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Variational approach to the Schrödinger equation with a delta-function potential

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Abstract

We obtain accurate eigenvalues of the one-dimensional Schrödinger equation with a Hamiltonian of the form $H_g = H + g\delta(x)$, where $\delta(x)$ is the Dirac delta function. We show that the well known Rayleigh–Ritz variational method is a suitable approach provided that the basis set takes into account the effect of the Dirac delta on the wavefunction. Present analysis may be suitable for an introductory course on quantum mechanics to illustrate the application of the Rayleigh–Ritz variational method to a problem where the boundary conditions play a relevant role and have to be introduced carefully into the trial function. Besides, the examples are suitable for motivating the students to resort to any computer-algebra software in order to calculate the required integrals and solve the secular equations.

Keywords: delta potential, variational method, perturbation theory, harmonic oscillator

(Some figures may appear in colour only in the online journal)

1. Introduction

A quantum-mechanical Hamiltonian operator H perturbed by a delta-function potential $g\delta(x)$ has received considerable attention [1–13]. In most cases H describes a free particle [1], a particle in a box [1–4] or the harmonic oscillator [1, 5–13]. Since in these cases the Schrödinger equation for H is exactly solvable one can obtain closed form expressions for the solutions to the Schrödinger equation for $H_g = H + g\delta(x)$ in several different ways. For example, from the eigenvalues and eigenfunctions of H [1, 8], by solving the eigenvalue equation left and right of the origin and matching those solutions at $x = 0$ [2, 3, 5, 9, 10] or by means of the Green function [11, 12]. In some cases the authors resorted to this kind of models to illustrate the application of approximate methods like perturbation theory [4, 9], WKB method [9], or variational approaches [9, 13]. Several such proposals have proved of pedagogical interest [1–4, 9, 10, 13] and a student may inquire about the possibility of solving examples in which the Schrödinger equation for H is not exactly solvable. The purpose of this paper is to address this point.

In most undergraduate courses on quantum mechanics and quantum chemistry the students become familiar with approximate methods like perturbation theory or variational techniques. For example, the Rayleigh–Ritz variational method is particularly useful in atomic and molecular physics [14]. Here, we show how to choose a suitable basis set that takes into account the effect of the Dirac-delta-function potential. The analysis carried out in this paper may be suitable for an introductory course on quantum mechanics. In section 2 we outline the model and some of the properties of the Schrödinger equation. In section 3 we describe the main ideas about the Rayleigh–Ritz variational method which we apply to a family of polynomial potentials in section 4. Finally, in section 5 we summarize the main results and draw conclusions.

2. The model

In what follows we restrict ourselves to the dimensionless Schrödinger equation in one dimension [15].

$$\psi''(x) = 2\left[V(x) + g\delta(x) - E\right]\psi(x), -\infty < x < \infty, \tag{1}$$

where $\delta(x)$ is the Dirac delta function. The delta-function potential determines the well known behaviour of the wavefunction at origin

$$\psi\left(0^-\right) = \psi\left(0^+\right) = \psi(0),\ \psi'\left(0^+\right) - \psi'\left(0^-\right) = 2g\psi(0). \tag{2}$$

According to the Hellmann–Feynman theorem [16, 17] every energy eigenvalue increases with the strength parameter of the delta potential as

$$\frac{\partial E}{\partial g} = |\psi(0)|^2, \quad \langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 = 1. \tag{3}$$

If the potential-energy function is parity invariant ($V(-x) = V(x)$) then the eigenfunctions are either even ($\psi_e(-x) = \psi_e(x)$) or odd ($\psi_o(-x) = -\psi_o(x)$) and the Hellmann–Feynman theorem tells us that the energies of the latter states do not change with g because $\psi_o(0) = 0$. In other words, the odd states are solutions to equation (1) with $g = 0$ which is consistent with the fact that $\psi_o'(x)$ is continuous at origin according to equation (2). The behaviour of the even states at origin becomes

$$\psi'(0^+) = g\psi(0), \tag{4}$$

and throughout this paper we consider that the wavefunction also satisfies $\psi(x \to \pm\infty) = 0$.

When $|g|$ is sufficiently small we can apply perturbation theory and obtain an expansion of the form

$$E_n(g) = \sum_{j=0}^{\infty} E_n^{(j)} g^j, \tag{5}$$

where the coefficients $E_n^{(j)}$ can be obtained in closed form provided that the eigenvalue equation for $H_0 = H$ is exactly solvable. Examples are given by the particle in a box [4] and the harmonic oscillator [9].

On the other hand, when $|g| \to \infty$ equation (4) yields $\psi(0) = 0$ and the solutions are the odd-parity states of H. An exception is the ground state when $g \to -\infty$ [9, 10]. We will discuss this point with more detail in the examples studied in section 4. Here, we just mention that there is a critical value g_0 such that $E_0(g) > 0$ if $g > g_0$ and $E_0(g) < 0$ if $g < g_0$ when $V(x) \geqslant 0$.

3. The Rayleigh–Ritz approach

In order to apply the Rayleigh–Ritz variational method to the Schrödinger equation $H\psi = E\psi$ we choose a suitable basis set $\{\varphi_j,\ j = 0, 1, \ldots\}$ and construct the trial function

$$\varphi = \sum_{j=0}^{N} c_j \varphi_j. \tag{6}$$

Then we obtain the minimum of the variational integral

$$W = \frac{\langle\varphi| H |\varphi\rangle}{\langle\varphi|\varphi\rangle}, \tag{7}$$

with respect to the expansion coefficients c_j

$$\frac{\partial W}{\partial c_j} = 0, \quad j = 0, 1, \ldots, N. \tag{8}$$

This approach is well described in many textbooks [14] so that we will only show the results here. The expansion coefficients c_j are solutions to the *secular equation*

$$\sum_{j=0}^{N} \left(H_{ij} - WS_{ij}\right) c_j = 0, \quad i = 0, 1, \ldots, N,$$

$$H_{ij} = \langle\varphi_i| H |\varphi_j\rangle, \quad S_{ij} = \langle\varphi_i|\varphi_j\rangle, \tag{9}$$

and there are nontrivial solutions only for those values of W that are roots of the *secular determinant*

$$|\mathbf{H} - W\mathbf{S}| = 0, \tag{10}$$

where $\mathbf{H}$ and $\mathbf{S}$ are $(N+1) \times (N+1)$ matrices with elements H_{ij} and S_{ij}, respectively. These roots $W_j^{[N]}$, $j = 0, 1, \ldots, N$, are real and satisfy $W_j^{[N]} \geqslant W_j^{[N+1]} \geqslant E_j$, where E_j is an eigenvalue of H [14].

4. Results

A suitable basis set for the class of polynomial potentials $V(x)$ discussed here is given by the Gaussian functions

$$\varphi_j = x^j \exp\left(-\frac{ax^2}{2}\right), \quad j = 0, 1, \ldots, a > 0. \tag{11}$$

However, if we require the trial function to satisfy (4) at origin then a more convenient basis set is

$$u_1(x) = (1 + gx)\exp\left(-\frac{ax^2}{2}\right), \;\; u_j = x^j \exp\left(-\frac{ax^2}{2}\right), \quad j = 2, 3, \ldots, x > 0, \tag{12}$$

and the trial function now reads

$$\varphi(x) = \sum_{j=1}^{N} c_j u_j(x), \quad x > 0. \tag{13}$$

For the application of the Rayleigh–Ritz variational method outlined above to present models we resort to the scalar product

$$\langle F|G\rangle = \int_0^\infty F(x)^* G(x)\,\mathrm{d}x, \tag{14}$$

because it is only necessary to take into account half the coordinate space, for example, $0 \leqslant x < \infty$, when $V(x)$ is parity invariant. For simplicity, we restrict ourselves to monomial potentials of the form

$$V(x) = A|x|^b, \quad A, b > 0, \tag{15}$$

so that all the integrals appearing in $\mathbf{H}$ and $\mathbf{S}$ are of the form

$$\int_0^\infty x^s \exp\left(-ax^2\right)\,\mathrm{d}x = \frac{1}{2}a^{-(s+1)/2}\Gamma\left(\frac{s+1}{2}\right), \tag{16}$$

where $\Gamma(z)$ is the gamma function.

The Rayleigh–Ritz variational method is quite general and has already been applied to far more challenging problems in atomic and molecular physics [14]. The application shown here is rather uncommon and the basis set (12) has been particularly designed for the one-dimensional delta-function potential.

In order to test the approach we first choose the harmonic oscillator

$$V(x) = \frac{1}{2}x^2, \tag{17}$$

because there are simple transcendental equations for its eigenvalues [1, 5, 6, 9–11]. Figure 1 shows the rate of convergence of the approach for the two lowest eigenvalues when $g = 1$. For simplicity, we have chosen $a = 1$ because it yields the correct asymptotic behaviour of $\varphi(x)$ at infinity.

Figure 2 shows similar results for $V(x) = x^4$ and $g = 1$. Since $x^4 \gg x^2$ for $x \gg 1$ we expect the eigenfunctions of the anharmonic oscillator to vanish asymptotically more rapidly; consequently, in this case we arbitrarily chose $a = 2$ to take into account this fact. It would be better to obtain the optimal value of a variationally but it would make the calculation rather more involved. Although in this case we do not have exact results for comparison, we are confident about the accuracy of the results because the roots of the secular equation converge to a limit from above. The actual eigenvalues given by the Rayleigh–Ritz variational method are available elsewhere [18].

The Rayleigh–Ritz variational method yields accurate results also for large $|g|$, the only exception being the ground state when $g \to -\infty$. We can estimate this energy eigenvalue by

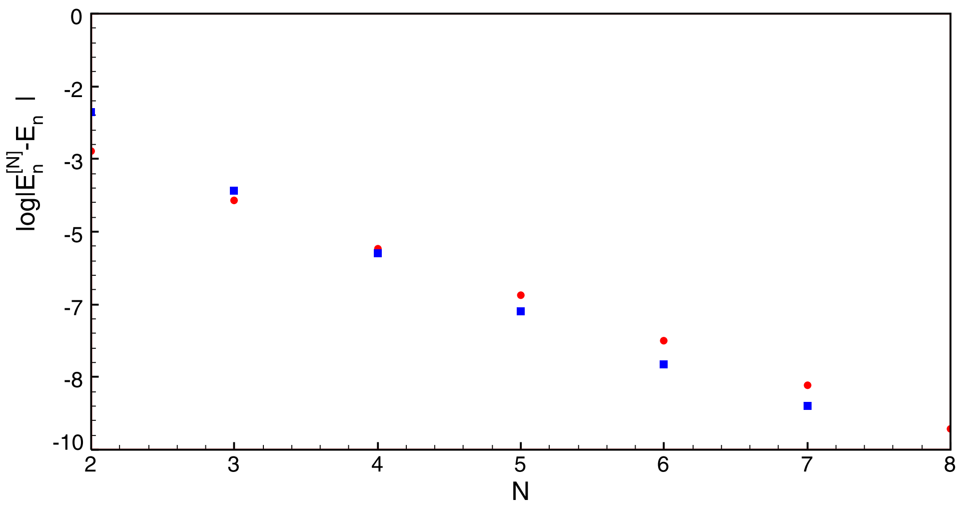

Figure 1. $\log|E_n^{[N]} - E_n|$ for $n = 0$ (red circles) and $n = 1$ (blue squares).

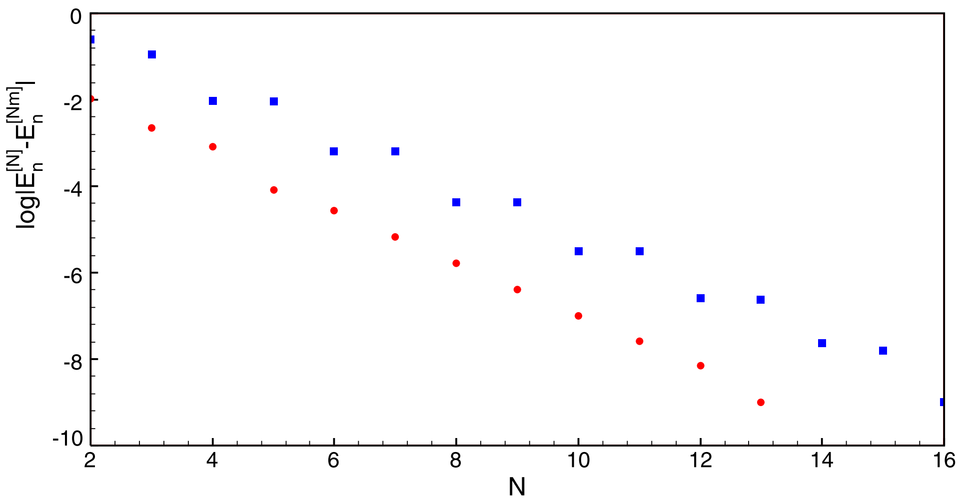

Figure 2. $\log|E_n^{[N]} - E_n^{[Nm]}|$ for $n = 0$ (red circles) and $n = 1$ (blue squares), where N_m indicates the maximum value of N in the calculation.

means of perturbation theory if we choose $V(x)$ to be the perturbation. In fact, by means of a simple scaling argument [15] we can easily prove that

$$E_0(g) = -\frac{|g|^2}{2} + \Gamma(b+1)A|g|^{-b} + \sum_{j=2}^{\infty} e_j A^j |g|^{-(b+2)j+2}, \tag{18}$$

for the family of potentials in equation (15).

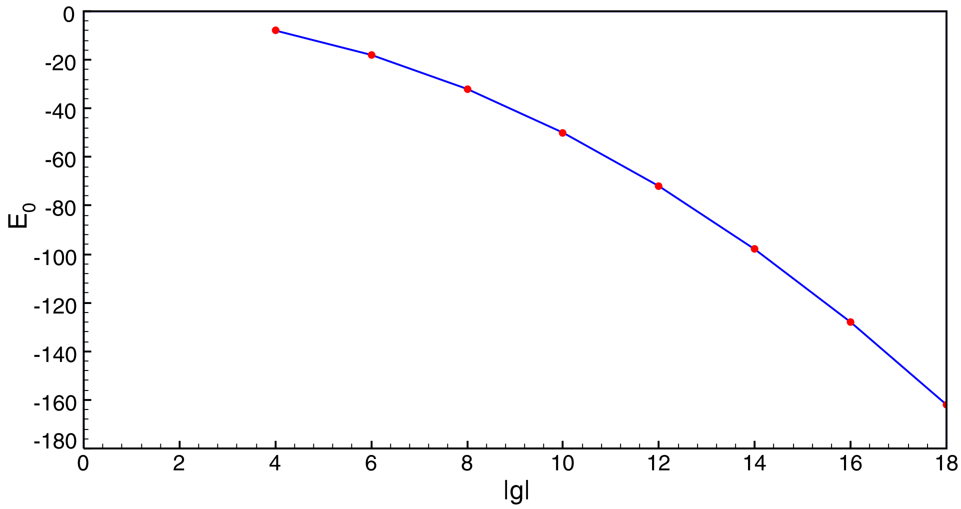

Figure 3. $E_0(g)$ for the harmonic oscillator calculated by means of perturbation theory (blue continuous line) and the Rayleigh–Ritz variational method (red points).

Figure 3 shows that present Rayleigh–Ritz variational results (with $N = 17$) agree with the perturbation expression

$$E_0(g) \approx -\frac{g^2}{2} + \frac{1}{g^2}, \tag{19}$$

for the harmonic oscillator (17) for moderately large values of $|g|$. Larger values of $|g|$ will require larger values of N in order to obtain results of similar accuracy.

Finally, it is worth mentioning that the Rayleigh–Ritz variational method is suitable for the calculation of the critical values g_0 mentioned at the end of section 2. We simply set $W = 0$ and solve the secular determinant (10) for g. We thus obtain $g_0^H = -0.675\,978\,2401$, $g_0^Q = -0.751\,594\,0253$ and $g_0^C = -0.765\,128\,1365$ for the harmonic, quartic and cubic potentials, respectively. The result for the harmonic oscillator agrees with the one predicted by the exact analytical expression for the eigenvalues [1, 8].

5. Conclusions

The results of this paper clearly show that the Rayleigh–Ritz variational method is a suitable tool for the treatment of the Schrödinger equation perturbed by a Dirac-delta-function potential provided that the trial function exhibits the correct behaviour at origin (or, in general, at the location of the delta function). This behaviour can be easily introduced into the basis set, at least for even-parity potentials. We have illustrated the application of the approach by means of three monomial potentials and a similar calculation for polynomial potentials is straightforward. In the case of non-polynomial potentials it may be necessary to calculate the matrix elements $H_{i,j}$ and $S_{1,j}$ numerically. This fact would make the calculation somewhat more involved but the method can still be applied as shown in the case of atoms and molecules [14].

The basis set chosen is suitable for moderate values of $|g|$ as suggested by the remarkable rate of convergence shown in figures 1 and 2 (see [18] for more explicit results). For large, positive values of g the performance of the variational method is similar because $\psi(0) \to 0$

as $g \to \infty$. The only difficulty may be found for the ground state when $g \ll -1$ because the wavefunction is expected to behave asymptotically as $\psi(x) \sim \exp\left(-g|x|\right)$. In this case it is required a large basis set of Gaussian functions or a more convenient set of functions. However, for most purposes the approach proposed here is sound.

The variational method proposed by Patil [9] and improved by Ghose and Sen [13] can also be applied to the models discussed above in the preceding section. However, this approach, based on just one trial function with adjustable parameters, only applies to the ground state. On the other hand, the Rayleigh–Ritz method outlined in this paper yields estimates for all the eigenvalues with the advantage that we can monitor the accuracy of the results because the roots of the secular determinant converge to the actual eigenvalues from above [18].

The application of the Rayleigh–Ritz variational method to problems of physical interest commonly requires resorting to suitable computer software for the calculation of the approximate eigenvalues and eigenfunctions. In our opinion, this is a good opportunity for introducing the students to any of the available computer-algebra software that enable one to calculate the integrals in the matrix elements and provide algorithms for the solution of the secular equations.

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