Spin symmetry in Dirac negative energy spectrum in density-dependent relativistic Hartree-Fock theory

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Abstract

The spin symmetry in the Dirac negative energy spectrum and its origin are investigated for the first time within the density-dependent relativistic Hartree-Fock (DDRHF) theory. Taking the nucleus 16O as an example, the spin symmetry in the negative energy spectrum is found to be a good approximation and the dominant components of the Dirac wave functions for the spin doublets are nearly identical. In comparison with the relativistic Hartree approximation where the origin of spin symmetry lies in the equality of the scalar and vector potentials, in DDRHF the cancellation between the Hartree and Fock terms is responsible for the better spin symmetry properties and determines the subtle spin-orbit splitting. These conclusions hold even in the case when significant deviations from the G-parity values of the meson-antinucleon couplings occur.

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I. INTRODUCTION

The relativistic Hartree approximation or relativistic mean field (RMF) theory \[1\] has received much attention due to its successful description of infinite nuclear matter as well as finite nuclei near and far away from the $\beta$ stability line \[2-4\]. One of its great success is the natural description of the nuclear spin-orbit potential, which leads to a remarkable spin-orbit splitting for the states with the same orbital angular momentum and opposite spins ($j = l \pm 1/2$), allowing for the understanding of the magic numbers and forming the basis of nuclear shell structure. Furthermore, the pseudo-spin symmetry \[5, 6\], i.e., the near degeneracy between two single-particle states with the quantum numbers ($n, l, j = l + 1/2$) and ($n - 1, l + 2, j = l + 3/2$), whose origin was a long mystery in nuclear physics \[7, 8\], is well interpreted within the relativistic scheme with local potentials (see Ref. \[9\] and references therein). The conservation and realization of pseudo-spin symmetry were discussed in detail within the RMF framework \[10-14\]. With the same origin, the spin symmetry in the Dirac negative energy spectrum (i.e., the single anti-nucleon spectrum) was proposed and investigated in RMF theory \[15, 16\].

As the Fock terms are missing and the one-pion exchange potential is not explicitly included in RMF, for the completeness of the theory, there have been attempts to include the Fock terms in the ground-state energy of nuclear systems over the past two decades \[17-20\]. Recently, the RHF theory with density-dependent nucleon-meson couplings (DDRHF) finally succeeded in the quantitative description of the ground-state properties of many nuclear systems on the same level as RMF \[21\]. Furthermore, it is found that the DDRHF theory can improve the descriptions of the nucleon effective mass and its isospin and energy dependences \[21\], as well as the shell evolution and closure with the inclusion of the one-pion exchange and $\rho$-tensor correlations \[22, 23\]. The pseudo-spin symmetry and its origin as well as the importance of the Fock terms have also been investigated before \[24, 25\]. Although the pseudo-spin symmetry is still found to be a good approximation in RHF, its mechanism becomes rather complicated by the presence of the non-local potentials.

In this paper, the Dirac negative energy spectrum or the single anti-nucleon spectrum in atomic nucleus such as $^{16}$O will be investigated within the DDRHF theory in order to understand the relativistic symmetry with non-local potentials. The corresponding spin symmetry and its origin will be examined, in particular the role of the Fock terms.
II. THEORETICAL FRAMEWORK

The starting point of the DDRHF theory is an effective Lagrangian density $\mathcal{L}$, which contains the degrees of freedom associated with the nucleon field ($\psi$), two isoscalar meson fields ($\sigma$ and $\omega$), two isovector meson fields ($\pi$ and $\rho$) and the photon field ($A$). Then the effective Hamiltonian $H$ is obtained with the general Legendre transformation. On the level of the mean field approximation, the energy functional $E$ is obtained by taking the expectation of the Hamiltonian $H$, where both the Hartree (direct) and Fock (exchange) terms are kept. Finally, the Dirac equations, i.e. the equations of motion of nucleons, are obtained via the variation of the energy functional $E$.

For spherical nuclei, the nucleon Dirac spinor can be written as,

$$f_\alpha(r) = \frac{1}{r} \begin{pmatrix} iG_{na}(r) & \mathcal{Y}_{ja}^a(\hat{r}) \\ -F_{na}(r) & \tilde{\mathcal{Y}}_{ja}^a(\hat{r}) \end{pmatrix} \chi_{\frac{1}{2}}(\tau_a),$$

where $\chi_{\frac{1}{2}}(\tau_a)$ is the isospinor, $\mathcal{Y}_{ja}^a$ is the spherical harmonics spinor and $\tilde{\mathcal{Y}}_{ja}^a(\hat{r}) = -\hat{\sigma} \cdot \hat{r} \mathcal{Y}_{ja}^a(\hat{r})$ with $\tilde{l}_a = 2j_a - l_a$. For the negative energy states, the lower component $F(r)$ is dominant. The states are labelled by $\{\tilde{n},\tilde{l},j\}$ with the relation

$$n = \tilde{n}, \text{ for } \kappa > 0, \quad n = \tilde{n} + 1, \text{ for } \kappa < 0,$$

in analogy to Ref. [26]. The spin symmetry concerns the near degeneracy of the states $(\tilde{n},\tilde{l},j = \tilde{l} \pm 1/2)$. In the following equations, the sub-index will be omitted for simplicity.

The radial Dirac equations are the coupled integro-differential ones due to the non-local Fock terms $X$ and $Y$,

$$EG(r) = -\left[\frac{d}{dr} - \frac{\kappa}{r}\right] F(r) + [M + \Sigma_S(r) + \Sigma_0(r)] G(r) + Y(r), \quad (3a)$$

$$EF(r) = +\left[\frac{d}{dr} + \frac{\kappa}{r}\right] G(r) - [M + \Sigma_S(r) - \Sigma_0(r)] F(r) + X(r). \quad (3b)$$

Introducing the effective local potentials $X_G, X_F, Y_G$ and $Y_F$ by the definitions,

$$X(r) = \frac{G(r)X(r)}{G^2 + F^2} G(r) + \frac{F(r)X(r)}{G^2 + F^2} F(r) \equiv X_G(r)G(r) + X_F(r)F(r), \quad (4a)$$

$$Y(r) = \frac{G(r)Y(r)}{G^2 + F^2} G(r) + \frac{F(r)Y(r)}{G^2 + F^2} F(r) \equiv Y_G(r)G(r) + Y_F(r)F(r), \quad (4b)$$


the integro-differential equations Eq. (3) can be formally rewritten as equivalent differential ones,

\[
\begin{align*}
\left[ \frac{d}{dr} - \frac{\kappa}{r} - Y_F(r) \right] F(r) - [V_+(r) - E] G(r) &= 0, \quad (5a) \\
\left[ \frac{d}{dr} + \frac{\kappa}{r} + X_G(r) \right] G(r) + [V_-(r) - E] F(r) &= 0, \quad (5b)
\end{align*}
\]

where \( V_+ \equiv V_+^D + Y_G, \ V_- \equiv V^D + X_F, \) and

\[
\begin{align*}
V_+^D &\equiv M + \Sigma_S + \Sigma_0, \quad V^D \equiv \Sigma_0 - \Sigma_S - M. \quad (6)
\end{align*}
\]

In the above expressions, \( \Sigma_S \) represents the scalar potential from the Hartree terms, \( \Sigma_0 \) is the time component of the vector potential, which contains the contributions from the Hartree terms and the rearrangement terms induced by the density-dependence of the meson-nucleon couplings \cite{21}, and \( X_G, X_F, Y_G, Y_F \) are the effective local potentials from the Fock terms. The equations Eq. (5) then can be solved self-consistently with the same numerical method as in RMF \cite{27}.

From the radial Dirac equation Eq. (5), the Schrödinger-type equation for the dominant component \( F(r) \) can be obtained as,

\[
\frac{1}{V_+ - E} \left\{ F'' + (V_1^D + V_1^E) F' + [V_{\text{CB}} + V_{\text{SOP}}^D + V_{\text{SOP}}^E] F \right\} + V^D F + V^E F = EF, \quad (7)
\]

where \( V_{\text{CB}} = \frac{\kappa(1-\kappa)}{r} \) and \( V_{\text{SOP}} \) correspond to the centrifugal barrier (CB) and spin-orbit potential (SOP), respectively. In the above equation, the Hartree and Fock terms for \( V_1, V_{\text{SOP}} \) and \( V \) read as

\[
\begin{align*}
V_1^D &= - \frac{V_+^D}{V_+ - E}, \quad V_1^E = X_G - Y_F - \frac{Y_F'}{V_+ - E}, \quad (8a) \\
V_{\text{SOP}}^D &= \frac{\kappa}{r} \frac{V_+^D}{V_+ - E}, \quad V_{\text{SOP}}^E = \frac{\kappa}{r} \left( \frac{Y_F'}{V_+ - E} - X_G - Y_F \right), \quad (8b) \\
V^D &= \Sigma_0 - \Sigma_S - M, \quad V^E = X_F + \frac{1}{V_+ - E} \left( Y_F \frac{V_+'}{V_+ - E} - Y_F' - X_G Y_F \right). \quad (8c)
\end{align*}
\]

One may note that the denominator \( V_+ - E \) contains a state dependent potential \( Y_G \). However, as the quantity \( Y_G \) is around a few MeV and is negligible in comparison with \( V_+ - E \) which is of the order of 1 GeV, the Eq. (7) is accurate enough to estimate the Hartree and Fock contributions. Similar argument also holds for the time component of the vector potential \( \Sigma_0 \) which contains the rearrangement term from Fock channels.
III. RESULTS AND DISCUSSION

Solving the DDRHF equations Eq. (5) with the parameter set PKO1 in coordinate space self-consistently as in RMF, the neutron and proton single-particle energies can be obtained. We take the nucleus $^{16}$O as an example to examine the negative energy spectrum and its spin symmetry.

![FIG. 1: (color online) Single neutron spectrum in the Dirac sea for $^{16}$O calculated by DDRHF with PKO1. The dash-dot line represents the Hartree potential $V^D$. For each pair of the spin doublets, the left levels are those with $j = \tilde{l} - 1/2$ and the right ones with $j = \tilde{l} + 1/2$.](image)

In Fig. 1 all the bound single neutron states in the Dirac sea for $^{16}$O are given. The dash-dot line represents the corresponding Hartree potential $V^D$ which is not strong enough for the $0s$ and $0p$ orbits, the importance and contribution of the Fock terms is thus illustrated. For each pair of the spin doublets, the left levels are those with $j = \tilde{l} - 1/2$ and the right ones with $j = \tilde{l} + 1/2$. It can be clearly seen that the spin symmetry is well conserved in the Dirac sea.

Taking $p$ orbits with $n = 0, 1, 2, 3$ as examples, the Dirac wave functions of spin partners are shown in Fig. 2. The dominant components $F(r)$ for the spin doublets are almost identical, whereas the small components $G(r)$ show dramatic deviations from each other due to the node relation given in Eq. (2). The features of the spin partners for both the energies and wave functions are similar to those in RMF. In the following, the origin and mechanisms of the spin symmetry will be investigated in comparison with those in RMF.

The spin-orbit splittings $\Delta E_{ls} = E_{n\tilde{l}_{i+1/2}} - E_{n\tilde{l}_{i-1/2}}$ in the negative energy spectrum of $^{16}$O versus the average binding energies $E_{av} = (E_{n\tilde{l}_{i+1/2}} + E_{n\tilde{l}_{i-1/2}})/2$ are given in Fig. 3.
FIG. 2: (color online) Radial Dirac wave functions of the spin doublets $p$ orbits in the negative energy spectrum of $^{16}$O calculated by DDRHF with PKO1. Panels (a), (b), (c), and (d) are for $0p$, $1p$, $2p$, and $3p$ spin doublets, respectively.

FIG. 3: (color online) Spin-orbit splitting $\Delta E_{ls} = E_{nl\tilde{l}+1/2} - E_{nl\tilde{l}-1/2}$ in the negative energy spectrum of $^{16}$O versus the average binding energy $E_{av} = (E_{nl\tilde{l}+1/2} + E_{nl\tilde{l}-1/2})/2$ calculated by DDRHF with PKO1. The vertical dashed line shows the continuum limit.

Comparison with the RMF results (see Fig. 2 in Ref. [15]), the DDRHF results have the following characteristics: 1) the spin-orbit splittings are smaller; 2) the spin-orbit splittings fluctuate with $E_{av}$, in contrast with the monotonous decreasing in the RMF case, when approaching the continuum limit; 3) in RMF the spin-down state ($j = \tilde{l} - 1/2$) is always lower than its spin-up partner ($j = \tilde{l} + 1/2$), while in DDRHF this occurs only for the $p$ orbits and states near the continuum limit.

In order to understand the origin of the spin symmetry in DDRHF and the relative positions of the spin-up state and its spin-down partner, the effective potentials $V$ in Eq.
as well as the relations between the centrifugal barrier and the spin-orbit potential will be investigated.

The effective potentials \( V \) for \( p, d, f, \) and \( g \) states in the negative energy spectrum of \( ^{16}\text{O} \) calculated by DDRHF with PKO1 are shown in Fig. 4, together with the Hartree part \( V^D \) (dash-dotted line). As seen in the Schrödinger-type equation Eq. (7), the effective potential \( V \) is composed of two parts, \( V^D \) the Hartree potential from the direct terms, and \( V^E \) the equivalent local potential from the exchange terms. The state dependence of the effective potential \( V \) comes from the contribution of the exchange terms.

Corresponding to the nodes of the dominant component \( F(r) \), there exist fluctuations in the effective potentials \( V \), which is brought in by the localization of non-local terms \( X \) and \( Y \) in Eq. (4). In addition, the contributions of Fock terms to the effective potentials tend to be slightly weaker when \( E_{\text{av}} \) approaches the continuum limit, or for larger orbital angular momenta \( \tilde{l} \).

Comparing the left and right panels of Fig. 4 it is found that the effective potentials at \( r = 0 \) are different between the spin partner states. This is due to the different asymptotic behaviors of the radial Dirac wave functions for spin doublets at \( r = 0 \),

\[
\lim_{r \to 0} \frac{G(r)}{F(r)} \propto r, \quad \text{for} \quad \kappa > 0, \\
\lim_{r \to 0} \frac{F(r)}{G(r)} \propto r, \quad \text{for} \quad \kappa < 0.
\] (9)
Within the RMF framework, it has been pointed out that the strong centrifugal barrier and weak spin-orbit potential lead to the pseudo-spin symmetry in the single nucleon spectrum \[10\] and the spin symmetry in the single anti-nucleon spectrum \[15\].

\[\text{FIG. 5: (color online) Centrifugal barriers } V_{\text{CB}} \text{ and spin-orbit potentials } V_{\text{SOP}} \text{ multiplied by the factor } \frac{\mp F^2}{(V_+ - E)} \text{ for the spin doublets } (\nu 0p_{1/2}, \nu 0p_{3/2}) \text{ (left panel) and } (\nu 3p_{1/2}, \nu 3p_{3/2}) \text{ (right panel) in the negative energy spectrum of } ^{16}\text{O}. \text{ The insets show the Hartree contributions of the spin-orbit potentials.}\]

\[\text{In Fig. 5 are shown the centrifugal barriers } V_{\text{CB}} \text{ and the spin-orbital potentials } V_{\text{SOP}} \text{ multiplied by the factor } \frac{\mp F^2}{(V_+ - E)} \text{ for the spin doublets } 0p \text{ and } 3p, \text{ and their integrals over } r \text{ are respectively proportional to their contributions to the single-particle energy. It is clearly shown that the contribution of the centrifugal barriers } V_{\text{CB}} \text{ is much larger than that of the spin-orbital potentials } V_{\text{SOP}}. \text{ Therefore, it can be concluded that similar reasons as in RMF lead to the spin symmetry in the negative energy spectrum in DDRHF, and the spin-orbit splitting is due to the different spin-orbit potentials } V_{\text{SOP}} \text{ of the spin doublets.}\]

\[\text{In the insets of Fig. 5 are given the Hartree contributions to the spin-orbit potentials. It is found that the contributions from the Fock terms to } V_{\text{SOP}} \text{ are one order of magnitude larger than those from the Hartree terms. Therefore, the Fock terms must play important roles in the spin-orbit splitting of the spin doublets.}\]

\[\text{From Eq. (7), the contributions to the single-particle energies } E \text{ from different channels can be estimated quantitatively. For example, the CB contribution can be calculated by}\]

\[\frac{1}{F^2} \int_0^\infty \int_0^\infty V_{\text{CB}} \frac{F^2}{V_+ - E} dr dE. \quad (10)\]

\[\text{In Table II are shown the contributions to the single-particle energies and spin-orbit splittings}\]
for the spin doublets 0\(p\) and 3\(p\). It is confirmed that the energy contributions from \(V_{\text{CB}}\) are much larger than those from \(V_{\text{SOP}}\) and the contribution from the Fock terms \(V_{\text{E}}^{E}\) is dominant in \(V_{\text{SOP}}\).

**TABLE I:** The contributions from different channels (see Eq. (7)) to the single-particle energies \(E\) as well as the spin-orbit splittings \(\Delta E\) for the spin doublets \((\nu0p_{1/2}, \nu0p_{3/2})\) and \((\nu3p_{1/2}, \nu3p_{3/2})\) in the negative energy spectrum of \(^{16}\text{O}\). The results are calculated by DDRHF with PKO1 and all units are in MeV.

| state     | \(F''\) | \(V_{\text{CB}}\) | \(V_{\text{D}}\) | \(V_{\text{D}}^{D}\) | \(V_{\text{D}}^{E}\) | \(V_{\text{E}}^{E}\) | \(V_{\text{E}}^{E}\) | \(E\)   |
|-----------|---------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-------|
| \(\nu0p_{1/2}\) | -45.32  | -41.92 0.21    | -0.26           | -416.00         | 5.35            | 3.65            | 151.87          | -342.43 |
| \(\nu0p_{3/2}\) | -45.41  | -42.19 0.21    | 0.53            | -415.68         | 2.52            | 8.18            | 149.49          | -342.37 |
| \(\Delta E\) | -0.09   | -0.27 0.00     | 0.79            | 0.32            | -2.83           | 4.53            | -2.38           | 0.06   |
| \(\nu3p_{1/2}\) | -211.40 | -38.44 0.01    | -0.12           | -611.42         | 4.77            | 0.90            | 55.82           | -799.91 |
| \(\nu3p_{3/2}\) | -211.39 | -38.42 0.01    | 0.24            | -611.47         | 3.80            | 2.00            | 55.41           | -799.84 |
| \(\Delta E\) | 0.01    | 0.02 0.00      | 0.36            | -0.05           | -0.97           | 1.10            | -0.41           | 0.07   |

In Table I, it is found that the contributions from \(V_{\text{D}}^{D}\), \(V_{\text{E}}^{E}\), \(V_{\text{D}}^{E}\) and \(V_{\text{E}}^{E}\) to the spin-orbit splitting are substantial. However, their contributions are counteracted by one another to preserve the spin symmetry. This kind of sophisticated cancellation implies that a weaker spin-orbit potential \(V_{\text{SOP}}\) does not mean better conserved spin symmetry, as for 0\(p\) and 3\(p\) orbits.

To further confirm the role of the Fock terms, the contributions from the Hartree and Fock channels to the spin-orbit splittings in the negative energy spectrum of \(^{16}\text{O}\) versus the average energies of the spin doublets are shown in Fig. 6 where the Fock part includes the contributions from the terms \(V_{\text{I}}^{E}\), \(V_{\text{SOP}}^{E}\) and \(V_{\text{E}}^{E}\) and the rest is gathered into the Hartree part. It is found that the absolute contributions from both Hartree and Fock parts decrease monotonously with the average energy \(E_{\text{av}}\). The contributions from the Hartree terms have an energy dependence similar to those in RMF [15]. The contributions from Fock terms have an opposite tendency and cancel with the Hartree ones, thus leading to better spin symmetry. The competition between the Hartree and Fock terms will determine the sign of the spin-orbit splitting and this explains why the spin-orbit splittings in DDRHF fluctuate with \(E_{\text{av}}\) in Fig. 3 instead of monotonously decreasing as in the RMF case.
FIG. 6: (color online) Hartree and Fock contributions to spin-orbit splitting in the negative energy spectrum of $^{16}$O versus the average energy of the spin doublets. The vertical dashed line shows the continuum limit.

In order to get a deeper understanding of the cancellation and competition between the Hartree and Fock terms, we first separate the different meson contributions to single-particle energies. It is found that in both Hartree and Fock contributions, the isoscalar mesons, $\sigma$ and $\omega$, play dominant roles in the spin-orbit splitting, while the contributions from the $\rho$-,$\pi$-mesons, and the rearrangement terms are negligible. Then, to make the mathematical structure simple and clear, one could replace the finite range Yukawa propagators with a pure delta function $\delta(r_1 - r_2)$ for these two heavy isoscalar mesons, but keeping their Dirac scalar and vector couplings. In this simple picture, it is found that the direct term of the $\sigma$-meson makes the spin-orbit splitting positive, whereas that of the $\omega$-meson makes the splitting negative. Since the attractive $\sigma$ field is slightly stronger than the repulsive $\omega$ field in realistic nuclei, the net Hartree contribution to the splitting is positive, as shown in the upper part of Fig. 6. Meanwhile, it is also found analytically that the effect of the $\sigma$ exchange term is roughly one half as the effect of its direct term, but with an opposite sign. The effect of the $\omega$ exchange term almost vanishes due to the cancellation between the time and space components. Therefore, the net Fock contribution to the splitting is negative and comparable to the Hartree contribution, as shown in the lower part of Fig. 6. All the above discussions for the case of $^{16}$O are also valid for heavier nuclei, e.g., $^{208}$Pb.

It is known that the presence of strong annihilation channels and various many-body effects could cause significant deviations from the G-parity values of the meson-antinucleon couplings and a global fits to antiprotonic X-rays and radiochemical data indicates the
In summary, the spin symmetry in the negative energy spectrum and its mechanism are investigated within the DDRHF theory by taking the nucleus $^{16}$O as an example.

Similarly to RMF, the spin symmetry in the negative energy spectrum is found to be...
a good approximation and the dominant components $F(r)$ of the Dirac wave functions for the spin doublets are nearly identical, as the centrifugal barrier is much stronger than the spin-orbit potential.

However, it is found that the Fock terms are dominant in the spin-orbit potential, which induce the state dependence of the effective potential and play essential roles in spin-orbit splitting.

Classifying the contributions to the spin-orbit splitting into the Hartree and Fock parts, it is found that the Hartree part has an energy dependence similar to those in RMF \[15\], while the Fock part has an opposite tendency and cancels with the Hartree part, thus leading to good spin symmetry.

The competition between the Hartree and Fock terms determines the subtle spin-orbit splitting, which explains the fluctuation of the spin-orbit splittings in DDRHF instead of monotonously decreasing with $E_{av}$ as in the RMF case.

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