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Spin symmetry in the Dirac sea derived from the bare nucleon–nucleon interaction

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ABSTRACT

The spin symmetry in the Dirac sea has been investigated with relativistic Brueckner–Hartree–Fock theory using the bare nucleon–nucleon interaction. Taking the nucleus ^{16}O as an example and comparing the theoretical results with the data, the definition of the single-particle potential in the Dirac sea is studied in detail. It is found that if the single-particle states in the Dirac sea are treated as occupied states, the ground state properties are in better agreement with experimental data. Moreover, in this case, the spin symmetry in the Dirac sea is better conserved and it is more consistent with the findings using phenomenological relativistic density functionals.

It is well known that in the nuclear system the spin symmetry is largely broken, that is, there exists a large spin–orbit (SO) splitting, which was introduced by Mayer [1] and Haxel et al. [2] in 1949. It formed the ground for the nuclear shell model. Twenty years later a new symmetry, the so-called pseudospin symmetry, was proposed to explain the near degeneracy between two single-particle (s.p.) states with the quantum numbers $(n, l, j = l + 1/2)$ and $(n - 1, l + 2, j = l + 3/2)$ [3,4]. The two states are regarded as the pseudospin doublets with the pseudospin quantum numbers $(\tilde{n} = n - 1, \tilde{l} = l + 1, j = \tilde{l} \pm 1/2)$.

By starting from the Dirac equation, it was found that the angular momentum of the pseudospin doublets $\tilde{l}$ is nothing but the orbital angular momentum of the lower component of the Dirac spinor, and the pseudospin symmetry is exact when the sum of vector and scalar potential $V + S$ vanishes [5]. The more general condition, $d(V + S)/dr = 0$, was proposed and can be approximately fulfilled in exotic nuclei [6,7]. The general condition for spin and pseudospin symmetry, namely that $V + S$ is a constant for pseudospin symmetry is confirmed in Ref. [8] and its connection to spin symmetry was also suggested there. Since then, pseudospin symmetry has been realized as a relativistic symmetry and much work has been done to investigate its origin and its properties using phenomenological single-particle Hamiltonians, relativistic mean field theory, or relativistic Hartree–Fock (RHF) theory [9–26].

If one starts with a Dirac Hamiltonian, there exist single-particle states not only with positive energy but also with negative energy, states in the so-called Dirac sea. It was shown in Ref. [27] that the pseudospin symmetry in the positive spectrum has the same origin as the spin symmetry in the Dirac sea. In other words, the SO doublets in the Dirac sea has the quantum number $(n, \tilde{l}, j = \tilde{l} \pm 1/2)$, and the spin symmetry breaking term is proportional to $d(V + S)/dr$, similar to the pseudospin symmetry in the positive spectrum. The spin symmetry in Dirac sea has also been investigated intensively afterwards [28–33]. For comprehensive reviews on the study of pseudospin and spin symmetries, see Refs. [34,35].

Up until now, all the studies on the pseudospin symmetry in nuclei or the spin symmetry in the Dirac sea have been started from phenomenological s.p. Hamiltonians, or relativistic density functionals using phenomenological parameters [36–40].

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It is therefore an interesting question to what extent spin symmetry in the Dirac sea is found in calculations starting from the bare nucleon–nucleon (NN) interaction which is fitted to the NN scattering data and deuteron properties. However, such *ab initio* calculations for nuclei are extremely difficult and most of them are performed in a nonrelativistic framework [41–47]. Only recently, a relativistic *ab initio* method has been developed for finite nuclei by extending Brueckner–Hartree–Fock theory to the relativistic framework, and it has been shown that relativistic effects are important to improve the agreement with the experimental data [48,49]. In particular, the effect of tensor force is well treated in the spin–orbit splittings, as demonstrated in neutron drops [50].

In this work, starting from a bare NN interaction and taking the nucleus ^{16}O as an example, we study the spin symmetry in the Dirac sea within relativistic Brueckner–Hartree–Fock (RBHF) theory. Special attention will be paid on the definition of the s.p. potential in Dirac sea. The results are compared with those obtained by phenomenological relativistic density functionals which are fitted to properties of finite nuclei and nuclear matter.

We use the relativistic version of the potential Bonn A. This is a relativistic one-boson-exchange NN interaction which has been carefully adjusted to the NN scattering data [51]. The corresponding Hamiltonian has the form:

$$H = \sum_{kk'} \langle k|T|k'\rangle b_k^\dagger b_{k'} + \frac{1}{2}\sum_{klk'l'} \langle kl|V|k'l'\rangle b_k^\dagger b_l^\dagger b_{l'} b_{k'}, \tag{1}$$

where the relativistic matrix elements are given by

$$\langle k|T|k'\rangle = \int d^3r\, \bar\psi_k(\mathbf{r})\, (-i\boldsymbol{\gamma}\cdot\nabla + M)\, \psi_{k'}(\mathbf{r}), \tag{2}$$

$$\langle kl|V_\alpha|k'l'\rangle = \int d^3r_1 d^3r_2\, \bar\psi_k(\mathbf{r}_1)\Gamma_\alpha^{(1)}\psi_{k'}(\mathbf{r}_1) \times D_\alpha(\mathbf{r}_1,\mathbf{r}_2)\bar\psi_l(\mathbf{r}_2)\Gamma_\alpha^{(2)}\psi_{l'}(\mathbf{r}_2). \tag{3}$$

The indices k, l run over a complete basis of Dirac spinors with positive and negative energies, as, for instance, over the eigensolutions of a Dirac equation with potentials of Woods–Saxon shape [52,49,53].

The two-body interaction V_α contains the exchange contributions of different mesons $\alpha = \sigma, \delta, \omega, \rho, \eta, \pi$. The interaction vertices Γ_α for particles 1 and 2 contain the corresponding γ-matrices for scalar (σ, δ), vector (ω, ρ), and pseudovector (η, π) coupling and the isospin matrices $\vec\tau$ for the isovector mesons δ, ρ, and π. For the Bonn interaction [51], a form factor of monopole-type is attached to each vertex and $D_\alpha(\mathbf{r}_1, \mathbf{r}_2)$ represents the corresponding meson propagator. Retardation effects were deemed to be small and were ignored from the beginning. Further details are found in Ref. [49].

The matrix elements of the bare nucleon–nucleon interaction are very large and difficult to be used directly in nuclear many-body theory. Within Brueckner theory, the bare interaction is replaced by an effective interaction in the nuclear medium, the G-matrix. It takes into account the short-range correlations by summing up all the ladder diagrams of the bare interaction [54] and it is deduced from the Bethe–Goldstone equation [55],

$$\bar G_{aba'b'}(W) = \bar V_{aba'b'} + \frac{1}{2}\sum_{cd} \frac{\bar V_{abcd}\bar G_{cda'b'}(W)}{W - e_c - e_d}, \tag{4}$$

where $\bar V_{aba'b'}$ are the anti-symmetrized two-body matrix elements (3) and W is the starting energy. In self-consistent RBHF theory the states $|a\rangle, |b\rangle, \ldots$ are solutions of the relativistic Hartree–Fock (RHF) equations,

$$(T+U)|a\rangle = e_a|a\rangle, \tag{5}$$

where $e_a = \varepsilon_a + M$ is the s.p. energy with the rest mass of the nucleon M. The intermediate states c, d in Eq. (4) run over all states above the Fermi surface with e_c, $e_d > e_F$, because the levels in the Fermi sea as well as those in the Dirac sea are occupied.

In the case of spherical symmetry, the s.p. wave function can be written as

$$|a\rangle = \frac{1}{r}\begin{pmatrix} F_{n_a\kappa_a}(r)\Omega^{l_a}_{j_a m_a}(\theta,\varphi) \\ iG_{n_a\tilde\kappa_a}(r)\Omega^{\tilde l_a}_{j_a m_a}(\theta,\varphi) \end{pmatrix}, \tag{6}$$

where $\Omega^l_{jm}(\theta,\varphi)$ are the spinor spherical harmonics. The radial, orbital angular momentum, total angular momentum, and magnetic quantum numbers are denoted by n, l, j, and m, respectively, while the quantum number κ is defined as $\kappa = \pm(j+1/2)$ for $j = l \mp 1/2$. Furthermore, $\tilde l = 2j - l$ is the orbital angular momentum for the lower component. The corresponding effective local radial Dirac equation reads

$$\begin{pmatrix} M+\Sigma(r) & -\frac{d}{dr}+\frac{\kappa}{r} \\ \frac{d}{dr}+\frac{\kappa}{r} & -M+\Delta(r) \end{pmatrix}\begin{pmatrix} F_a(r) \\ G_a(r) \end{pmatrix} = e_a \begin{pmatrix} F_a(r) \\ G_a(r) \end{pmatrix}, \tag{7}$$

with $\Sigma = V + S$ and $\Delta = V - S$ are the sum and difference of vector and scalar potentials.

The self-consistent s.p. potential U in Eq. (5) is defined by the G-matrix with the usual Hartree–Fock prescription. The problem is the starting energy W. Several methods have been introduced in the literature and we use here the method proposed in Refs. [56,57]. These were nonrelativistic investigations and therefore one had here only matrix elements $\langle a|U|b\rangle$ for s.p. states $|a\rangle$, $|b\rangle$ in the Fermi sea and above the Fermi level. In our earlier relativistic work [49] we treated in this context s.p. states $|a\rangle$, $|b\rangle$ in the Dirac sea as unoccupied, i.e. in a similar way as the states above the Fermi level. This leads to the following definition of the starting energy W in the matrix elements of the self-consistent s.p. potential U:

$$\langle a|U|b\rangle = \begin{cases} \frac{1}{2}\sum_{i=1}^{A}\langle ai|\bar G(e_a+e_i) + \bar G(e_b+e_i)|bi\rangle, & 0 < (e_a, e_b) \le e_F \\ \sum_{i=1}^{A}\langle ai|\bar G(e_a+e_i)|bi\rangle, & 0 < e_a \le e_F,\ e_b > e_F \text{ or } e_b < 0 \\ \sum_{i=1}^{A}\langle ai|\bar G(e'+e_i)|bi\rangle, & e_a, e_b > e_F \text{ or } < 0. \end{cases} \tag{8}$$

where the index i runs over the occupied states in the Fermi sea (*no-sea* approximation). In the above equations, e' is somewhat uncertain in the (R)BHF framework and it has been fixed as an energy among the occupied states in Ref. [49]. The difference of the results by fixing e' as the highest and as the lowest energy of the occupied states in the Fermi sea has been discussed therein. As discussed in Ref. [49] the various matrix elements of the matrix $\bar G(W)$ are determined by interpolation and with this choice the starting energy W is limited as a sum of two single-particle energies in the Fermi sea.

From Eq. (8) it can be seen that in Ref. [49] the matrix elements $\langle a|U|b\rangle$ with s.p. states $|a\rangle$ and/or $|b\rangle$ in the Dirac sea (with $e < 0$) have been treated in the same way as those with states in unoccupied particle states ($e > e_F$). This is technically less time consuming as one does not need to calculate $\bar G(W)$ for values $W < 0$. One should recall that there is no "right" or "wrong" choice for the s.p. potential in (R)BHF theory, as (R)BHF theory can be viewed as the 2 hole-line expansion in the more general hole-line expansion