Variation Principle for a Linear Potential

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Abstract

We introduce the student to the Quantum Mechanic linear potential (constant force) using new variation wave functions for the ground state and the first excited one. This approach use simple wave functions to describe the exact Airy solution.

1.   Introduction

Simple systems in quantum mechanics are very useful in education because they introduce important principles of quantum mechanics to the students and also prepare them to the study the hydrogen atom and other systems of physical interest. The simplest model problem is provided by a particle in a one-dimensional box (PIB) of length L, in which the particle is constrained to remain between two infinite potential walls. Inside the box the potential is constant and usually taken as the zero of energy. The exact solutions of this problem are known, and have been extensively investigated [1–13]. The experimental application of a PIB model lies, for example, in Semiconductor Nanocrystals [14] and in the layered structure AlGaAs-GaAs-AlGaAs, where the separation between the layers is 10–100 nm (thickness of the GaAs layer). This case may be modeled by a finite one-dimensional square well potential with a depth on the order of a mV—sufficient to be viewed as infinity. The low density of electrons allows the problem to be treated using a one-electron approximation [15]. In the present work we consider a one-dimensional potential that can be written in the form: $V(x) = \infty$ for $x < 0$ and $V(x) = kx$ for $x \geq 0$, where k is a constant. This linear potential, or constant force, describes the motion of a particle falling under gravity: the force in this case is -mg, where m is the mass and g the acceleration due to gravity. So the potential is mgz, where z is the height above ground.

Another example of a linear potential could be an electron placed in a constant electric field of a thin capacitor; in which case $V = -qEx$ between the plates of a capacitor. Here k is the negative of the electric force ($k = -qE$).

2. Discussion

2.1. Determination of eigenvalues and eigenfunctions for the linear potential problem

The literature for the quantum linear potential case [16–18] is scarcer than that for the PIB problem. Winter [19] calculated the ground state linear potential problem via a variation approach, and found a ground state energy 6% higher than the true value. In the following presentation, we set the atomic units $h = e = m = 1$ and seek solution to the Schrödinger Equation:

$$-\frac{1}{2}\frac{d^2}{dx^2}\psi(x) + kx\psi(x) = E\psi(x).$$ (1)

Equation (1) may be transformed into the form

$$\frac{d^2\eta}{d\zeta^2} - \zeta\eta = 0.$$ (2)

using the substitutions

$$\zeta = \left(x - \frac{E}{k}\right)(2k)^{1/3} \text{ and } \eta(\zeta) = \psi(x).$$ (3)

General solution of Equation (2) is a linear combination of the Airy functions $Ai(\zeta)$ and $Bi(\zeta)$, however, as a proper study of Airy functions would require an extensive detour [19], we give here only the essential properties required. The first point to note is that, as $\zeta \to \infty$, the lim $Ai(\zeta) = 0$ and lim $Bi(\zeta) = \infty$, so the $Bi(\zeta)$ functions have an inappropriate asymptotic form and thus play no role in the present context—a situation which is analogous to that in solving the second-order differential equation for the PIB model. Here the cosine functions have zero weight on account of the boundary condition at the origin when the origin is at the left end of the box. Thus, the solution of Equation (2) takes the form

$$\eta(\zeta) = Ai(\zeta).$$ (4)
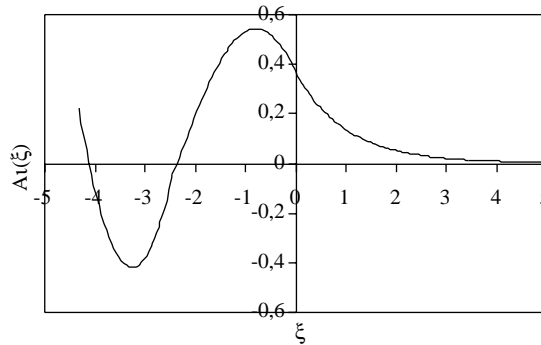
A plot of equation (4) is given in Figure 1.

Figure 1. Plot of the Airy function $Ai(\zeta)$ vs. ζ.

We now establish the relation between $\eta(\zeta)$ (the Ai (ζ) function) and $\psi(x)$, the solution of Equation (1). Using relations (3), we obtain

$$\eta(\zeta) = \eta\left(\left[x - \frac{E}{k}\right]\left\{2k^{1/3}\right\}\right) = \psi(x).$$ (5)

However, since the boundary condition at the origin requires that $\psi(0) = 0$, we deduce from Equation (5) that

$$\eta(\zeta) = \eta\left(\left[x - \frac{E}{k}\right]\{2k\}^{1/3}\right) = 0. \tag{6}$$

It is now obviously that Equation (6) is satisfied for the values of ζ corresponding to the roots of the Airy function (pure real numbers). If we designate these numbers by ζ_n and denote the associated quantified energies by E_n, then we conclude that ζ_n and E_n are related by the function

$$\left[-\frac{E_n}{k}\right](2\,k)^{1/3} = \zeta_n. \tag{7}$$

We therefore obtain the values of E_n as

$$E_n = -\zeta_n(k^2/2)^{1/3}. \tag{8}$$

and since the ζ_n are negative, we write Equation (8) as:

$$E_n = -|\zeta_n|\left(k^2/2\right)^{1/3}. \tag{9}$$

where $|\zeta_n|$ is the absolute value of each root.

The first two roots of the Airy function are $\zeta_1 = -2.3381$ and $\zeta_2 = -4.0879$, as can be seen in reference [19] and also in Figure 1.

For illustration, and as we employ Mathematica to for computations, we set $k = 1$ to simplify the result. Thus the exact energies for the ground and the first excited states are $E_1^{\text{exact}} = 1.85575$ and $E_2^{\text{exact}} = 3.24457$, respectively.

The eigenfunctions for the ground and first excited states were obtained using Equations (4) and (5) as well as the values found for the exact energies and the first two roots of the Airy functions. Then:

$$\psi_1^{\text{Exact}}(x) = Ai\left(2^{1/3}x - 2.3381\right) \tag{10}$$

$$\psi_2^{\text{Exact}}(x) = Ai\left(2^{1/3}x - 4.0879\right) \tag{11}$$

These eigenfunctions (unnormalized and scaled) are the shifted Airy functions, as can be seen in Figure 2.
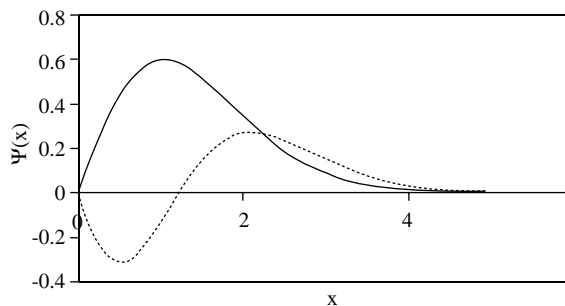

Figure 2. The ground and first excited states for the linear potential problem with $k = 1$.

2.2. The variation approach by Winter

The variation approach by Winter [19] is based on the normalized trial function

$$\psi(x) = 2\gamma^{3/2}\,x\,\exp(-\gamma x). \tag{12}$$

Solving the derivative of the energy quotient, we get

$$\frac{d}{d\gamma} \frac{\langle \psi H \psi \rangle}{\langle \psi \psi \rangle} = 0. \tag{13}$$

Winter obtains $\gamma = (3/2)^{1/3}$ and $E_1(W) = 1.96552$. This value is 6% higher than those found for the exact energy for the ground state ($E_1^{\text{exact}} = 1.85575$).

2.3. Improving the variation wave function

Now we will try to improve the trial wave function by examining the behavior of the Airy function in Equation (4) when $\zeta \to +\infty$. From reference [19] we see that when $\zeta \to +\infty$ the Airy function can be written as

$$Ai(\zeta) \approx \frac{1}{2\sqrt{\pi}\zeta^{1/4}} \exp\left(-\frac{2}{3}\zeta^{3/2}\right). \tag{14}$$

On the basis of this asymptotic behavior, we now take the (unnormalized) variation wave function in the form

$$\Psi(x) = x \exp\left(-ax^{3/2}\right). \tag{15}$$

Minimization of the energy, using the method of trial and error, yields an optimum value for a of 0.665. The value found for the associated ground state energy is $E_1^{var_1} = 1.863$, which differs from the value for the exact energy in the ground state ($E_1^{\text{exact}} = 1.85575$) by 0.39%.

2.4. Further Improvement of the ground state energy.

We next decided to perform a further calculation in which the value 3/2 in Equation (15) is replaced by a second parameter, b. So the new trial wave function is written as

$$\Psi(x) = x \exp\left(-ax^b\right). \tag{16}$$

When the energy is minimized with this wave function we found that the optimum values of the variation parameters a and b are 0.5245 and 1.747, respectively. This lead to an improved energy $E_1^{var_2} = 1.85587$, which is 0.006% higher than the exact energy in the ground state ($E_1^{\text{exact}} = 1.85575$).

2.5. The first excited state energy

Finally, we use a trial wave function to calculate the energy for the first excited state. The trial wave function proposed in this case is

$$\Psi(x) = \left(Ax^2 + Bx\right) \exp\left(-ax^b\right). \tag{17}$$

In this wave function the parameters a and b are the same as those used in the previous calculation ($a = 0.5245$ and $b = 1.747$). On the other hand, Equation (17) remains orthogonal to Equation (16) by taking $B/A = -1.23703$. The value of the energy for the first excited state is $E_2^{var} = 3.50128$ which is 8% higher than the exact energy for the first excited state ($E_2^{\text{exact}} = 3.24457$). However, although increased flexibility is desirable, it is always more difficult to optimize the energy of the first excited state than the ground state.

3. Conclusions

The use of simple wave functions to describe the exact Airy solution for the Quantum Mechanic linear potential problem allows one to find energies for the ground state and the first excited that are, respectively, 0.006% and 8% higher than the exact energies. The energy for the ground state found in this work is better than the energy previously reported by Winter [19].

Acknowledgments

References

[1] J. I. Casaubon and G. Doggett, *J. Chem. Educ.*, **77**, (2000), 1221.

[2] E. Besalú and J. Martí, *J. Chem. Educ.*, **75**, (1998), 105.

[3] I. N. Levine, *Quantum Chemistry*, (Prentice-Hall: Englewood Cliffs, NJ, 1991).

[4] B. H. Bransden, and C. J. Joachain, *Introduction to Quantum Mechanics*, (Longman: Harlow, UK, 1989).

[5] G. L. Bendazzoli, *J. Chem. Educ.*, **70**, (1993), 912.

[6] L. J. A. Martins, *J. Chem. Educ.*, **65**, (1988), 861.

[7] S. K. Knudson, *J. Chem. Educ.*, **74**, (1997), 930.

[8] B. D. Andersen, *J. Chem. Educ.*, **74**, (1997), 985.

[9] D. Keeports, *J. Chem. Educ.*, **66**, (1989), 314.

[10] C. W. David, *J. Chem. Educ.*, **78**, (2001), 682.

[11] J. Gea-Banacloche, *Am. J. Phys*, **70**, (2002), 307.

[12] D. F. Styer, *Am. J. Phys.*, **69**, (2001), 56.

[13] R. W. Robinett, *Am. J. Phys.*, **68**, (2000), 410.

[14] T. Kippeny, *J. Chem. Educ.*, **79**, (2002), 1094.

[15] P. Tamborena, Private communication.

[16] J. R. Hiller, *Am. J. Phys.*, **70**, (2002), 522.

[17] M. A. Doncheski and R. W. Robinett, *Am. J. Phys.*, **69**, (2001), 1084.

[18] G. Vandegrift, *Am. J. Phys.*, **68**, (2000), 576.

[19] R. G. Winter, *Quantum Physics*, (Faculty Publishing, Inc.: Davis, California, 1986) p. 92 and p. 333.