin{pmatrix} G_i^{\kappa_2} \\ F_i^{\kappa_2} \end{pmatrix}_{r'},$$

where terms P and Q read as

$$P_G^{\kappa_1,\kappa_2;\sigma} = \sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^G_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^\sigma_{\lambda_p}(r) \frac{\partial g^\sigma_{\lambda'}}{\partial \rho^b_{\lambda_d}}(r') \tilde{D}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'},$$

with similar expressions for other components. For time components of vector couplings, similar expressions are obtained by replacing propagator expansion terms R_σ with corresponding ones, and plus signs in Y_G, X_F, P_G, and Q_F terms should be changed to minus. Note that for isovector -V coupling, factor $\delta_{\tau\tau'}$ is replaced by $(2-\delta_{\tau\tau'})$. For Coulomb interaction, there is no rearrangement term and only $\lambda_p = \lambda' = 0$ terms remain for nonlocal self-energies [see Eqs. (A18)].

For space components of vector couplings, we take ω-V coupling as an example, with others deduced similarly. To write expressions compactly, we introduce symbols $\tilde{B}$:

$$\tilde{B}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'} \equiv \sum_{\lambda_d\lambda_d'} \left[Q^{\kappa_1' m',\kappa_1 m}_{\lambda_d\mu\sigma} Q^{\kappa_2' m',\kappa_2 m}_{\lambda_d'\mu\sigma} \Theta^{\lambda_d\lambda_p}_{\lambda_y\mu} + \bar{Q}^{\kappa_1' m',\kappa_1 m}_{\lambda_d\bar{\mu}\sigma} \bar{Q}^{\kappa_2' m',\kappa_2 m}_{\lambda_d'\bar{\mu}\sigma} \Theta^{\lambda_d\lambda_p}_{\lambda_y\bar{\mu}} \right],$$

with similar definitions for other sign combinations. Thus, nonlocal self-energies can be expressed as

$$Y_G^{\kappa_1,\kappa_2;\omega} = +\sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^G_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^\omega_{\lambda_p}(r) g^\omega_{\lambda'}(r') \tilde{B}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'},$$

$$Y_F^{\kappa_1,\kappa_2;\boldsymbol{\omega}} = -\sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^F_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^{\omega}_{\lambda_p}(r) g^{\omega}_{\lambda'}(r') \tilde{B}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'},$$

$$X_G^{\kappa_1,\kappa_2;\boldsymbol{\omega}} = -\sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^G_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^{\omega}_{\lambda_p}(r) g^{\omega}_{\lambda'}(r') \tilde{B}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'},$$

$$X_F^{\kappa_1,\kappa_2;\boldsymbol{\omega}} = +\sum_{\pi'm'} \delta_{\tau\tau'} \sum_{\kappa_1'\kappa_2'} R^F_{\kappa_1'\kappa_2',\pi'm'}(r,r') \sum_{\lambda_p\lambda'} g^{\omega}_{\lambda_p}(r) g^{\omega}_{\lambda'}(r') \tilde{B}^{\kappa_1\kappa_2 m;\kappa_1'\kappa_2' m'}_{\lambda_p\lambda'}.$$

Here, bold type $\boldsymbol{\omega}$ represents the space component. In terms of these nonlocal self-energies, the energy functional from the space component of ω-V coupling reads as

$$E^{E,\text{space}}_{\omega\text{-V}} = \int dr\, dr' \sum_{\kappa_1\kappa_2} \begin{pmatrix} G_i^{\kappa_1} & F_i^{\kappa_1} \end{pmatrix} \begin{pmatrix} Y_G^{\kappa_1,\kappa_2;\boldsymbol{\omega}} & Y_F^{\kappa_1,\kappa_2;\boldsymbol{\omega}} \\ X_G^{\kappa_1,\kappa_2;\boldsymbol{\omega}} & X_F^{\kappa_1,\kappa_2;\boldsymbol{\omega}} \end{pmatrix}_{\pi m} \begin{pmatrix} G_i^{\kappa_2} \\ F_i^{\kappa_2} \end{pmatrix}_{r'}.$$

For rearrangement terms, contributions to self-energy can be similarly expressed as

$$\Sigma^{R,\omega}_{E,\lambda_d} = \int dr' \sum_{\kappa_1\kappa_2} \begin{pmatrix} G_i^{\kappa_1} & F_i^{\kappa_1} \end{pmatrix} \begin{pmatrix} P_G^{\kappa_1,\kappa_2;\omega} & Q_G^{\kappa_1,\kappa_2;\omega} \\ P_F^{\kappa_1,\kappa_2;\omega} & Q_F^{\kappa_1,\kappa_2;\omega} \end{pmatrix}_{\pi m,\lambda_d} \begin{pmatrix} G_i^{\kappa_2} \\ F_i^{\kappa_2} \end{pmatrix}_{r'},$$

where P and Q terms are analogous to those for σ-S coupling but with ω couplings and $\tilde{B}$ symbols. For other vector couplings, expressions are obtained by replacing propagator and coupling strength terms with relevant ones. For isovector -V coupling, replace isospin factor $\delta_{\tau\tau'}$ with $(2-\delta_{\tau\tau'})$, and for Coulomb interaction only $\lambda_p = \lambda' = 0$ terms remain.

For π-PV coupling, the situation becomes more complicated due to gradient operations on the propagator, which can be expressed as

$$\nabla_r \nabla_{r'} D_\pi(r,r') = m_\pi^2 \sum_{\lambda_y\lambda_y'} \sum_{\mu_y\sigma_y} C^{\lambda_y'0}_{\lambda_y 0 L 0 1} C^{\lambda_y'\mu_y}_{\lambda_y\mu_y 1\sigma_y} Y_{\lambda_y\mu_y}(\vartheta,\phi)\mathbf{e}_{\sigma_y} \sum_{\mu_y'\sigma_y'} (-1)^{\mu_y'} C^{L0}_{\lambda_y'-\mu_y' 1\sigma_y'} Y_{\lambda_y'-\mu_y'}(\vartheta',\phi')\mathbf{e}_{-\sigma_y'} V_{\lambda_y\lambda_y'}(m$$

where radial terms read as

$$V_{\lambda_y\lambda_y'}(m_\pi;r,r') \equiv -R_{\lambda_y\lambda_y'}(m_\pi;r,r') + \frac{\pi}{r^2}\delta(r-r').$$

To obtain compact expressions, we introduce symbols P and $\bar{P}$:

$$P^{\kappa_1' m', \kappa_1 m}_{\lambda_p, L\lambda_y; \mu\sigma} \equiv \sum_{\lambda_d \mu_d} C^{\lambda_d 0}_{\lambda_y 0 L 0 1} C^{\lambda_d \mu_d}_{\lambda_y \mu 1 \sigma} Q^{\kappa_1' m', \kappa_1 m}_{\lambda_d \mu_d \sigma} \Theta^{\lambda_d \lambda_p}_{\lambda_y \mu},$$

$$\bar{P}^{\kappa_1' m', \kappa_1 m}_{\lambda_p, L\lambda_y; \bar{\mu}\sigma} \equiv \sum_{\lambda_d \mu_d} C^{\lambda_d 0}_{\lambda_y 0 L 0 1} C^{\lambda_d \mu_d}_{\lambda_y \bar{\mu} 1 \sigma} \bar{Q}^{\kappa_1' m', \kappa_1 m}_{\lambda_d \mu_d \sigma} \Theta^{\lambda_d \lambda_p}_{\lambda_y \bar{\mu}},$$

and further symbols $\tilde{A}$ for combinations of P and $\bar{P}$:

$$\tilde{A}^{\kappa_1 \kappa_2 m; \kappa_1' \kappa_2' m'}_{\lambda_p \lambda'} \equiv \sum_{\sigma\sigma'} \left[P^{\kappa_1' m', \kappa_1 m}_{\lambda_p, L\lambda_y; \mu\sigma} P^{\kappa_2' m', \kappa_2 m}_{\lambda', L\lambda_y'; \mu'\sigma'} + \bar{P}^{\kappa_1' m', \kappa_1 m}_{\lambda_p, L\lambda_y; \bar{\mu}\sigma} \bar{P}^{\kappa_2' m', \kappa_2 m}_{\lambda', L\lambda_y'; \bar{\mu}'\sigma'} \right],$$

with $\mu + \sigma = \mu' + \sigma' = m - m'$ and $\bar{\mu} + \sigma = \bar{\mu}' + \sigma' = m + m'$. With these definitions, self-energies from π-PV coupling can be expressed as

$$Y^{\kappa_1, \kappa_2; \pi}_G = \sum_{\pi' m'} (2 - \delta_{\tau\tau'}) \sum_{\kappa_1' \kappa_2'} R^G_{\kappa_1' \kappa_2', \pi' m'}(r, r') \sum_{\lambda_p \lambda'} f^\pi_{\lambda_p}(r) f^\pi_{\lambda'}(r') \sum_{\lambda_y \lambda_y'} V_{\lambda_y \lambda_y'}(m_\pi; r, r') \tilde{A}^{\kappa_1 \kappa_2 m; \kappa_1' \kappa_2' m'}_{\lambda_p \lambda'},$$

with similar expressions for other components. The energy functional from π-PV coupling reads as

$$E^E_{\pi\text{-PV}} = \int dr\, dr' \sum_{\kappa_1 \kappa_2} \begin{pmatrix} G^{\kappa_1}_i & F^{\kappa_1}_i \end{pmatrix} \begin{pmatrix} Y^{\kappa_1, \kappa_2; \pi}_G & Y^{\kappa_1, \kappa_2; \pi}_F \\ X^{\kappa_1, \kappa_2; \pi}_G & X^{\kappa_1, \kappa_2; \pi}_F \end{pmatrix}_{\pi m} \begin{pmatrix} G^{\kappa_2}_i \\ F^{\kappa_2}_i \end{pmatrix}_{r'}.$$

Similarly, rearrangement term $\Sigma^{R,\pi}_{E,\lambda_d}$ can be expressed as

$$\Sigma^{R,\pi}_{E,\lambda_d} = \int dr' \sum_{\kappa_1 \kappa_2} \begin{pmatrix} G^{\kappa_1}_i & F^{\kappa_1}_i \end{pmatrix} \begin{pmatrix} P^{\kappa_1, \kappa_2; \pi}_G & Q^{\kappa_1, \kappa_2; \pi}_G \\ P^{\kappa_1, \kappa_2; \pi}_F & Q^{\kappa_1, \kappa_2; \pi}_F \end{pmatrix}_{\pi m, \lambda_d} \begin{pmatrix} G^{\kappa_2}_i \\ F^{\kappa_2}_i \end{pmatrix}_{r'},$$

where P and Q terms involve $\partial f^\pi_{\lambda_p} / \partial \rho^b_{\lambda_d}$.

Besides, a contact term is introduced to compensate the zero-range term in $V^\pi_{\lambda_y \lambda_y'}$ [see Eq. (A37)]. Hartree contributions from the contact term are zero, and Fock contributions read as

$$E^\delta_{\pi\text{-PV}} = -\sum_{ii'} (2 - \delta_{\tau_i \tau_{i'}}) \int dr\, dr' \left[f_\pi \bar{\psi}_{\nu\pi m} \gamma_5 \gamma^\mu \partial_\mu \psi_{\nu'\pi' m'} \right] \left[f_\pi \bar{\psi}_{\nu'\pi' m'} \gamma_5 \gamma^\nu \partial_\nu \psi_{\nu\pi m} \right]_{r'} \delta(r - r'),$$

where the δ function can be decomposed as

$$\delta(r-r') = \frac{\delta(r-r')}{r^2}\sum_{LM}(-1)^M Y_{LM}(\vartheta,\phi)Y_{L-M}(\vartheta',\phi').$$

To express the contact term compactly, we introduce symbols $\tilde{B}$ analogous to those for space components but with L replacing λ_y and using Q symbols directly. The energy functional of the contact term can be expressed as

$$E^{\delta}_{\pi\text{-PV}} = \int dr \sum_{\kappa_1\kappa_2} \begin{pmatrix} G_i^{\kappa_1} & F_i^{\kappa_1} \end{pmatrix} \begin{pmatrix} Y_G^{\kappa_1,\kappa_2;\pi\delta} & Y_F^{\kappa_1,\kappa_2;\pi\delta} \\ X_G^{\kappa_1,\kappa_2;\pi\delta} & X_F^{\kappa_1,\kappa_2;\pi\delta} \end{pmatrix}_{\pi m} \begin{pmatrix} G_i^{\kappa_2} \\ F_i^{\kappa_2} \end{pmatrix}_r,$$

where self-energies involve $f_\pi^2(r)$ and $\tilde{B}$ symbols evaluated at $r' = r$. The rearrangement term in the self-energy can be derived similarly with $\partial f^{\pi}_{\lambda_p}/\partial\rho^{b}_{\lambda_d}$.

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

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