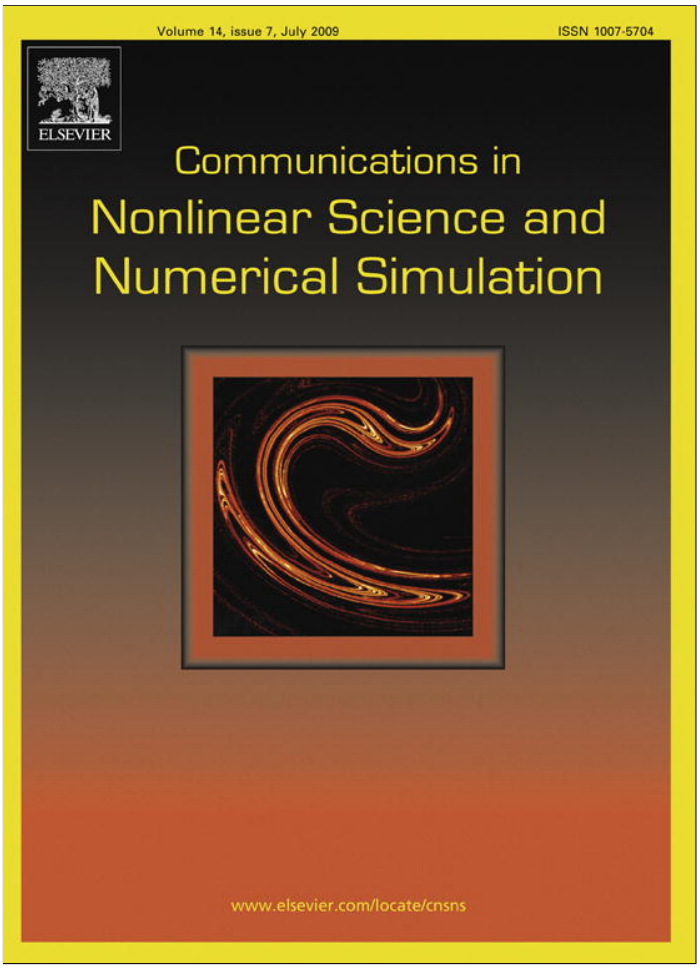

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A semi-inverse variational method for generating the bound state energy eigenvalues in a quantum system: The Schrödinger equation

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ABSTRACT

This paper deals with the semi-inverse variational method to extract the structures of bound states of the Schrödinger equation in a quantum environment. From realistic examples, some state configurations are presented to illustrate the effectiveness and the exactitude of the proposed method.

1. Introduction

In recent years the analysis of structures of the Schrödinger equation has gained considerable momentum and a particular attention. Several important physical problems in quantum system require solving the Schrödinger equation to determine the eigenenergies and the eigenfunctions. There are relatively few quantum mechanical problems for which the Schrödinger equation is exactly solvable.

Over the past years, a great deal of approximate schemas and numerical approaches have appeared to calculate the quantum quantities of the Schrödinger equation for numerous potential functions [1–13]. The scope of this area remains until now a more active field of diverse problems.

The main part of this work serves to the construction of a specific functional in the framework of spherically symmetric potentials by using the semi-inverse variational method [14,15]. In the application, a special attention is focused on the Coulomb potential. This last is chosen among other forms because it has been the subject of intense study and plays a central role in quantum physics.

The content of this paper is organized as follows. In Section 2, we present the necessary arguments which underlie the variational formulation in connection with the problems of quantum nature. In Section 3, some applications are proposed to concretize the method and conclusion and trends for future work are made in Section 4.

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2. Variational formulation: semi-inverse method

Hereby we begin with the radial Schrödinger equation for any spherically symmetric potential $V(r)$, i.e., a particle moving under the influence of a central potential, but this argument remains applicable also for arbitrary interactions.

$$-\frac{\hbar^2}{2mr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+(w(r)-E)R=0 \tag{1}$$

where $w(r)=V(r)+\frac{\hbar^2 l(l+1)}{2mr^2}$ is the effective potential, l denotes the angular momentum quantum number, $\hbar$ is called the reduced Planck constant (also known as Dirac's constant), $m(E)$ is the mass (energy) of the particle. In next section, for the examples, $V(r)$ is taken to be of Coulomb potential-type as $V(r)=-\frac{Ze^2}{4\pi\varepsilon r}$, where Z is the atomic number, and e is the charge of the particle.

However, we can rewrite Eq. (1) in the form

$$U(r;R;R';R'')\equiv-\frac{\hbar^2}{2m}\frac{d^2R}{dr^2}-\frac{\hbar^2}{mr}\frac{dR}{dr}+(w(r)-E)R=0 \tag{2}$$

where the superscripts $\prime$ and $\prime\prime$ denote the derivatives with respect to r. The consistency conditions for the existence of a functional integral are described in [16,17]. For the one-dimensional (1D) case, we have

$$\frac{\partial U}{\partial R'}=\frac{d}{dr}\left(\frac{\partial U}{\partial R''}\right) \tag{3}$$

We apply the consistency condition (3) to Eq. (2), it is easy to verify that this condition is not satisfied. Consequently, we use an auxiliary factor $g(r)$ and rewrite Eq. (2) as:

$$Y(r;R;R';R'')\equiv g(r)U(r;R;R';R'')=0 \tag{4}$$

and in Eq. (3), U is replaced by Y. Now the consistency condition is satisfied provided that $g(r)=r^2$.

Now, the differential equation (4) can be derived from a specific functional as stationary conditions.To find this functional, we apply the semi-inverse method which provides until now the best technique to establish variational principles for numerous physical problems. The basic idea of the semi-inverse method is illustrated as follows [18].

We construct in an alternative form a general trial functional for Eq. (4) as:

$$J(R)=\int_0^{+\infty}L dr \tag{5}$$

in which L is a trial-Lagrange function, which reads

$$L=a\frac{\hbar^2}{2m}\left(r\frac{dR}{dr}\right)^2+b(w(r)-E)(rR)^2+F \tag{6}$$

where F is an unknown function of R and/or its derivatives, a and b are arbitrary constants to be determined. Requiring to the trial functional (6), the stationary condition, yields the following trial-Euler equation

$$-a\frac{\hbar^2}{m}r^2\frac{d^2R}{dr^2}-2a\frac{\hbar^2}{m}r\frac{dR}{dr}+2b(w(r)-E)r^2R+\frac{\delta F}{\delta R}=0 \tag{7}$$

we refer to $\delta F/\delta R$ as the variational derivative of F with respect to R, expressed by

$$\frac{\delta F}{\delta R}=\frac{\partial F}{\partial R}-\frac{d}{dr}\left(\frac{\partial F}{\partial R'}\right)+\frac{d^2}{dr^2}\left(\frac{\partial F}{\partial R''}\right)-\cdots \tag{8}$$

We search for such an F, a and b so that Eq. (7) turns out to be the original equation. Now the unknown F, a and b, can be identified as follows:

$$a=b=\frac{1}{2},\quad F=0 \tag{9}$$

Finally we obtain the needed variational principle of Eq. (6), which reads

$$J(R)=\int_0^{+\infty}\frac{1}{2}\left\{\frac{\hbar^2}{2m}\left(\frac{dR}{dr}\right)^2+(w(r)-E)R^2\right\}r^2dr \tag{10}$$

It can often be quite instructive to consider some alternative examples which can be considered from pedagogical point of view as a testbed. This point is shown in the next section.

3. Illustrative examples

To illustrate how this method works, and see whether it is robust, a good test may be made by examining two concrete physical examples. To be more precise, we use therefore the case of the angular momentum $l = 0$ (s-wave setting) and $l = 1$ (p-wave setting) and we denote by p the energy E and by z the atomic number Z.

From the asymptotic behaviors of solutions in regard to the large distances and near the origin, we can guess the solutions by making the following ansatz to the radial wavefunctions for both examples:

$$R(r) = e^{-kr} r^l \sum_{j=0}^{m} A_j r^j \tag{11}$$

where k and A_j are constant quantities to be determined, and are used as free variational parameters of the problem under consideration. These variational parameters are inferred from the variational functional $J(R)$ (Eq. (9)) subject to the minimization condition

$$\delta J(R) = 0 \tag{12}$$

with respect to specific variational parameters.

The optimization condition (12) yields sets of algebraic equations in terms of the variational parameters. In order to identify the different configurations we need to add some subscripts to the solutions $R(r)$ as: $R_{n,l}(r)$. Throughout the examples we adopt a system of atomic units in which $\hbar = m = \frac{e^2}{4\pi\varepsilon} = 1$.

3.1. First test example: case $l = 0$ and $m = 2$

The solution we are looking for is expressed in the form:

$$R(r) = e^{-kr}(a + br + cr^2) \tag{13}$$

substituting ansatz (13) into (10), then using the minimization condition (12) with respect to a, b, c and k and with the help of symbolic software packages in *Mathematica*, we can get a system of algebraic equations for a, b, c, k and p

$$\begin{aligned}
&-6c(2p + kz) + 2ak^2(k^2 - 2p - 2kz) + bk(k^2 - 6p - 4kz) = 0\\
&3c(k^2 - 10p - 4kz) + ak^2(k^2 - 6p - 4kz) + 2bk(k^2 - 6p - 3kz) = 0\\
&c(3k^2 - 30p - 10kz) - 2ak^2(2p + kz) + bk(k^2 - 10p - 4kz) = 0\\
&2k^2(2abk(k^2 - 12p - 6kz) + 3b^2(k^2 - 10p - 4kz) + a^2k^2(k^2 - 6p - 4kz)) + 45c^2(k^2 - 14p - 4kz)\\
&\quad + 24ck(b(k^2 - 15p - 5kz) - ak(5p + 2kz)) = 0
\end{aligned} \tag{14}$$

for which, we obtain with the aid of *Mathematica*, a variety of solutions

$$\begin{cases} b = 0 \\ c = 0 \\ k = z \\ p = -\frac{z^2}{2} \end{cases} \tag{15}$$

$$\begin{cases} b = -\frac{az}{2} \\ c = 0 \\ k = \frac{z}{2} \\ p = -\frac{z^2}{8} \end{cases} \tag{16}$$

and

$$\begin{cases} b = -\frac{2az}{3} \\ c = \frac{2az^2}{27} \\ k = \frac{z}{3} \\ p = -\frac{z^2}{18} \end{cases} \tag{17}$$

where the parameter a is easily evaluated from the following normalization condition for the wavefunction $\int_0^\infty |R(r)|^2 r^2 dr = 1$.

From these results, we identify the following configuration states: the first, the second and the third variant give, respectively, the states $1s, 2s$ and $3s$, i.e., $R_{1,0}, R_{2,0}$ and $R_{3,0}$, respectively.

3.2. Second test example: case $l = 1$ and $m = 1$

We seek the solutions in the form

$$R(r) = e^{-kr} r(a + br) \tag{18}$$

Similarly, substituting ansatz (18) into (10), we can deduce the following system of algebraic equations with respect to a, b, k and p

$$\begin{aligned} &b(3k^2 - 10p - 4kz) + 2ak(k^2 - 2p - kz) = 0 \\ &5b^2(7k^2 - 42p - 12kz) + 8abk(3k^2 - 15p - 5kz) + 2a^2k^2(3k^2 - 10p - 4kz) = 0 \\ &b(7k^2 - 30p - 10kz) + ak(3k^2 - 10p - 4kz) = 0 \end{aligned} \tag{19}$$

Solving the set of Eq. (19) with the help of *Mathematica*, we distinguish two sets of parameters given by

$$\begin{cases} b = 0 \\ k = \frac{z}{2} \\ p = -\frac{z^2}{8} \end{cases} \tag{20}$$

and

$$\begin{cases} b = -\frac{az}{6} \\ k = \frac{z}{3} \\ p = -\frac{z^2}{18} \end{cases} \tag{21}$$

Similarly, from these results, we identify the following configuration states: the first and the second variant give, respectively, the states $2p$ and $3p$, i.e., $R_{2,1}$ and $R_{3,1}$, respectively.

Indeed, it may be noted that the eigenenergies and the wavefunctions obtained for this potential are exact compared with those obtained by the power series method reported in the literature. As illustration, we sketch the variation of the s-wave states versus r to represent the three unnormalized wavefunctions $R_{1,0}(r)$, $R_{2,0}(r)$ and $R_{3,0}(r)$ in Fig. 1. Similarly, the plot of the two wave functions $R_{2,1}(r)$ and $R_{3,1}(r)$ versus r for the p-wave states is displayed in Fig. 2. We can finally underline that, the behavior of wavefunctions is very well outlined and preserved for all the states considered.

Remark. Phrased in its more general form, the specific functional may be used to deduce the Rayleigh quotient $E(\psi) = \frac{(\psi, H\psi)}{(\psi, \psi)}$ which is a key quantity of the variational principle in a quantum environment. E is the energy, H is the Hamiltonian of the system and ψ is the full wave function.

4. Conclusion

In this work, the semi-inverse variational method is applied to the Schrödinger wave equation. The aim to obtain exact wave solutions of the Schrödinger equation by using some specific examples has been achieved. Using some illustrative examples, it was shown that the semi-inverse variational method is a powerful and straightforward solution method to find closed-form for Schrödinger-type equations.

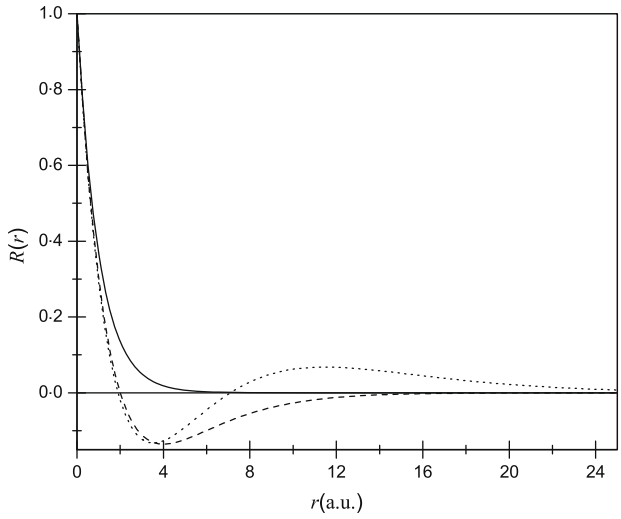

Fig. 1. Representation of the unnormalized wavefunction $R(r)$ obtained with the present method, where r is in a.u. for the Coulomb potential. Solid curve (configuration: 1s), dash curve (configuration: 2s), dot curve (configuration: 3s).

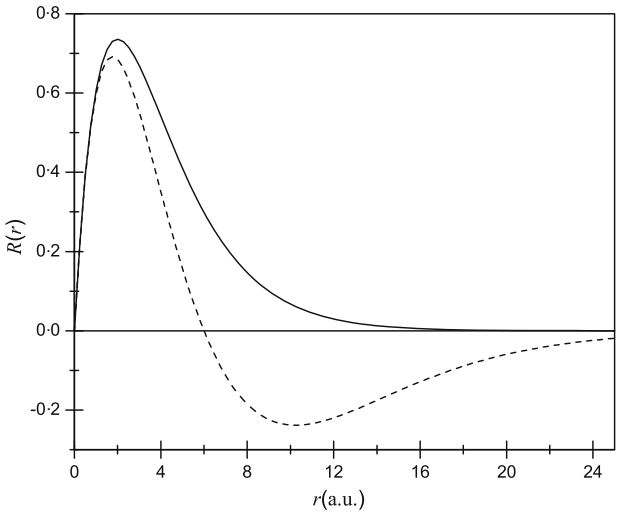

Fig. 2. Representation of the unnormalized wavefunction $R(r)$ obtained with the present method, where r is in a.u. for the Coulomb potential. Solid curve (configuration: $2p$), dash curve (configuration: $3p$).

In this paper, we have shown a possible connection between the semi-inverse variational method and the evaluation of solutions of a given quantum system. Specially, we have introduced the Coulomb potential as testbed to obtain simultaneously some bound energies and the associated quantum states. Furthermore, we have proposed some ansatz for the solutions for several configurations and we have demonstrated that the trial Lagrangian build by this approach has provided an exact aspect of solutions that are the same as those obtained by the power series method. However this technique may be applied successfully to other operators such as Dirac Hamiltonian. This matter will be discussed in a future work and will constitute a sequel to this paper.

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