

Variational-Iterative Solution of Ground State for Central Potential*

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Abstract *The newly developed iterative method based on Green function defined by quadratures along a single trajectory is combined with the variational method to solve the ground state quantum wave function for central potentials. As an example, the method is applied to discuss the ground state solution of Yukawa potential, using Hulthen solution as the trial function.*

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1 Introduction

Recently an iterative solution of the ground state for the one-dimensional double-well potential is obtained^[1] based on the Green function method developed in Ref. [2]. This Green function is defined along a single trajectory, from which the ground state wave function in N -dimension can be expressed by quadratures along the single trajectory. This makes it possible to develop an iterative method for obtaining the ground state wave function, starting from a properly chosen trial function. The convergence of the iterative solution depends very much on the choice of the trial function.^[1] Therefore the key of this new method is to find the best trial function as the starting point of the iteration process.

On the other hand the variational method is a well-known approximate approach to solve Schrödinger equation starting from a trial function with a set of variational parameters. By minimizing the expectation value of the Hamiltonian respect to the set of parameters of the trial function, the variational solution could be obtained. If the starting trial function is properly chosen the solution could be a very good approximation for the equation. However, it is difficult to further improve the accuracy of this approximate solution.

In this paper the two methods are combined to get a variational-iterative solution. The result is obviously more accurate than the variational one. It has been shown in Ref. [1] that the final iterative solution is convergent if the trial function is properly chosen. As an example the variational-iterative method is applied to solve Yukawa potential, using the solution of a Hulthen potential as the trial function. The obtained result up to the second order is compared to those based on the pure variational procedure, starting from the same trial function. The solution

of the combined method is improved significantly.

In Sec. 2, a brief introduction is given about the Green function method based on the single trajectory quadrature and the corresponding iterative formula for central potentials. The variational-iterative solution for Yukawa potential is given in Sec. 3. The numerical results and discussions are given in Sec. 4.

2 Green Function and Its Iterative Solution for a Central Potential

2.1 Green Function

We discuss a particle with unit mass, moving in a central potential $V(r)$. The ground state wave function $\Psi(r)$ satisfies

$$\left[-\frac{1}{2}\nabla^2 + V(r)\right]\Psi(r) = E\Psi(r). \quad (1)$$

The boundary condition for $\Psi(r)$ is set as

$$\Psi(0) = 1 \quad \text{and} \quad \Psi(\infty) = 0. \quad (2)$$

Now a trial function $\Phi(r)$, satisfying the same boundary condition as $\Psi(r)$, is introduced into the following Schrödinger equation

$$\left[-\frac{1}{2}\nabla^2 + V_0(r)\right]\Phi(r) = E_0\Phi(r). \quad (3)$$

The trial function should be chosen so that the difference of the two potentials

$$U(r) = V(r) - V_0(r) \quad (4)$$

is small. Defining a Green function D satisfying the following equation^[2]

$$\left[-\frac{1}{2}\nabla^2 + V_0(r) - E_0\right]D = 1, \quad (5)$$

then the solution $\Psi(r)$ can be formally expressed as

$$\Psi = \Phi - D(U - \Delta)\Psi \quad (6)$$

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with $\Delta = E - E_0$. Express $\Psi = \Phi f$, and f satisfies

$$f = 1 - \bar{D}(U - \Delta)f, \quad (7)$$

where

$$\bar{D} = \Phi^{-1}D\Phi. \quad (8)$$

Following the same procedure as in Ref. [2], in the spherical coordinate system with variables (r, θ, ϕ) the single trajectory is chosen as the radial coordinate r and correspondingly we define

$$\begin{aligned} h_r^2 &= [(\nabla r)^2]^{-1} = 1, \\ h_\theta^2 &= [(\nabla \theta)^2]^{-1} = r^2, \\ h_\phi^2 &= [(\nabla \phi)^2]^{-1} = r^2 \sin^2 \theta, \\ h_\omega &= h_\theta h_\phi = r^2 \sin \theta \end{aligned} \quad (9)$$

with the volume element

$$d\tau = h_r h_\omega dr d\theta d\phi. \quad (10)$$

Introducing a step function

$$(r|\Theta|r') \equiv \begin{cases} 1, & \text{for } r > r' > 0, \\ 0, & \text{for } 0 < r < r', \end{cases} \quad (11)$$

or

$$(r|\Theta|r') \equiv \begin{cases} 0, & \text{for } r > r' > 0, \\ -1, & \text{for } 0 < r < r'. \end{cases} \quad (12)$$

It can be proved^[2] that the Green function is

$$\begin{aligned} \bar{D} &\equiv -2\Theta\Phi^{-2}\frac{h_r}{h_\omega}\Theta\Phi^2h_rh_\omega \\ &= -2\Theta\Phi^{-2}r^{-2}\Theta\Phi^2r^2. \end{aligned} \quad (13)$$

According to the boundary condition of the wave functions we have

$$f = 1 \quad \text{at } r = 0, \quad \text{and } f = \text{finite} \quad \text{at } r \rightarrow \infty. \quad (14)$$

Using the definitions of the step functions (11) and (12) to express the first and the second Θ -function in Eq. (13), respectively, f has the following integral form

$$\begin{aligned} f(r) &= 1 - 2 \int_0^r \Phi^{-2}(r')r'^{-2} dr' \int_{r'}^\infty \Phi^2(r'') \\ &\quad \times (U(r'') - \Delta)f(r'')r''^2 dr'' \end{aligned} \quad (15)$$

and $\Psi(r) = \Phi(r)f(r)$ is the solution of Eq. (1). Considering the definitions in Eqs. (9) and (10), the corresponding energy correction Δ can be expressed as

$$\Delta = \frac{\int_0^\infty \Phi^2(r)U(r)f(r)r^2 dr}{\int_0^\infty \Phi^2(r)f(r)r^2 dr}, \quad (16)$$

which can be formally expressed as

$$\Delta = [Uf]/[f] \quad (17)$$

with $[F]$ defined as

$$[F] = \int_0^\infty \Phi^2(r)F(r)r^2 dr. \quad (18)$$

2.2 Iterative Solution

Based on Eqs. (7) and (17), two iterative sequences $\{f_n\}$ and $\{\Delta_n\}$ are introduced as

$$\begin{aligned} f_0 &= 1, f_1, f_2, f_3, \dots, f_n, \dots, \\ \Delta_0 &= 0, \Delta_1, \Delta_2, \Delta_3, \dots, \Delta_n, \dots \end{aligned} \quad (19)$$

We require

$$\begin{aligned} f_n &= 1 - \bar{D}(U - \Delta_n)f_{n-1}, \\ \Delta_n &= [Uf_{n-1}]/[f_{n-1}]. \end{aligned} \quad (20)$$

In the explicit form,

$$\begin{aligned} f_n(r) &= 1 - 2 \int_0^r \Phi^{-2}(r')r'^{-2} dr' \int_{r'}^\infty \Phi^2(r'') \\ &\quad \times (U(r'') - \Delta_n)f_{n-1}(r'')r''^2 dr'' \end{aligned} \quad (21)$$

with

$$\Delta_n = \frac{\int_0^\infty \Phi^2(r)f_{n-1}(r)U(r)r^2 dr}{\int_0^\infty \Phi^2(r)f_{n-1}(r)r^2 dr}. \quad (22)$$

For a properly chosen trial function $\Phi(r)$ this iterative procedure will approach the solution

$$\begin{aligned} f(r) &= \lim_{n \rightarrow \infty} f_n(r), \quad \text{for all } r \geq 0, \\ \Delta &= \lim_{n \rightarrow \infty} \Delta_n, \end{aligned} \quad (23)$$

and $\Psi(r) = \Phi(r)f(r)$, $E = E_0 + \Delta$.

3 Variational-Iterative Solution of Ground State for Yukawa Potential

The variational solution of Yukawa potential has been widely discussed in details.^[3] In Ref. [3] using a Hulthen solution as the trial function the result based on variational method is compared to the results from different methods. In our paper starting from the Hulthen solution we first give the traditional variational result. Using it as the trial function of the iterative procedure the further improvement can be obtained. The Hamiltonian for the Yukawa potential is

$$H = -\frac{1}{2m}\nabla^2 - g^2 \frac{e^{-\alpha r}}{r}. \quad (24)$$

To simplify the notation, based on the following rescaling:^[3]

$$\frac{\alpha}{mg^2} \rightarrow \alpha, \quad mg^2r \rightarrow r, \quad \frac{E}{mg^4} \rightarrow E, \quad (25)$$

the Hamiltonian can be expressed as

$$H = -\frac{1}{2}\nabla^2 - \frac{e^{-\alpha r}}{r}, \quad H\Psi(r) = E\Psi(r). \quad (26)$$

Introducing the trial function

$$\Phi_\lambda(r) = \frac{1 - e^{-\lambda r}}{r} e^{-r + \lambda r/2} \quad (27)$$

with a variational parameter λ , which satisfies the Schrödinger equation with a Hulthen potential

$$\begin{aligned} H_\lambda &= -\frac{1}{2}\nabla^2 - \frac{\lambda e^{-\lambda r}}{1 - e^{-\lambda r}}, \\ H_\lambda \Phi_\lambda(r) &= E_\lambda \Phi_\lambda(r), \end{aligned} \quad (28)$$

where

$$E_\lambda = -\frac{1}{2} + \frac{1}{4}\lambda - \frac{1}{8}\lambda^2. \quad (29)$$

Based on the variational method the approximate solution of Eq. (26) can be obtained by minimizing the expectation value of H in Eq. (26),

$$\begin{aligned} \bar{H} &= \frac{\int_0^\infty r^2 \Phi_\lambda(r) \left(-\frac{1}{2}\nabla^2 - \frac{e^{-\alpha r}}{r} \right) \Phi_\lambda(r) dr}{\int_0^\infty \Phi_\lambda^2(r) r^2 dr}, \\ \frac{\partial \bar{H}}{\partial \lambda} &= 0. \end{aligned} \quad (30)$$

Now using the obtained wave function $\Phi_\lambda(r)$ as the zero-th order solution, we introduce the formal Green function expression of $\Psi(r) = \Phi_\lambda(r)f(r)$ in the following way. We can define Green function D and \bar{D} satisfying

$$(H_\lambda - E_\lambda)D = 1, \quad (31)$$

$$\bar{D} = \Phi_\lambda^{-1} D \Phi_\lambda. \quad (32)$$

As in Sec. 2, introducing the energy difference $\Delta = E - E_\lambda$ and the potential difference of Hamiltonians (26) and (28)

$$U(r) = \frac{\lambda e^{-\lambda r}}{1 - e^{-\lambda r}} - \frac{e^{-\alpha r}}{r}, \quad (33)$$

we obtain expressions for f and Δ similar to Eqs. (7) and (17). The Green function is

$$\bar{D} = -2\Theta\Phi_\lambda^{-2}r^{-2}\Theta\Phi_\lambda^2r^2. \quad (34)$$

Introducing the iterative series $\{f_n\}$ and $\{\Delta_n\}$ as Eqs. (19) and (20), the successive terms can be expressed as

$$\begin{aligned} \Delta_0 &= 0, & f_0 &= 1, \\ \Delta_1 &= \frac{[U]}{[1]}, & f_1 &= 1 - \bar{D}(U - \Delta_1), \\ \Delta_2 &= \frac{[Uf_1]}{[f_1]}, & f_2 &= 1 - \bar{D}(U - \Delta_2)f_1, \\ &\dots & &\dots \\ \Delta_n &= \frac{[Uf_{n-1}]}{[f_{n-1}]}, & f_n &= 1 - \bar{D}(U - \Delta_n)f_{n-1}. \end{aligned} \quad (35)$$

Here the trial function for the iterative procedure is the variational wave function Φ_λ . In the explicit form, for the

first order, we have

$$\begin{aligned} \Delta_1 &= \int_0^\infty \Phi_\lambda^2(r)U(r)r^2 dr / \int_0^\infty \Phi_\lambda^2(r)r^2 dr, \\ E_1 &= E_\lambda + \Delta_1, \end{aligned} \quad (36)$$

and

$$\begin{aligned} f_1(r) &= 1 - 2 \int_0^r \Phi_\lambda^{-2}(r')r'^{-2} dr' \int_{r'}^\infty \Phi_\lambda^2(r'') \\ &\quad \times (U(r'') - \Delta_1)r''^2 dr''. \end{aligned} \quad (37)$$

It is interesting to compare this first order result to the variational energy and the first order perturbation result. From Eq. (30)

$$\bar{H} = \frac{\int_0^\infty r^2 \Phi_\lambda(r)(H_\lambda + U)\Phi_\lambda(r) dr}{\int_0^\infty \Phi_\lambda^2(r)r^2 dr} = E_\lambda + \Delta_1, \quad (38)$$

which is the same as the first order result of the iterative method. If applying the perturbation method, the first order perturbation also gives the same energy. However, to further improve the above result the perturbation method would meet the problem of the unknown excited unperturbed states which are necessary for the calculation of the crossing-matrix elements in the second order calculation. For the iterative method, in principle, there is no problem for the higher order calculation. In general, for the n -th order, we have

$$\Delta_n = \frac{\int_0^\infty \Phi_\lambda^2(r)f_{n-1}(r)U(r)r^2 dr}{\int_0^\infty \Phi_\lambda^2(r)f_{n-1}(r)r^2 dr}, \quad (39)$$

$$E_n = E_\lambda + \Delta_n,$$

and

$$\begin{aligned} f_n(r) &= 1 - 2 \int_0^r \Phi_\lambda^{-2}(r')r'^{-2} dr' \int_{r'}^\infty \Phi_\lambda^2(r'') \\ &\quad \times (U(r'') - \Delta_n)f_{n-1}(r'')r''^2 dr''. \end{aligned} \quad (40)$$

In the next section the numerical results of E_1 and E_2 are given and compared to the result from the variational method for different α of the Yukawa potential in Eq. (26).

4 Numerical Results and Discussions

For the Yukawa potential with different parameter α , the variational parameter λ of a Hulthen potential can be obtained by minimizing the expectation value of the Hamiltonian Eq. (26) vs. λ . The values of λ corresponding to different α are listed in the first two columns of Table 1. For the Hulthen potential the upper limit of λ to have a bound state is $\lambda < 2$. Considering this limitation the highest value of α is taken to be $\alpha = 1.15$ which corresponds to $\lambda = 1.9473$. For different $\{\alpha, \lambda\}$ pairs the obtained zero-th order energy E_λ , the first order energy correction Δ_1 , and the corresponding binding energy of

the ground state $E_1 = E_\lambda + \Delta_1$ in the first order iteration are listed in columns 3–5 of Table 1. As mentioned in Sec. 3 the values of E_1 for different $\{\alpha, \lambda\}$ are exactly the same as the variational result in Ref. [3]. In columns 6–7 of Table 1 are given the values of the energy correction Δ_2 and the obtained binding energy of the ground state $E_2 = E_\lambda + \Delta_2$ after the second order iteration. For larger

α , the correction in the second order iteration is visible. Comparing to the numerical exact solution in column 8 taken from Ref. [4] the values after the second order iteration are obviously improved. In principle, the iteration process could go on to get more accurate result if the integrations in the iteration procedure could be performed properly.

Table 1 Ground state energy of Yukawa potential calculated based on variational-iterative method.

α	λ	$-E_\lambda$	$-\Delta_1$	$-E_1$	$-\Delta_2$	$-E_2$	Numeric.
0.1	0.2296	0.391790	0.015628	0.407058	0.015268	0.407058	0.4071
0.2	0.4358	0.305840	0.020968	0.326808	0.020968	0.326809	0.3268
0.25	0.5327	0.269121	0.021796	0.290918	0.021798	0.290920	0.2909
0.3	0.6263	0.235881	0.021753	0.257634	0.021757	0.257639	
0.4	0.8052	0.178443	0.019918	0.198362	0.019933	0.198376	
0.5	0.9750	0.131328	0.016756	0.148084	0.016789	0.148117	0.1481
0.6	1.1377	0.0929452	0.0131321	0.106077	0.0131915	0.106137	
0.7	1.2944	0.0622339	0.0095107	0.0717446	0.0096002	0.0718341	
0.8	1.4461	0.0383507	0.0062364	0.0445871	0.0063520	0.0447027	
0.9	1.5936	0.0206451	0.00353503	0.0241802	0.0036677	0.0243128	
1.0	1.7374	0.00861985	0.00153843	0.0101583	0.00165138	0.0102712	0.01029
1.05	1.8081	0.00460320	0.00083757	0.00544078	0.00093748	0.00554068	
1.1	1.8780	0.00186050	0.00034306	0.00220356	0.00041866	0.00227916	
1.15	1.9473	0.000347161	0.000065800	0.000412961	0.000068335	0.000415496	

It is possible to solve some excited states based on this method if the proper variational solution can be found. For example, since the variational solution of the excited S -states for the Hulthen potential is known,^[3] the corresponding solution for the Yukawa potential can be obtained by the iteration procedure. This method can also be extended to multi-dimensional cases as long as one can choose the proper variational solution and find the single trajectory to define the Green function and perform the necessary quadratures.^[1,2]

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