Pseudo-spin symmetry in density-dependent relativistic Hartree-Fock theory

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The pseudo-spin symmetry (PSS) is investigated in the density-dependent relativistic Hartree-Fock theory by taking the doubly magic nucleus 132Sn as a representative. It is found that the Fock terms bring significant contributions to the pseudo-spin orbital potentials (PSOP) and make it comparable to the pseudo-centrifugal barrier (PCB). However, these Fock terms in the PSOP are counteracted by other exchange terms due to the non-locality of the exchange potentials. The pseudo-spin orbital splitting indicates that the PSS is preserved well for the partner states (ν3s1/2, ν2d3/2) of 132Sn in the relativistic Hartree-Fock theory.

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The pseudo-spin symmetry (PSS), quasi-degeneracy of two single particle states with the quantum numbers (n, l, j = l + 1/2) and (n − 1, l + 2, j = l + 3/2), was firstly discovered more than thirty years ago in spherical nuclei1,2 and later in deformed nuclei3,4. During the past ten years, many efforts have been made to investigate the origin of PSS5,6,7,8 and the conservation conditions9,10,11,12 within the framework of relativistic mean field (RMF) theory. In Ref. 5, the PSS was interpreted as the relativistic symmetry in the Dirac equation, which arises from the cancellation between an attractive scalar potential ΣS and a repulsive vector potential Σ0, i.e., ΣS + Σ0≈0, and the pseudo-orbit number ̄l is nothing but the orbital angular momentum of the lower component of the Dirac wave function. However, in this limit there is no bound states in the mean field, at variance with reality. More realistic conditions were discussed for the conservation of the PSS in Refs.9,10,12.

In the framework of the RMF theory13,14,15,16,17,18,19,20, i.e., the relativistic Hartree-Fock

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approach with a no-sea approximation, the nucleons interact via the exchange of mesons and photons. For the description of nuclear structure, the relevance of relativity is not in the need of relativistic kinematics but it lies in a covariant formulation which maintains the distinction between scalar and vector fields (more precisely, the zeroth component of the Lorentz four-vector field). The representations with large scalar and vector fields in nuclei (of the order of a few hundred MeV) provide more efficient descriptions of nuclear systems than non-relativistic approaches, for example the origin of the nuclear spin-orbit potential [21] and that of the PSS [5, 9].

Although there exist some attempts to include the exchange terms in the relativistic description of nuclear matter and finite nuclei [22, 23, 24], the relativistic Hartree-Fock (RHF) method was still not comparable with the RMF theory in the quantitative description of nuclear systems. Recently, it was shown that the density-dependent relativistic Hartree-Fock (DDRHF) theory [25] gives a successful quantitative description of nuclear matter and finite nuclei at the same level as the RMF [26]. Compared with RMF, the relevance of the relativity is still kept well in DDRHF although the covariant formulation becomes much more complicated due to the exchange terms. Since the DDRHF describes quite well nuclear systems, it is worthwhile to investigate the role of exchange terms in the PSS, especially the influence of the non-locality on the conservation of the PSS. In this work, we study the role of the Fock terms on the conservation of PSS in the covariant relativistic Hartree-Fock theory. The numerical study is done with the effective Lagrangian PKO1 [25] in the case of DDRHF, and the results are compared with those obtained with the RMF model PKDD [20].

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

\[ f_a(r) = \frac{1}{r} \left( \begin{array}{c}
  iG_a(r) \mathcal{Y}_{j a m_a}^l(a) \\
  -F_a(r) \mathcal{Y}_{j a m_a}^{l'}(a)
\end{array} \right) \chi_{1/2}^\tau(a), \]  

(1)

where \( \chi_{1/2}^\tau(a) \) is the isospinor, \( G_a \) and \( F_a \) correspond to the radial parts of upper and lower components, respectively. \( \mathcal{Y}_{j a m_a}^l \) is the spinor spherical harmonics and \( \mathcal{Y}_{j a m_a}^{l'}(\hat{r}) = -\hat{\sigma} \cdot \hat{r} \mathcal{Y}_{j a m_a}^l(\hat{r}) \) with \( l_a = 2j_a - l \). In the spherical nuclei, the total angular momentum \( j_a \), its projection on the \( z \) axis \( m_a \) and \( \hat{\kappa} = -\hat{\beta}(\hat{\sigma} \cdot \hat{L} + 1) \) are conserved. The eigenvalues of \( \hat{\kappa} \) are \( \kappa_a = \pm (j_a + \frac{1}{2}) \) (− for \( j_a = l_a + \frac{1}{2} \) and + for \( j_a = l_a - \frac{1}{2} \)). In the following, the sub-index \( a \) will be omitted in the notations.

Within the DDRHF, the radial Dirac equations, i.e., the relativistic Hartree-Fock equations for
spherical nuclei, are expressed as the coupled differential-integral equations

\[
EG(r) = - \left[ \frac{d}{dr} - \frac{\kappa}{r} \right] F(r) + [\Sigma_S(r) + \Sigma_0(r)] G(r) + Y(r), \tag{2a}
\]

\[
EF(r) = + \left[ \frac{d}{dr} + \frac{\kappa}{r} \right] G(r) - [2M + \Sigma_S(r) - \Sigma_0(r)] F(r) + X(r), \tag{2b}
\]

where the scalar potential \(\Sigma_S\) and the time component of the vector potential \(\Sigma_0\) contain the contributions from the direct terms and the rearrangement term due to the density-dependence of the meson-nucleon couplings. The \(X\) and \(Y\) functions represent the results of the non-local Fock potentials acting on \(F\) and \(G\), respectively \[26\]. By introducing the functions \(X_G, X_F, Y_G\) and \(Y_F\) as in Ref. \[22\],

\[
X(r) = \frac{G(r)X(r)}{G^2 + F^2} G(r) + \frac{F(r)X(r)}{G^2 + F^2} F(r)
\]

\[
\equiv X_G(r)G(r) + X_F(r)F(r), \tag{3a}
\]

\[
Y(r) = \frac{G(r)Y(r)}{G^2 + F^2} G(r) + \frac{F(r)Y(r)}{G^2 + F^2} F(r)
\]

\[
\equiv Y_G(r)G(r) + Y_F(r)F(r), \tag{3b}
\]

the coupled differential-integral equations \[24\] can be transformed into the equivalent local ones,

\[
\left[ \frac{d}{dr} - \frac{\kappa}{r} - Y_F(r) \right] F(r) - [\Delta(r) - E] G(r) = 0, \tag{4a}
\]

\[
\left[ \frac{d}{dr} + \frac{\kappa}{r} + X_G(r) \right] G(r) + [V(r) - E] F(r) = 0, \tag{4b}
\]

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

\[
\Delta^D \equiv \Sigma_S + \Sigma_0; \quad V^D \equiv \Sigma_0 - \Sigma_S - 2M. \tag{5a}
\]

The coupled equations \[4\] can be solved by using the same numerical method as in RMF \[27\]. In Eqs. \[4\], the functions \(X_G, X_F, Y_G\) and \(Y_F\) might be taken as the effective potentials from the exchange (Fock) terms in the DDRHF. Eqs. \[4\] must be solved iteratively since the potentials depend on the solution \((G, F)\).

From the radial Dirac equations \[4\], the Schrödinger-type equation for the lower component \(F\) is obtained as,

\[
\frac{d^2}{dr^2} F + V_1 \frac{d}{dr} F + (V_{PCB} + V_{PSO} + V_2) F
\]

\[
= - (V^D - E) (\Delta^D - E) F, \tag{6}
\]
with

\[ V_1 \equiv (X_G - Y_F) - \frac{1}{\Delta - E} \frac{d\Delta}{dr}, \]  
\[ V_2 \equiv Y_F \frac{1}{\Delta - E} \frac{d\Delta}{dr} - X_G Y_F - \frac{d}{dr} Y_F \]
\[ + Y_G (V^D - E) + X_F (\Delta - E), \]  
\[ V_{PSO} \equiv \kappa \left[ \frac{1}{\Delta - E} \frac{d\Delta}{dr} - (X_G + Y_F) \right], \]  
\[ V_{PCB} \equiv \kappa (1 - \kappa) \frac{1}{r^2}, \]

where \( V_{PCB} \) and \( V_{PSO} \) correspond to the pseudo-centrifugal barrier (PCB) and pseudo-spin orbital potential (PSOP), respectively. In the limit of \( V_{PSO} = 0 \), the pseudo-spin becomes a good symmetry and the PSS can be labeled by the pseudo radial number \( \tilde{n} = n - 1 \), pseudo-orbit \( \tilde{l} = l' \), and pseudo-spin \( \tilde{s} = s = \frac{1}{2} \), with the total angular momentum \( j = \tilde{l} \pm \tilde{s} \) for the two partner states. For instance, the partners are \((ns_{1/2}, (n - 1)d_{3/2})\) for \( \tilde{l} = 1 \), \((np_{3/2}, (n - 1)f_{5/2})\) for \( \tilde{l} = 2 \), etc. Notice that \( X_G \) and \( Y_F \) in the \( V_{PSO} \) are new contributions from the Fock terms compared with RMF. The potential \( V_2 \) entirely originates from the Fock contributions. The direct (Hartree) and exchange (Fock) contributions of the PSOP and \( V_1 \) can be separated as,

\[ V^D_{PSO} = \kappa \frac{1}{r} \frac{d\Delta^D}{dr}, \]  
\[ V^E_{PSO} = \kappa \left[ \frac{1}{\Delta - E} \frac{dY_G}{dr} - (X_G + Y_F) \right], \]  
\[ V^D_1 = - \frac{1}{\Delta - E} \frac{d\Delta^D}{dr}, \]  
\[ V^E_1 = (X_G - Y_F) - \frac{1}{\Delta - E} \frac{dY_G}{dr}, \]

while \( \Delta \) comes from both the Hartree and Fock contributions.

To have better a understanding of the pseudo-spin orbital splitting, especially the effects of Fock terms, it will be more transparent to rewrite Eq. (6) as,

\[ \frac{1}{V^D - E} \frac{d^2}{dr^2} F + \frac{1}{V^D - E} \left[ V_{PCB} + \hat{V}^D + \hat{V}^E \right] F \]
\[ + \Delta^DF = EF \]

where the operators \( \hat{V}^D \) and \( \hat{V}^E \) are

\[ \hat{V}^D = \frac{1}{V_1^D} \frac{d}{dr} + V^D_{PSO}, \]
\[ \hat{V}^E = \frac{1}{V_1^E} \frac{d}{dr} + V^E_{PSO} + V_2. \]

Let us discuss the PSS by taking the doubly magic nucleus \(^{132}\text{Sn}\) as a representative. In Fig. we are shown the neutron single-particle energies calculated by the DDRHF with PKO1, compared
with those given by the RMF with PKDD and the experimental data [28]. Among the neutron single-particle states shown in Fig. 1 there are four pseudo-spin partners $1\tilde{p}$, $1\tilde{d}$, $1\tilde{f}$ and $2\tilde{p}$, which correspond to the pairs $(\nu 2s_{1/2}, \nu 1d_{3/2})$, $(\nu 2p_{3/2}, \nu 1f_{5/2})$, $(\nu 2d_{5/2}, \nu 1g_{7/2})$ and $(\nu 3s_{1/2}, \nu 2d_{3/2})$, respectively. From Fig. 1 one can find a good PSS in the partners $\nu 3s_{1/2}$ and $\nu 1d_{3/2}$ both in the DDRHF and RMF.

From the single-particle energies, the pseudo-spin orbital splitting is estimated as $\Delta E_{PSO} = (E_{lj=\tilde{l}-1/2} - E_{lj=\tilde{l}+1/2})/(2\tilde{l} + 1)$ for the pseudo-spin partners $1\tilde{p}$, $1\tilde{d}$, $1\tilde{f}$ and $2\tilde{p}$. The results are shown in Fig. 2 as a function of the average binding energy $\bar{E}_{PSO} = (E_{lj=\tilde{l}-1/2} + E_{lj=\tilde{l}+1/2})/2$.

For both DDRHF (filled symbols) and RMF (open symbols) results, the pseudo-spin splitting between $\nu 3s_{1/2}$ and $\nu 2d_{3/2}$ is more than ten times smaller than that between $\nu 2s_{1/2}$ and $\nu 1d_{3/2}$. As shown in Fig. 1 and Fig. 2 there exist some differences in the single-particle energies (especially the deeply bound states) between the DDRHF and RMF, whereas the monotonous decreasing behavior of $\Delta E_{PSO}$ with the decreasing binding energies is observed in the both models. As a reference, the spin-orbit splitting $\Delta E_{SO} = (E_{lj=l-1/2} - E_{lj=l+1/2})/(2l + 1)$ versus the average binding energy $\bar{E}_{SO} = (E_{lj=l-1/2} + E_{lj=l+1/2})/2$ is also shown in Fig. 2 for the spin-orbit partners $1p$, $1d$, $1f$, and $1g$, and $2p$, $2d$. A clear difference between the pseudo-spin orbital and spin-orbit splittings can be seen in their energy-dependence, i.e., a strong energy-dependence is found for the pseudo-spin orbital splitting, while the spin-orbit splitting shows a weak energy-dependence. This difference can be understood from the comparison between the expressions for the PSOP and the corresponding spin-orbit potential. The energy $E$ and the potential $\Delta$ in the denominator $\Delta - E$ of Eq. 7 are comparable so that it brings a strong energy-dependence for the PSOP. On the other hand, the corresponding denominator of the spin-orbit potential in RHF is $V - E$, which...
which gives much weaker energy-dependence because the single-particle energy $E$ is much smaller than the potential $V$: the value of $E$ is a few tens MeV while $V$ is several hundred MeV.

![Image of Dirac wave function and pseudo-spin partners](image)

**FIG. 2:** The pseudo-spin orbital splitting $\Delta E_{PSO} = (E_{lj=I-1/2} - E_{lj=I+1/2})/(2I + 1)$ versus the average binding energy $E_{PSO} = (E_{lj=I-1/2} + E_{lj=I+1/2})/2$ for the neutron states in $^{132}$Sn. The pseudo-spin partners $1\tilde{p}^1, 1\tilde{d}^1, 1\tilde{f}^2$ and $2\tilde{p}$ correspond to $(\nu 2s_{1/2}, \nu 1d_{3/2}), (\nu 2p_{3/2}, \nu 1f_{5/2}), (\nu 2d_{5/2}, \nu 1g_{7/2})$ and $(\nu 3s_{1/2}, \nu 2d_{3/2})$ states, respectively. The spin-orbit splitting $\Delta E_{SO} = (E_{lj=I-1/2} - E_{lj=I+1/2})/(2l + 1)$ are also given for $(\nu 1p_{3/2}, \nu 1p_{1/2}), (\nu 1d_{5/2}, \nu 1d_{3/2}), (\nu 1f_{7/2}, \nu 1f_{5/2}), (\nu 1g_{9/2}, \nu 1g_{7/2})$ and $(\nu 2p_{3/2}, \nu 2p_{1/2}), (\nu 2d_{5/2}, \nu 2d_{3/2})$ pairs as a function of $E_{SO} = (E_{lj=I+1/2} + E_{lj=I-1/2})/2$. The results are obtained by the DDRHF with PKO1 (filled symbols) and the RMF with PKDD (open symbols), respectively.

Let us discuss the effects of Fock terms, especially the non-locality effect on the conservation of the PSS by considering the pseudo-spin partners $1\tilde{p}$ and $2\tilde{p}$. The left panel of **Fig. 3** shows the radial wave function (upper and lower components $G, F$) for the pseudo-spin partners $(\nu 2s_{1/2}, \nu 1d_{3/2})$ and $(\nu 3s_{1/2}, \nu 2d_{3/2})$. The lower components of the partner states $\nu 2s_{1/2}$ $(\nu 3s_{1/2})$ and $\nu 1d_{3/2}$ $(\nu 2d_{3/2})$ are very close each other in both the shape and magnitude whereas the upper components are quite different. Comparisons of the upper and lower components between the partner states indicate that the approximate PSS exists in the lower components for both partners $1\tilde{p}$ and $2\tilde{p}$ although the upper component of the total Dirac wave function dominate. The functions $X(r)$ $(Y(r))$ introduced in Eq. (2) and representing the action of the Fock potentials on $F$ $(G)$ are also given in the right panel of **Fig. 3** for the pseudo-spin partners $1\tilde{p}$ and $2\tilde{p}$. It is interesting to find that the radial dependence of the functions $X$ and $Y$ are very similar to those of the lower and upper components, respectively.

In Eq. (3), the Fock-related terms $X$ and $Y$ are divided into two products of effective potentials times the Dirac wave functions to obtain the equivalent local Dirac equations (1). **Fig. 4** shows these effective potentials $(X_G, Y_G)$, and $(X_F, Y_F)$ for the pseudo-spin partners $(\nu 2s_{1/2}, \nu 1d_{3/2})$ and $(\nu 3s_{1/2}, \nu 2d_{3/2})$. The local peaks and dips in the figures are due to the localization of the exchange
terms in Eq. (3) reflecting the nodes of the upper components in the denominator. It is seen in Fig. 4 that the radial dependence of $Y_F$ is almost identical to that of $X_G$ since the shapes of $(X, Y)$ and $(G, F)$ are very close each other. Because the peaks and dips in Fig. 4 are due to the nodes of upper components, their contributions to the single-particle energies will be smoothed out by the corresponding nodes. Thus, one can ignore the non-locality represented by the peaks or dips for the discussion on the PSS. Besides the peaks, one can find that in the inner part of the nucleus the effects of the non-locality are significant on $X_G$ and $Y_F$ and give a strong state dependence with different signs, while it shows fairly weak effects on $Y_G$. The $X_F$ is just due to the nodes of the upper component.

In RMF it has been proved that the PSS is well obeyed if the PCB is much stronger than the PSOP [9]. Fig. 5 shows the PCB and PSOP multiplied by the factor $F^2/(V^D - E)$ for the pseudo-spin partners $(\nu 2s_{1/2}, \nu 1d_{3/2})$ and $(\nu 3s_{1/2}, \nu 2d_{3/2})$ in $^{132}$Sn. Due to the denominator $\Delta - E$ in Eq. (4), there exists singular points at $r \simeq 6$ fm for the partner $(\nu 2s_{1/2}, \nu 1d_{3/2})$, and at $r \simeq 7.5$ fm...
for \((\nu 3s_{1/2}, \nu 2d_{3/2})\). The other local peaks in the PSOP are due to the nodes of upper component \(G\). For the \(s\) states \((l = 0)\), the PCB is much stronger than the PSOP since the contributions for the PSOP around the nodes or the singular points are more or less mutually cancelling. On the other hand, for the \(d\) states, the PSOP are comparable to the PCB even after taking account of the cancellation around the nodes or singular points. Comparing the shapes of the PSOP in Fig. 5 and \(X_G, Y_F\) in Fig. 4 one can find that the Fock terms present significant contributions to the PSOP, especially for the \(d\) states in the inner part of the nucleus. It is also seen that the Fock terms in Fig. 6 have substantial contributions to the PSOP in Fig. 5.

FIG. 5: The PCB and PSOP multiplied by the factor \(F^2/(V^D - E)\) for the pseudo-spin partners \((\nu 2s_{1/2}, \nu 1d_{3/2})\) and \((\nu 3s_{1/2}, \nu 2d_{3/2})\) in \(^{132}\text{Sn}\). The PCB contributions are drawn by the dashed lines, while the PSOP are shown by the solid lines. The DDRHF with PKO1 is used for the calculations. See the text for details.

From Eq. 9, one can estimate the contributions of the potentials \(V_{\text{PCB}}, \hat{V}^D\) and \(\hat{V}^E\) to the single-particle energy \(E\). For example, the PCB contribution can be expressed as,

\[
\frac{1}{\int_0^\infty F^2dr} \int_0^\infty \frac{V_{\text{PCB}}}{V^D - E} F^2dr.
\]

The results calculated by the DDRHF with PKO1 and the RMF with PKDD are shown in Table 1 for the pseudo-spin partners \(1\bar{p}\) and \(2\bar{p}\). For both the DDRHF and RMF, the terms \(F''\), \(\Delta^D\) and \(\hat{V}^D\) in Eq. 9 show substantial differences between the partner states \((\nu 2s_{1/2}, \nu 1d_{3/2})\) and \((\nu 3s_{1/2}, \nu 2d_{3/2})\) whereas the differences in the PCB and the exchange terms \(\hat{V}^E\) are negligible. The differences in \(F''\) and \(\Delta^D\) reflect those of the lower components in the two pseudo-spin partners as shown in the left panel of Fig. 3.

The large differences between the partner states can be seen in the \(F''\), \(\Delta^D\) and \(\hat{V}^D\) contributions. However, these three terms cancel largely one another and the PSS is preserved to a good degree, especially in the partners \((\nu 3s_{1/2}, \nu 2d_{3/2})\) in both DDRHF and DDRMF. The Fock terms \(\hat{V}^E\) become small although each term on the right hand side of Eq. 10b shows appreciable differences.
TABLE I: The single-particle energies $E$ and the contributions from different terms in the left hand side of Eq. (9) given by the DDRHF with PKO1, in comparison with those by the RMF with PKDD. All units are in MeV.

| Model | Orbit  | $E$  | $E'$ | $\Delta^D$ | $V_{PCB}$ | $\tilde{V}^D$ | $\tilde{V}^E$ |
|-------|--------|------|------|-------------|-----------|--------------|--------------|
| DDRHF | $\nu 2s_{1/2}$ | -31.41 | 18.11 | -75.35 | 9.30 | -2.99 | 19.51 |
| PKO1  | $\nu 1d_{3/2}$ | -34.90 | 14.87 | -79.01 | 9.54 | 0.44 | 19.26 |
| DDRMF | $\nu 3s_{1/2}$ | -8.33 | 34.25 | -72.00 | 11.11 | 0.09 | 18.22 |
| PKDD  | $\nu 2d_{3/2}$ | -8.66 | 31.93 | -73.96 | 11.32 | 3.89 | 18.17 |

Let us now discuss the reason why the cancellations among the exchange terms occur. From
the similar radial dependence between the non-local terms $X(Y)$ and Dirac wave functions $F(G)$ in Fig. 3 we might be able to validate the following relations,

$$X(r) \simeq X_0(r)F(r), \quad Y(r) \simeq Y_0(r)G(r),$$  \hspace{1cm} (12)

where $X_0$ and $Y_0$ are supposed to be state-independent potentials due to the Fock terms. Using Eq. (12), the non-local RHF equations can be reduced to local ones similar to the RMF equations in which the terms $X_G$ and $Y_F$ do not appear in the PSOP. Thus, the realization of the PSS will be similar to the RMF case. Therefore, the cancellation of the Fock contributions in Table I is not occasional but it is because of the similar radial dependence between the Fock-related terms $(X,Y)$ and the wave functions $(F,G)$.

In summary, the PSS in the DDRHF theory was investigated in the doubly magic nucleus $^{132}$Sn. The PSOP was derived by transforming the coupled radial Dirac equations into the Schrödinger type equation of the lower component properly taking account of the non-local Fock terms. The analyses of the single particle spectrum and the pseudo-spin orbital splitting indicate that the PSS is preserved as a good symmetry for the pseudo-spin partner $(\nu^3s_{1/2}, \nu^2d_{3/2})$ of $^{132}$Sn in the DDRHF on the same level as RMF, although the Fock terms bring substantial contributions to the PSOP. These contributions to the pseudo-spin orbital splitting, however, are cancelled by the other terms due to the non-locality of the exchange potentials. The physical mechanism of these cancellations was discussed in relation to the similarity between the exchange potentials and the Dirac wave functions.

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