First attempt to overcome the disaster of Dirac sea in imaginary time step method[*]

ZHANG Ying(张颖)[1]   LIANG Hao-Zhao(梁豪兆)[1,2]   MENG Jie(孟杰)[1,3,4,5;1]

1 (School of Physics and State Key Laboratory of Nuclear Physics and Technology, Peking University, Beijing 100871, China)
2 (Institut de Physique Nucléaire, IN2P3-CNRS and Université Paris-Sud, F-91406 Orsay, France)
3 (Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China)
4 (Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou, 730000, China)
5 (Department of Physics, University of Stellenbosch, Stellenbosch, South Africa)

Abstract Efforts have been made to solve the Dirac equation with axially deformed scalar and vector Woods-Saxon potentials in the coordinate space with the imaginary time step method. The results of the single-particle energies thus obtained are consistent with those calculated with the basis expansion method, which demonstrates the feasibility of the imaginary time step method for the relativistic static problems.

Key words imaginary time step method, Dirac equation, Woods-Saxon potential, axially deformed, coordinate space

PACS 02.60.Cb, 03.65.Pm, 21.10.-k

1 Introduction

The relativistic mean field (RMF) theory[1] has received lots of attention due to its successful description of numerous nuclear phenomena from infinite nuclear matter to finite nuclei[2, 3]. It is also one of the best candidates for the theoretical description of exotic nuclei[4]. To describe the extremely weakly binding properties of these exotic nuclei, it is desired to solve the Dirac equation directly in coordinate space. For spherical system, the conventional shooting method could solve the Dirac equation without any difficulties. However, when it comes to deformed system, the shooting method for coupled channels[5] or Woods-Saxon basis expansion method[6] becomes more complicated and difficult.

On the other hand, the imaginary time step (ITS) method[7] is an alternative to solve the static problems in coordinate space, which has been well-developed in non-relativistic framework on 3-dimensional Cartesian mesh[8]. This method is a kind of gradient methods[9, 10], which searches for the direction of steepest descent of energy and follows it in

iterative steps until the local minimum on the energy surface is reached.

Therefore, it is natural to introduce the ITS method to the deformed relativistic system. However, its feasibility has been doubted for years due to the existence of negative energy solutions of Dirac equation. Since ITS method always starts from finding the lowest state in the equation of motion, it becomes a disaster as there is no bottom in the Dirac sea.

In this paper, we attempt to adopt the ITS method to solve the Dirac equation with axially deformed scalar and vector Woods-Saxon potentials in the coordinate space, and try to overcome the disaster of Dirac sea.

In Section 2, the principle of ITS method and its application in relativistic framework are presented. Section 3 is devoted to numerical details and the corresponding results. The summary and conclusions are given in Section 4.

2 Imaginary time step method to solve deformed Dirac equation

The imaginary time step (ITS) method[7] is

inspired by the technique employed to solve the time-dependent Hartree-Fock (TDHF) equation,

$$i\hbar\frac{\partial\varphi_j}{\partial t} = \hat{h}(t)\varphi_j(t), \qquad j = 1,...,A. \qquad (1)$$

The solution $\{\varphi_j^{(n+1)}\}$ of the above equation at time $t_{n+1} = (n+1)\Delta t$ can be approximated by

$$|\varphi_j^{(n+1)}\rangle = \exp\left(-\frac{i}{\hbar}\Delta t\hat{h}^{(n+\frac{1}{2})}\right)|\varphi_j^{(n)}\rangle, \qquad (2)$$

in which $\hat{h}^{(n+\frac{1}{2})}$ is the numerical approximation to the single-particle hamiltonian $\hat{h}(t)$ at time $(n+\frac{1}{2})\Delta t$.

If the time step Δt is real, the operator $\exp\left(-\frac{i}{\hbar}\Delta t\hat{h}^{(n+\frac{1}{2})}\right)$ indicates a unitary transformation between the wave functions at two immediate time steps, which could guarantee the orthogonality of the initial set of wave functions, and thus the conservation of the total energy during the time evolution.

When the real time step Δt in Eq. (2) is replaced by an imaginary one $-i\Delta t$ (Δt is still real in this expression, $\lambda \equiv \Delta t/\hbar$), the transformation Eq. (2) reads

$$|\Psi_j^{(n+1)}\rangle = \exp\left(-\lambda\hat{h}^{(n+\frac{1}{2})}\right)|\varphi_j^{(n)}\rangle =$$
$$\left(1 - \lambda\hat{h}^{(n+\frac{1}{2})}\right)|\varphi_j^{(n)}\rangle + O(\lambda^2). \qquad (3)$$

In this case, the operator in Eq. (3) does not guarantee the orthogonality of wave functions during the time evolution. Then, it could be demonstrated that after orthogonalization the total energy will decrease as the time evolves, until it converges to a stable state, which is the static solution of the Hartree-Fock equation.

The attempt here will be made to apply ITS method to solve Dirac equation with given potentials,

$$\{\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta[m + S(\boldsymbol{r})] + V(\boldsymbol{r})\}\varphi_i = \varepsilon_i\varphi_i. \qquad (4)$$

When an axial deformation is adopted for the system, the Dirac spinor φ_i takes the form of[11]

$$\varphi_i = \frac{1}{\sqrt{2\pi}}\begin{pmatrix} f_i^+(z,r_\perp)e^{i(\Omega_i-1/2)\phi} \\ f_i^-(z,r_\perp)e^{i(\Omega_i+1/2)\phi} \\ ig_i^+(z,r_\perp)e^{i(\Omega_i-1/2)\phi} \\ ig_i^-(z,r_\perp)e^{i(\Omega_i+1/2)\phi} \end{pmatrix}\chi_{\tau_i}(\tau), \qquad (5)$$

where $f_i^\pm$ and $g_i^\pm$ are the upper and lower components, Ω_i is the projection of total angular momentum along the symmetry axis, $\chi_{\tau_i}(\tau)$ is the pauli matrix for isospin. Correspondingly, the Dirac equation Eq. (4) in the cylindrical coordinates could be reduced to

$$\begin{pmatrix} V+M^* & 0 & \partial_z & \partial_{r_\perp}+\dfrac{\Omega+\frac{1}{2}}{r_\perp} \\ 0 & V+M^* & \partial_{r_\perp}-\dfrac{\Omega-\frac{1}{2}}{r_\perp} & -\partial_z \\ -\partial_z & -\left(\partial_{r_\perp}+\dfrac{\Omega+\frac{1}{2}}{r_\perp}\right) & V-M^* & 0 \\ -\left(\partial_{r_\perp}-\dfrac{\Omega-\frac{1}{2}}{r_\perp}\right) & \partial_z & 0 & V-M^* \end{pmatrix}\begin{pmatrix} f_i^+ \\ f_i^- \\ g_i^+ \\ g_i^- \end{pmatrix} = \varepsilon_i\begin{pmatrix} f_i^+ \\ f_i^- \\ g_i^+ \\ g_i^- \end{pmatrix}, \qquad (6)$$

with $M^* = m + S(z,r_\perp)$. The 4×4 matrix operator on the l.h.s. in Eq. (6) is thus the single-particle hamiltonian $\hat{h}$ which could be used in the imaginary time evolution in Eq. (3).

Referring to the application of ITS method in nonrelativistic framework, we rewrite the above Dirac equation Eq. (6) to Schrödinger-like equation for the upper component, then evolve the upper components as Eq. (3), and obtain the lower components by the

relation of

$$\begin{pmatrix} g_i^+ \\ g_i^- \end{pmatrix} = \frac{-1}{M_i^*}\begin{pmatrix} \partial_z & \partial_{r_\perp}+\dfrac{\Omega+\frac{1}{2}}{r_\perp} \\ \partial_{r_\perp}-\dfrac{\Omega-\frac{1}{2}}{r_\perp} & -\partial_z \end{pmatrix}\begin{pmatrix} f_i^+ \\ f_i^- \end{pmatrix}, \qquad (7)$$

where $M_i^* = M^* - V + \varepsilon_i$.

3 Numerical details and results

As a first attempt, the scalar and vector potentials in Dirac equation Eq. (4) take the form of axially de-

formed Woods-Saxon potentials[12]. In this case, the single-particle states are labeled by good quantum numbers (Ω,π). To evolve the single-particle wave functions, we take the axially deformed Harmonic Oscillator bases for the upper components, and zero for the lower components as a set of orthogonal initial wave functions,

$$f_i^{\pm}(z,r_{\perp}) \to \phi_{n_z}(z)\phi_{n_r}^{m_l}(r_{\perp})\chi_{\pm\frac{1}{2}}(s), \qquad (8a)$$

$$g_i^{\pm}(z,r_{\perp}) \to 0, \qquad (8b)$$

where

$$\phi_{n_z}(z) = \frac{\mathcal{N}_{n_z}}{\sqrt{b_z}}H_{n_z}(\zeta)e^{-\zeta^2/2},$$

$$\left(\zeta = \frac{z}{b_z}, \ \mathcal{N}_{n_z} = \frac{1}{\sqrt{\sqrt{\pi}2^{n_z}n_z!}}\right), \quad (9a)$$

$$\phi_{n_r}^{m_l}(r_{\perp}) = \frac{\mathcal{N}_{n_r}^{m_l}}{b_{\perp}}\sqrt{2}\eta^{m_l/2}L_{n_r}^{m_l}(\eta)e^{-\eta/2},$$

$$\left(\eta = \frac{r_{\perp}^2}{b_{\perp}^2}, \ \mathcal{N}_{n_r}^{m_l} = \sqrt{\frac{n_r!}{(n_r+m_l)!}}\right). \ (9b)$$

During the time evolution, the wave functions are confined in a box $(0 \leqslant r_{\perp} \leqslant L_{r_{\perp}}, \ -L_z \leqslant z \leqslant L_z)$, with mesh sizes $dr_{\perp}$ and dz respectively.

After the evolution in Eq. (3), the set of wave functions $\{\Psi_j^{(n+1)}\}$ is orthogonalized by Gram-Schmidt orthogonalization method. Then a new set of orthogonal wave functions $\{\varphi_j^{(n+1)}\}$ is obtained, which will go on for the next step of evolution and orthogonalization. The above procedure is iterated until the final convergence is reached.

Table 1 shows the single-particle energies calculated by the ITS method compared with the basis expansion method for the nucleus ^{16}O. In the present calculation, we take a deformation $\beta = 0.1$ for the scalar and vector Woods-Saxon potentials, with the Coulomb interaction included for protons. For the ITS method, the box size is $L_{r_{\perp}} = L_z = 12$ fm, with the mesh $dr_{\perp} = dz = 0.3$ fm, the corresponding imaginary time step is $\Delta t = 5 \times 10^{-26}$ s. In the basis expansion method, we take 8 shells for both fermion and boson.

It can be seen from the comparison in Table 1 that the ITS method could give the results consistent with those calculated by the basis expansion method within the precision tolerance.

Table 1.   Single-particle energis for neutron and proton calculated by ITS method compared with basis expansion (BE) method for the nucleus ^{16}O in Woods-Saxon potentials with $\beta = 0.1$.

	neutron		proton	
	ITS	BE	ITS	BE
$(\Omega)^{\pi}$	ε_i/MeV	ε_i/MeV	ε_i/MeV	ε_i/MeV
$\left(\frac{1}{2}\right)^{+}$	−43.547	−43.216	−40.386	−40.096
$\left(\frac{1}{2}\right)^{-}$	−25.668	−25.524	−23.441	−23.310
$\left(\frac{3}{2}\right)^{-}$	−24.111	−24.085	−21.788	−21.773
$\left(\frac{1}{2}\right)^{-}$	−19.015	−18.871	−18.283	−18.146
$\left(\frac{1}{2}\right)^{+}$	−8.636	−8.541	−6.825	−6.733
$\left(\frac{3}{2}\right)^{+}$	−7.819	−7.831	−5.939	−5.954
$\left(\frac{5}{2}\right)^{+}$	−6.637	−6.587	−4.666	−4.619
$\left(\frac{1}{2}\right)^{+}$	−3.703	−3.273	−2.640	−2.339
$\left(\frac{1}{2}\right)^{+}$	−1.812	−1.455	−1.277	−0.962
$\left(\frac{3}{2}\right)^{+}$	−0.715	−0.386	−0.128	0.074

4   Summary and conclusions

The first attempt has been made to apply the imaginary time step method, which has been widely used in non-relativistic static problems, for the Dirac equation with axially deformed scalar and vector Woods-Saxon potentials. First results obtained show that this method is also feasible in the relativistic framework. The single-particle energies obtained in this way are consistent with the conventional basis expansion method. More systematical investigations along this line including the numerical checks and details of the calculation are in preparation and will be published elsewhere.

References

1   Serot B D, Walecka J D. Adv. Nucl. Phys., 1986, **16**: 1
2   Ring P, Prog. Part. Nucl. Phys., 1996, **37**: 193
3   Vretenar D, Afanasjev A V, Lalazissis G A, Ring P. Phys. Rep., 2005, **409**: 101
4   MENG J, Toki H, ZHOU S G, ZHANG S Q, LONG W H, GENG L S. Prog. Part. Nucl. Phys., 2006, **57**: 470
5   Price C E, Walker G E. Phys. Rev. C, 1987, **36**: 354
6   ZHOU S G, MENG J, RING P. Phys. Rev. C, 2003, **68**: 034323

7   Davies K T R, Flocard H, Krieger S J, Weiss M S. Nucl. Phys. A, 1980, **342**: 111
8   Bonche P, Flocard H, Heenen P H, Krieger S J, Weiss M S. Nucl. Phys. A, 1985, **443**: 39
9   Kelemen A. Nucl. Phys. A, 1974,**220**: 391
10   MANG H J, Samadi B, Ring P. Z. Phys. A, 1976, **279**: 325
11   Ring P, Gambhir Y K, Lalazissis G A. Com. Phys. Com., 1997, **105**: 77
12   Koepf W, Ring P. Z. Phys. A, 1991, **339**: 81