Solving the Dirac equation with nonlocal potential by Imaginary Time Step method *

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Abstract

The Imaginary Time Step (ITS) method is applied to solve the Dirac equation with the nonlocal potential in coordinate space by the ITS evolution for the corresponding Schrödinger-like equation for the upper component. It is demonstrated that the ITS evolution can be equivalently performed for the Schrödinger-like equation with or without localization. The latter algorithm is recommended in the application for the reason of simplicity and efficiency. The feasibility and reliability of this algorithm are also illustrated by taking the nucleus $^{16}$O as an example, where the same results as the shooting method for the Dirac equation with localized effective potentials are obtained.

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With the operating of the worldwide new Radioactive Ion Beam (RIB) facilities and the developments in the detection techniques, a lot of novel aspects of nuclear structure and entirely unexpected features have been found in the exploration of “exotic nuclei” [1, 2, 3, 4]. The extreme neutron richness of exotic nuclei and the physics related to the low density in the tails of nuclear matter distributions provide both demand and challenge to solve complex many-body problem in coordinate space.

As one of the best candidates for the description of exotic nuclei, the Relativistic Mean Field (RMF) approach [5] has achieved lots of success in describing many nuclear phenomena during the past years [6, 7, 8]. In particular, the Relativistic Continuum Hartree-Bogoliubov (RCHB) theory [9] provides a fully self-consistent treatment of pairing correlations in the presence of the continuum and thus gives a reliable description of nuclei far away from the line of $\beta$-stability, which suggests a new mechanism for the formation of the halo phenomena [10].

Within the RMF approach, however, the Fock terms of the energy density functional are neglected under the Hartree approximation. The recent development of density-dependent relativistic Hartree-Fock (DDRHF) theory [11] resumes the Fock terms and obtains quantitatively comparable precision with the RMF theory for nuclear matter and finite nuclei [11, 12]. Moreover, within the DDRHF theory, the importance of the Fock terms is evidenced by the improvement on the descriptions of the nuclear shell structures [12] and their evolutions [13], the excellent reproduction of the spin-isospin resonance based on the self-consistent random phase approximation [14], as well as the influences on isospin properties of nuclear matter and neutron stars at high densities [15]. More recently, as an extension of the DDRHF theory, the relativistic Hartree-Fock-Bogoliubov theory with density dependent meson-nucleon couplings (DDRHFB) is developed for the description of the exotic nuclei [16].

For the future study, one of the natural extensions of the RCHB or DDRHFB theory is the exploration of deformed exotic nuclei, which will provide the decisive conclusion on the existence of deformed halo. Efforts along this line have been made in the past several years. Due to the difficulty in solving the coupled channel differential equations for deformed system in coordinate space [17], the method for expansion in Woods-Saxon basis was proposed [18], which becomes very time consuming for the heavy system.

The Imaginary Time Step (ITS) method [19] is another effective approach to solve the nonrelativistic problems in coordinate space and has achieved lots of success in the conventional mean field approach [20]. More importantly, its extension from spherical to deformed
systems is straightforward. It is therefore worthwhile to adopt this method for the relativistic system. Naively, one may assume that the ITS method will result in a great disaster due to the Dirac sea. Fortunately, it has been demonstrated that this disaster can be avoided by the ITS evolution for the Schrödinger-like or charge-conjugate Schrödinger-like equation for the solution respectively in the Fermi or Dirac sea [21].

For the application of the ITS method in the relativistic Hartree-Fock theory, one has to solve the Dirac equation with nonlocal potential due to the Fock terms. The corresponding Dirac equation will be a set of coupled integro-differential equations, which cannot be solved by the conventional shooting method directly.

In this letter, the ITS method will be applied to solve the Dirac equation with the nonlocal potential in coordinate space following the success in solving the Dirac equation with the local potential by the ITS evolution for the corresponding Schrödinger-like equation for the upper component [21]. It will be demonstrated that the ITS evolution can be equivalently performed for the Schrödinger-like equation with or without localization, and the latter algorithm is recommended for the reason of simplicity and efficiency.

In the relativistic Hartree-Fock approach, the main issue is to solve the Dirac equation

\[
\{ \alpha \cdot p + \beta [M + S(r)] + V(r) \} \varphi_a(r) + \int dr' U(r, r') \varphi_a(r') = \varepsilon_a \varphi_a(r),
\]

(1)

with the local (scalar and vector) potentials \( S(r) \) and \( V(r) \), and the nonlocal potential \( U(r, r') \). For clarity and simplicity, \( V(r) \pm S(r) \) are assumed to be the spherical Woods-Saxon potentials similar as in Ref. [18], and thus the Dirac spinor takes the form,

\[
\varphi_a(r) = \frac{1}{r} \begin{pmatrix} iF_a(r) \mathcal{Y}_{j_a m_{j_a}}^l(\Omega) \\ -G_a(r) \mathcal{Y}_{j_a m_{j_a}}^{l'}(\Omega) \end{pmatrix} \chi^{1/2}(q_a), \ l_a + l'_a = 2j_a,
\]

(2)

with the isospinor \( \chi^{1/2}(q_a) \) and the spherical spinor \( \mathcal{Y}_{j_a m_j}(\Omega) \). The single-particle state is labeled by the quantum numbers \( \{ n_a, l_a, \kappa_a, j_a \} \) of the upper component, where \( \kappa_a = \pm |j_a + 1/2| \) for \( l_a = j_a \pm 1/2 \).

Similar as in Ref. [22], the nonlocal potential \( U(r, r') \) is expanded as,

\[
U(r, r') = \sum_l \frac{u_l(r, r') 2l + 1}{4\pi} P_l(\cos \omega),
\]

(3)

where \( P_l \) is the Legendre polynomial and \( \omega \) is the angle between \( r \) and \( r' \). More explicitly,
if \( U(r, r') \) takes the same form as in Ref. \[22\],

\[
U(r, r') = \frac{\sqrt{u(r)u(r')}}{(\pi \gamma^2)^{\frac{1}{2}}} e^{-(r-r')^2/\gamma^2},
\]

the expansion coefficient \( u_l(r, r') \) can be obtained as,

\[
u_l(r, r') = \frac{2\sqrt{rr'} \gamma}{\gamma^2} u(r)u(r') e^{-\frac{r^2+r'^2}{\gamma^2}} I_{l+\frac{1}{2}} \left( \frac{2rr'}{\gamma^2} \right),
\]

where \( I_{l+\frac{1}{2}} \) is the modified Bessel function of the first kind. In practice, the central part \( u(r) \) could take the shape of Woods-Saxon type,

\[
u(r) = -\frac{V_0}{1 + e^{(r-R)/a}}, R = r_0A^{1/3},
\]

with the parameters, \( V_0, r_0, \alpha \) and the nonlocality parameter \( \gamma \).

With the expansion as in Equation \[3\], the Dirac equation with nonlocal potential can be reduced as

\[
\begin{pmatrix}
V + S + M & -\frac{d}{dr} + \frac{\kappa a}{r} \\
\frac{d}{dr} + \frac{\kappa a}{r} & V - (S + M)
\end{pmatrix}
\begin{pmatrix}
F_a(r) \\
G_a(r)
\end{pmatrix}
+ \begin{pmatrix}
X_a(r) \\
Y_a(r)
\end{pmatrix} = \varepsilon_a \begin{pmatrix}
F_a(r) \\
G_a(r)
\end{pmatrix},
\]

where the nonlocal terms are

\[
X_a(r) = \int dr' U_X (r, r') F_a(r'), \quad U_X (r, r') \equiv u_{l_a} (r, r'),
\]

\[
Y_a(r) = \int dr' U_Y (r, r') G_a(r'), \quad U_Y (r, r') \equiv u_{l_a} (r, r').
\]

The coupled integro-differential equations in Equation\[7\] cannot be directly solved by the conventional shooting (Runge-Kutta) method unless they are transformed to homogeneous differential equations by localization \[23\]. For example, one can rewrite Equation \[7\] as

\[
\begin{pmatrix}
V + S + M + X_{a,F_a} & -\frac{d}{dr} + \frac{\kappa a}{r} + X_{a,G_a} \\
\frac{d}{dr} + \frac{\kappa a}{r} + Y_{a,F_a} & V - (S + M) + Y_{a,G_a}
\end{pmatrix}
\begin{pmatrix}
F_a(r) \\
G_a(r)
\end{pmatrix}
= \varepsilon_a \begin{pmatrix}
F_a(r) \\
G_a(r)
\end{pmatrix},
\]

with the localized effective potentials,

\[
X_{a,F_a} \equiv \frac{F_a(r)X_a}{F_a^2(r) + G_a^2(r)}, \quad X_{a,G_a} \equiv \frac{G_a(r)X_a}{F_a^2(r) + G_a^2(r)},
\]

\[
Y_{a,F_a} \equiv \frac{F_a(r)Y_a}{F_a^2(r) + G_a^2(r)}, \quad Y_{a,G_a} \equiv \frac{G_a(r)Y_a}{F_a^2(r) + G_a^2(r)},
\]

then Equation\[9\] could be solved iteratively from an initial guess of the wave function by the shooting method.
For the ITS method, as demonstrated in Ref. [21], the evolution can be performed by using the effective single-particle Hamiltonian for the upper component $\hat{h}_{\text{eff}}$. With the relation between the upper and lower components in Equation (9),

$$G_a = \frac{1}{M_L} \left( \frac{dF_a}{dr} + \frac{\kappa_a}{r} F_a + Y_{a,F_a} F_a \right),$$

where $M_L = M - (V - S) - Y_{a,G_a} + \varepsilon_a$,  

(11)

the Schrödinger-like equation for the upper components is, $\hat{h}_{\text{eff}} F_a = \varepsilon_a F_a$, with

$$\hat{h}_{\text{eff}} F_a = -\frac{1}{M_L} \frac{d^2 F_a}{dr^2} + \left[ -\frac{1}{M_L} (Y_{a,F_a} - X_{a,G_a}) + \frac{1}{M_L^2} \frac{dM_L}{dr} \right] \frac{dF_a}{dr}$$

$$+ \left[ \frac{1}{M_L} \frac{\kappa_a (\kappa_a + 1)}{r^2} + \frac{1}{M_L} \frac{\kappa_a}{r} \left( \frac{1}{M_L} \frac{dM_L}{dr} + Y_{a,F_a} + X_{a,G_a} \right) \right] F_a$$

$$+ \left( -\frac{1}{M_L} \frac{dY_{a,F_a}}{dr} + \frac{1}{M_L^2} \frac{dM_L}{dr} Y_{a,F_a} + \frac{1}{M_L} X_{a,G_a} Y_{a,F_a} \right) + (V + S + M + X_{a,F_a}) \right] F_a.$$  

(12)

On the other hand, one could also obtain the relation between the upper and lower components from Equation (7),

$$G_a = \frac{1}{M_+} \left( \frac{dF_a}{dr} + \frac{\kappa_+}{r} F_a + Y_a \right),$$

where $M_+ = M - (V - S) + \varepsilon_a$,  

(13)

and the corresponding Schrödinger-like equation for the upper component gives

$$\hat{h}_{\text{eff}} F_a = -\frac{1}{M_+} \frac{d^2 F_a}{dr^2} + \frac{1}{M_+^2} \frac{dM_+}{dr} \frac{dF_a}{dr} + \left[ (V + S + M) + \frac{1}{M_+^2} \frac{dM_+}{dr} \frac{\kappa_+}{r} + \frac{1}{M_+} \frac{\kappa_+ (\kappa_+ + 1)}{r^2} \right] F_a$$

$$-\frac{1}{M_+} \frac{dY_a}{dr} + \frac{1}{M_+^2} \frac{dM_+}{dr} Y_a + \frac{1}{M_+} \frac{\kappa_+}{r} Y_a + X_a.$$  

(14)

Although the right-hand sides are different, Equation (14) is exactly the same as Equation (12). Moreover, one should note that the ITS evolution involves only the operation $\hat{h}_{\text{eff}} F_a$. Therefore, the nonlocalized ITS evolution for Equation (14) is equivalent to the localized one for Equation (12). For the reason of simplicity and efficiency, the nonlocalized ITS evolution for Equation (14) will be used.

In the numerical calculations, the ITS evolution starts from the initial orthogonal wave functions $\{ \varphi_a^{(0)} \}$ with spherical Bessel function for the upper components and zero for the lower components. Together with the given nonlocal potentials (5), the initial $X_{a}^{(0)}(r)$ and $Y_{a}^{(0)}(r)$ are constructed according to Eqs. (8a) and (8b). Then the operation $\hat{h}_{\text{eff}} F_a$ in Equation (14) is obtained and applied to evolve the single-particle wave functions, which is carried out in coordinate space within a spherical box $[0, R]$ with the box size $R = 20$ fm.
mesh size $dr = 0.1$ fm and a typical time step $\Delta t = 10^{-26}$ s. The set of wave functions thus obtained is then orthogonalized by the standard Gram-Schmidt procedure to provide a new set of orthogonal single-particle wave functions which will be used for the next ITS evolution. This process is repeated till the final convergence.

Take the state $\nu 1s_{1/2}$ in $^{16}$O as an example, the nonlocal potentials $U_X(r, r')$ and $U_Y(r, r')$ defined in Eqs. (8a) and (8b) are shown in Fig. 1. The detailed parameters for the nonlocal potentials chosen tentatively to give a reasonable single-particle spectrum in $^{16}$O can be found in the corresponding caption. The nonlocal potentials $U_X(r, r')$ and $U_Y(r, r')$ are state-dependent with different orbital angular momentum quantum numbers $l_a$ and $l'_a$ for the upper and lower components, respectively.

The ITS evolutions of the single-particle wave function and the nonlocal terms $X(r), Y(r)$ for $\nu 1s_{1/2}$ in $^{16}$O are illustrated in Fig. 2. The initial single-particle wave function which is assumed to be spherical Bessel function for the upper component and zero for the lower component, together with the corresponding $X(r)$ and $Y(r)$ are denoted by the thin solid line, which are followed by the results at $2 \times 10^3$ (dotted lines) and $4 \times 10^3$ (dash-dotted lines) iterations. Finally, the evolution results converge to the same ones obtained by the shooting method. The results from shooting method are obtained by solving the Dirac equation with the localized effective potentials from the converged $X(r)$ and $Y(r)$ in the ITS evolution.

Similarly, the neutron single-particle spectrum of $^{16}$O can be obtained by the ITS method as shown in Fig. 3 where the the evolutions of the corresponding single-particle energies are also illustrated. It can be seen that different levels converge at different speeds. The deeper the level lies, the faster the evolution converges. Most levels converge monotonously except the level $2s_{1/2}$, which evolves with fluctuation at the beginning due to the orthonormalization with respect to the level $1s_{1/2}$.

In summary, the ITS method is applied for solving the Dirac equation with nonlocal potential. Similar as in Ref. [21], the evolution is performed for the corresponding Schrödinger-like equation for the upper component. It is demonstrated that the ITS evolution can be equivalently performed for the Schrödinger-like equation with or without localization. The nonlocalized ITS evolution is much more simple and efficient, and thus is recommended for future application. These conclusions are further supported by the numerical solution of the Dirac equation with nonlocal potential reasonably chosen for $^{16}$O. The present algorithm provides the same results as the shooting method for the Dirac equation with the localized
effective potentials. The investigation here demonstrates the possibility of the ITS method in the relativistic Hartree-Fock theory.

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FIG. 1: (color online) The nonlocal potentials $U_X(r, r')$ and $U_Y(r, r')$ for $\nu 1s_{1/2}$ state in nucleus $^{16}$O. The parameters in Eqs. (5) and (6) are chosen as $V_0 = 10$ MeV, $r_0 = 1.04$ fm, $\alpha = 0.65$ fm and $\gamma = 1.0$ fm.

FIG. 2: (color online) The evolutions of the single-particle wave functions $F(r)$, $G(r)$ and the nonlocal terms $X(r)$, $Y(r)$ for $\nu 1s_{1/2}$ in nucleus $^{16}$O. The evolutions are illustrated at the initial (thin solid lines), $2 \times 10^3$ (dotted lines), $4 \times 10^3$ (dash-dotted lines) iterations. The converged results (thick solid lines) of the ITS evolution are compared with the results by shooting method (dashed lines).
FIG. 3: (color online) The evolutions of the single-particle energies and the final convergent neutron single-particle spectrum of nucleus $^{16}$O obtained by the ITS method.