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2000 J. Phys. A: Math. Gen. 33 9265

(http://iopscience.iop.org/0305-4470/33/50/310)

J. Phys. A: Math. Gen. **33** (2000) 9265–9272. Printed in the UK PII: S0305-4470(00)15618-5

On the Coulomb-type potential of the one-dimensional Schrödinger equation

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Received 11 July 2000

Abstract. By means of the Laplace transform and a series expansion, exact solutions of the bound state for the one-dimensional Schrödinger equation with a potential $-Ze^2/x$ are given. We found that the energy levels are proportional to $1/n^2$ ($n = 1, 2, 3, \ldots$) and the value of the wavefunction of the bound state at the origin is zero. The reasons for the wrong answer that the energy levels are proportional to $(n + \frac{1}{2})^{-2}$ with n an integer are analysed.

1. Introduction

Recently, much theoretical effort has been devoted to studying the one-dimensional (1D) Coulomb-type potentials of the Schrödinger equation, including the symmetric potential $-Ze^2/|x|$ and the antisymmetric potential $-Ze^2/x$. The reason for the great deal of interest in discussing the 1D hydrogen atom potential $-Ze^2/|x|$ is partly due to its wide applications to different physical topics involving excitons in high-temperature superconductivity [1], semiconductors [2, 3], polymers [4, 5], 1D electron gas at the helium surface and the Wigner crystal [6, 7], and partly due to contradictory conclusions regarding stationary eigenfunctions. The eigenfunctions of the 1D hydrogen atom can have a definite parity because of its symmetric potential. However, whether the even eigenfunctions and the odd eigenfunctions are true bound states remains an open question. Flugge and Marschall [8] concluded that only the odd states were bound solutions, while Loudon [9] argued that the even states were solutions, too. Andrews [10] objected to the existence of Loudon's ground state and Dai [11] claimed that only eigenstates with even parity exist. Even though many wrangles still exist concerning the eigenfunctions of the 1D hydrogen atom, all authors agree that the eigenvalues, i.e. the energy levels of the 1D hydrogen atom, are proportional to $1/n^2$ ($n = 1, 2, 3, \ldots$) [8–14].

In contrast to the potential $-Ze^2/|x|$, another Coulomb-type potential $-Ze^2/x$ seems not to have been investigated widely yet, even though it may have applications in semiconductors or insulators [15]. Employing the Laplace and Fourier transformations in momentum space, Reyes and del Castillo-Mussot [15] claimed that the eigenenergies for the potential $-Ze^2/x$ are proportional to $\left(n + \frac{1}{2}\right)^{-2}$ with n an integer. Because of its antisymmetry and singular character, it is of interest to discuss this potential in more detail.

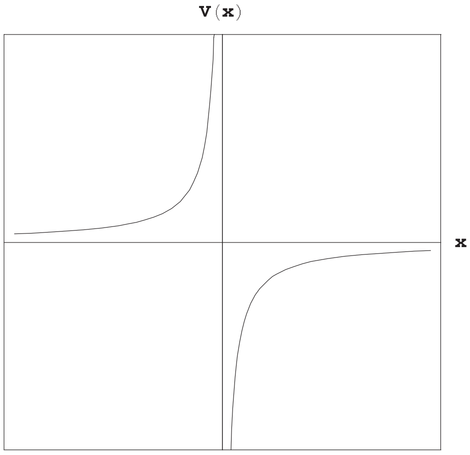

Figure 1. Potential $V(x)$.

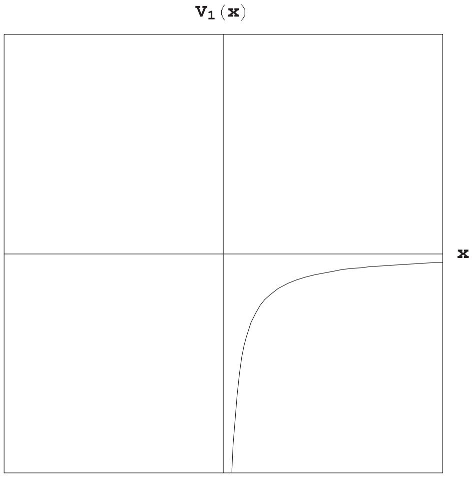

Figure 2. Potential $V_1(x)$.

To investigate the bound states of the potential

$$V(x) = -Ze^2/x \tag{1}$$

we compare the behaviour of $V(x)$ with an imaginary potential

$$V_1(x) = \begin{cases} -Ze^2/x & x > 0 \\ \infty & x \leqslant 0. \end{cases} \tag{2}$$

First, we sketch these two potentials in figures 1 and 2. Obviously, potential $V(x)$ and $V_1(x)$ will have different scattering states because of the different barriers. However, for the bound states, they will be the same because the bound states are determined by the potential well of the right-half space and the boundary condition $\psi(0)$ completely. The barriers of the left-half space cannot affect the bound states and the boundary condition $\psi(0)$, as will be shown below, also equals zero for potential $V(x)$. As is well known, instead of $-\left(n+\frac{1}{2}\right)^{-2}$, the eigenenergies of the potential $V_1(x)$ are proportional to $-1/n^2$ [16]. This result is different to that of [15]. The objective of this paper is to study this problem, in particular concerning the bound state energies, in detail. We will prove that the conclusion concerning the energy levels given by [15] is incorrect.

To illustrate our conclusion, we will employ the Laplace transform and the virial theorem to discuss this problem and obtain the wavefunctions and the energy levels of bound states in section 2. In section 3, to confirm our conclusion we will use a series expansion to find the exact solutions of $V(x)$. Instead of an input $\psi(0) = 0$ for the Laplace transform, in this section $\psi(0) = 0$ is an output from the series expansion solution. In section 4 we will analyse why a Fourier transform used in [15] gave the wrong answer, $E_n \propto -\left(n+\frac{1}{2}\right)^{-2}$. We will point out that the correct Fourier transform will reduce to a Laplace transform in this problem because the wavefunction $\psi(x) = 0$ in the regions $-\infty < x \leqslant 0$.

2. Laplace transform

By means of the virial theorem of quantum mechanics [16], we find

$$E = \frac{1}{2}\langle V(x)\rangle = -\frac{1}{2}Ze^2\int_{-\infty}^{\infty}\frac{|\psi(x)|^2}{x}\,\mathrm{d}x \tag{3}$$

for the Coulomb-type potential $V(x)$, where $\psi(x)$ is the wavefunction of bound states. If $\psi(x)$ does not tend to zero when $x \to 0$, the integral of equation (3) will diverge and E will approach negative infinity. This situation of course cannot be accepted and we come to the conclusion that $\psi(0) = 0$. This boundary condition $\psi(0) = 0$ implies that we can take a Laplace transform to solve this problem safely.

The 1D Schrödinger equation for the potential $V(x)$ is given by

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} - \frac{Ze^2}{x}\psi(x) = E\psi(x). \tag{4}$$

Introducing variable transformations

$$\begin{aligned}\zeta &= \frac{\sqrt{-2mE}}{\hbar}x \\ \gamma &= -\frac{Ze^2\sqrt{-2mE}}{\hbar E} > 0\end{aligned} \tag{5}$$

we rewrite equation (4) as

$$\frac{\mathrm{d}^2\psi(\zeta)}{\mathrm{d}\zeta} + \left(\frac{\gamma}{\zeta} - 1\right)\psi(\zeta) = 0. \tag{6}$$

Performing the Laplace transform of equation (6) in the positive ζ regions yields

$$(s^2 - 1)\phi_1(s) + \gamma\int_s^{\infty}\phi_1(s')\,\mathrm{d}s' - \frac{\mathrm{d}\psi(0^+)}{\mathrm{d}\zeta} = 0 \tag{7}$$

where

$$\phi_1(s) = \int_0^{\infty}\psi(\zeta)\,\mathrm{e}^{-s\zeta}\,\mathrm{d}\zeta \tag{8}$$

is the Laplace transform of $\psi(\zeta)$ and

$$\frac{\mathrm{d}\psi(0^+)}{\mathrm{d}\zeta} = \lim_{\Delta\zeta\to 0^+}\frac{\psi(0+\Delta\zeta) - \psi(0)}{\Delta\zeta} \tag{9}$$

is the derivative of $\psi(\zeta)$ when $\zeta \to 0^+$. In above calculation, we have used the property

$$L[\psi(x)/x] = \int_s^{\infty}\phi(s')\,\mathrm{d}s'. \tag{10}$$

The solution of equation (7) reads

$$\phi_1(s) = \frac{B}{s^2 - 1}\left(\frac{s-1}{s+1}\right)^{\gamma/2}. \tag{11}$$

Note that $\left(\frac{s-1}{s+1}\right)^{\gamma/2}$ is a multi-valued function and the wavefunction $\phi_1(s)$ is required to be single-valued, we must take

$$\gamma = 2n \qquad n = 1, 2, 3, \ldots \tag{12}$$

and then $\phi_1(s)$ becomes

$$\phi_1(s) = \frac{B}{s^2-1}\left(\frac{s-1}{s+1}\right)^n \tag{13}$$

where $B = \frac{\mathrm{d}\psi(0^+)}{\mathrm{d}\zeta}$.

In order to obtain the wavefunctions of coordinate space, we must perform an inverse Laplace transform of equation (13). By using the expansion theorem we obtain

$$\psi(\zeta) = B\,\mathrm{Res}\left[\frac{(s-1)^{n-1}}{(s+1)^{n+1}}\mathrm{e}^{s\zeta}\right]\Bigg|_{s=-1} = B\zeta\mathrm{e}^{-\zeta}F(1-n,2;2\zeta) \qquad (\zeta > 0) \tag{14}$$

where $F(1-n,2;2\zeta)$ is the confluent hypergeometric function or Kummer function.

Extending the above calculation of the bound state to the negative ζ region, we introduce a transformation $t = -\zeta > 0$, and rewrite equation (6) as

$$\frac{\mathrm{d}^2\psi(t)}{\mathrm{d}t^2} + \left(-\frac{\gamma}{t} - 1\right)\psi(t) = 0. \tag{15}$$

By means of the same procedure, we find the solution of equation (15) as

$$\phi_2(s) = \frac{C}{s^2-1}\left(\frac{s+1}{s-1}\right)^n \tag{16}$$

and its inverse Laplace transform as

$$\psi(t) = C\mathrm{e}^t t\left[1 + \sum_{k=1}^{n-1}\frac{(n-1)(n-2)\cdots(n-k)}{k!(k+1)!}(2t)^k\right]. \tag{17}$$

We see when $t \to \infty$, i.e. $s \to -\infty$, $\psi(t) \to \infty$. The natural boundary condition of bound state solutions that $\psi\ (t \to \infty)$ is finite requires $C = 0$. We only have a zero solution in the negative ζ region for a bound state. This result is in agreement with our previous discussion of $V(x)$ and $V_1(x)$ in section 1. The barrier on the left-hand side would not affect the bound state solutions.

In summary, we obtain the wavefunction

$$\psi(\zeta) = \begin{cases} B\mathrm{e}^{-\zeta}\zeta F(1-n,2;2\zeta) & \zeta > 0 \\ 0 & \zeta \leqslant 0 \end{cases} \tag{18}$$

and the energy levels which are given by the condition (12) as

$$E_n = -\frac{mZ^2e^4}{2\hbar^2n^2} \qquad n = 1,2,3,\ldots. \tag{19}$$

3. Exact solution

To confirm the results given by the last section, we will use another method, namely a series expansion, to solve the Schrödinger equation (6) in coordinate space exactly. We would like to emphasize that instead of the input $\psi(0) = 0$ for introducing the Laplace transform in the last section, the condition $\psi(0) = 0$ will be a natural conclusion, i.e. an output, in the series expansion. According to the argument of Landau and Lifshiz [17] on a singular potential, the matching conditions at $x = 0$ read: the wavefunction is continuous and the derivative of the wavefunction may be discontinuous because $x = 0$ is the first-order singularity. We will use this matching condition as well as the natural boundary conditions at $x \to \pm\infty$ to determine the bound state solutions of equation (6).

3.1. The region $\zeta > 0$

For large ζ, we can neglect the term γ/ζ in comparison with 1, equation (6) becomes

$$\frac{d^2\psi}{d\zeta^2} - \psi = 0. \tag{20}$$

It has the asymptotic integrals $\psi = e^{\pm\zeta}$. Since the wavefunction ψ must remain finite when $\zeta \to +\infty$, the solution must be taken as $\psi = e^{-\zeta} = e^{-t/2}$ where $t = 2\zeta$. Therefore, it is natural to make equation (6) the substitution

$$\psi(\zeta) = e^{-t/2}U(t). \tag{21}$$

The equation of function $U(t)$ reads

$$tU''(t) - tU'(t) + \tfrac{1}{2}\gamma U(t) = 0. \tag{22}$$

Equation (22) is a Kummer equation, its two linearly independent solutions being

$$U_1(t) = tF(1 - \tfrac{1}{2}\gamma, 2; t) \tag{23}$$

$$U_2(t) = tF(1 - \tfrac{1}{2}\gamma, 2; t)\ln t - \tfrac{1}{2}\gamma + \sum_{n=2}^{\infty} a_n t^n \tag{24}$$

where

$$a_n = \frac{(1-\frac{1}{2}\gamma)(2-\frac{1}{2}\gamma)\cdots(n-1-\frac{1}{2}\gamma)}{n!(n-1)!}\left[\frac{1}{1-\frac{1}{2}\gamma} + \frac{1}{2-\frac{1}{2}\gamma} + \cdots + \frac{1}{n-1-\frac{1}{2}\gamma} \right.$$
$$\left. - \frac{3}{1\times 2} - \frac{5}{2\times 3} - \cdots - \frac{2n-1}{(n-1)n}\right]. \tag{25}$$

The general solutions of equation (22) are

$$U(t) = B_1U_1(t) + B_2U_2(t) \tag{26}$$

where B_1 and B_2 are arbitrary constants. When $t \to \infty$ (i.e. $\zeta \to \infty$) and $n \to \infty$, $F(1 - \frac{1}{2}\gamma, 2; t) \approx e^t$ and $\sum_{n=2}^{\infty} a_n t^n \approx e^t$. The solution which satisfies the conditions at infinity is obtained only for $\gamma = 2n$, $n = 1, 2, 3, \ldots$ and $B_2 = 0$. Hence the wavefunction is given by

$$\psi(\zeta) = B_1 e^{-\zeta}U_1(2\zeta) = 2B_1\zeta e^{-\zeta}F(1-n, 2; 2\zeta) \qquad (\zeta > 0) \tag{27}$$

and the eigenenergies E_n are still given by equation (19).

3.2. The region $\zeta < 0$

The same procedure can also be employed to discuss the solution in the region $\zeta \leqslant 0$. With the aid of the function transformation $\psi(\zeta) = e^{-s/2}U(s)$, $s = -2\zeta > 0$, we have

$$sU''(s) - sU'(s) - \tfrac{1}{2}\gamma U(s) = 0. \tag{28}$$

The general solutions are

$$U(s) = CU_3(s) + DU_4(s) \tag{29}$$

where

$$U_3(s) = sF(1 + \tfrac{1}{2}\gamma, 2; s)$$

$$U_4(s) = sF(1 + \tfrac{1}{2}\gamma, 2; s)\ln s + \tfrac{1}{2}\gamma + \sum_{n=2}^{\infty} b_n s^n$$

are two linearly independent solutions and

$$b_n = \frac{(1+\frac{1}{2}\gamma)(2+\frac{1}{2}\gamma)\cdots(n-1+\frac{1}{2}\gamma)}{n!(n-1)!}\left[\frac{1}{1+\frac{1}{2}\gamma}+\frac{1}{2+\frac{1}{2}\gamma}+\cdots+\frac{1}{n-1+\frac{1}{2}\gamma}\right.$$
$$\left.-\frac{3}{1\times 2}-\frac{5}{2\times 3}-\cdots-\frac{2n-1}{(n-1)n}\right]. \tag{30}$$

Because of $\gamma > 0$, $U_3(s)$ and $U_4(s)$ are all divergent when $\zeta \to \infty$, we must choose $B_3 = B_4 = 0$, and obtain zero solution $\psi(\zeta) = 0$ in the $\zeta \leqslant 0$ region.

In summary, we come to the conclusion that

$$\psi(\zeta) = \begin{cases} 2B_1\zeta \mathrm{e}^{-\zeta} F(1-n, 2; 2\zeta) & \zeta > 0 \\ 0 & \zeta \leqslant 0. \end{cases} \tag{31}$$

The coefficients B in equation (18) and $2B_1$ in equation (31) are normalized constants. We can easily prove that the wavefunctions have

$$\psi(0^+) = \psi(0^-) = \psi(0) = 0 \tag{32}$$

$$\frac{\mathrm{d}\psi(0^+)}{\mathrm{d}\zeta} = 2B_1 \qquad \frac{\mathrm{d}\psi(0^-)}{\mathrm{d}\zeta} = 0. \tag{33}$$

The matching condition at $\zeta = 0$ is indeed satisfied.

4. On the Fourier transform

As we have mentioned in section 1, the energy levels of the potential $-Ze^2/x$ given by [15] are proportional to $\left(n+\frac{1}{2}\right)^{-2}$, which is different from our conclusion, $1/n^2$, given in sections 2 and 3. The basic method employed by [15] is the Fourier transform. The authors of [15] took a Fourier transform over the whole coordinate space to find the wavefunctions in momentum space and the energy levels. In this section we hope to analyse their treatment and discuss their result in detail.

Obviously, the first problem in the Fourier transform for the potential $V(x) = -Ze^2/x$ is how to calculate the Fourier integral of $1/x$. In [15] they used

$$r(p) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{\zeta}\mathrm{e}^{-\mathrm{i}p\zeta}\,\mathrm{d}\zeta = -\tfrac{1}{2}\mathrm{i}\,\mathrm{sign}(p) \tag{34}$$

as the Fourier transform of $1/\zeta$. Equation (34) refers to the principal value only, in general, the exact Fourier integral of $1/\zeta$ is given by

$$r(p) = \frac{1}{2\pi}\lim_{\epsilon\to 0^+}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}p\zeta}}{\zeta\pm\mathrm{i}\epsilon}\mathrm{d}\zeta = \frac{1}{2\pi}\left[P\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}p\zeta}}{\zeta}\,\mathrm{d}\zeta \mp \mathrm{i}\pi\right]$$
$$= -\tfrac{1}{2}\mathrm{i}\,\mathrm{sign}(p) \mp \tfrac{1}{2}\mathrm{i} \tag{35}$$

where $P\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}p\zeta}}{\zeta}\,\mathrm{d}\zeta$ is the principal value of the integral. The additional term $\mp\frac{1}{2}\mathrm{i}$ will give a contribution to the momentum expression of $1/x$. Instead of equation (34), if we use equation (35) to perform the Fourier transform and employ the same procedure as [15] to find the wavefunctions in momentum space, we shall obtain an incorrect answer. In fact, following [15], the Fourier transform of equation (6) reads

$$-\left(p^2+1\right)\phi(p) + \gamma\int_{-\infty}^{\infty} r(p-p')\phi(p')\,\mathrm{d}p' = 0 \tag{36}$$

where

$$\phi(p) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(\zeta)\, \mathrm{e}^{-\mathrm{i}p\zeta}\, \mathrm{d}\zeta \tag{37}$$

is the wavefunction in momentum space. Define

$$G(p) = \int_0^p \phi(p')\, \mathrm{d}p'. \tag{38}$$

Substituting equations (35) and (38) into equation (36) and using the same treatment as [15], we find

$$G(p) = G(-\infty) - A\mathrm{e}^{-\mathrm{i}\gamma \arctan p} \tag{39}$$

where A is in principle an arbitrary constant to be determined from the normalization condition. Another equation by taking the lower plus sign of equation (35) is the same as that of equation (39) if we notice

$$G(+\infty) - G(-\infty) = \psi(0) = 0. \tag{40}$$

Evaluating equation (39) in $-\infty$, we arrive at the conclusion that only a zero solution exists because

$$A\mathrm{e}^{-\mathrm{i}\gamma\pi/2} = 0 \tag{41}$$

then $A = 0$. This is a trivial solution and, indeed, we cannot obtain a bound state solution. Of course this is incorrect because the exact bound state solutions have been found in sections 2 and 3.

Now we are in a position to investigate further why the Fourier transform used by [15] cannot give us a correct answer for this problem. Noting that the exact solution of the bound state given by equation (31) has the important property that $\psi(\zeta) = 0$ when $\zeta \leqslant 0$. This property will affect the Fourier transform of equation (6) and make equation (36) incorrect. In fact, considering $\psi(\zeta) = 0$ for $\zeta \leqslant 0$, the Fourier transform of $\frac{\mathrm{d}^2\psi}{\mathrm{d}\zeta^2}$ and $\frac{\psi(\zeta)}{\zeta}$ becomes

$$\begin{aligned} F\left[\frac{\mathrm{d}^2\psi}{\mathrm{d}\zeta^2}\right] &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}^2\psi}{\mathrm{d}\zeta^2} \mathrm{e}^{-\mathrm{i}p\zeta}\, \mathrm{d}\zeta = \frac{1}{2\pi} \int_0^{\infty} \frac{\mathrm{d}^2\psi}{\mathrm{d}\zeta^2} \mathrm{e}^{-\mathrm{i}p\zeta}\, \mathrm{d}\zeta \\ &= -p^2\phi(p) - \frac{1}{2\pi} \frac{\mathrm{d}\psi(0)}{\mathrm{d}\zeta} \end{aligned} \tag{42}$$

$$\begin{aligned} F\left[\frac{1}{\zeta}\psi(\zeta)\right] &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\psi(\zeta)}{\zeta} \mathrm{e}^{-\mathrm{i}p\zeta}\, \mathrm{d}\zeta = \frac{1}{2\pi} \int_0^{\infty} \frac{\psi(\zeta)}{\zeta} \mathrm{e}^{-\mathrm{i}p\zeta}\, \mathrm{d}\zeta \\ &= -\mathrm{i} \int_0^p \phi(p')\, \mathrm{d}p' + \frac{1}{2\pi} \int_0^{\infty} \frac{\psi(\zeta)}{\zeta}\, \mathrm{d}\zeta \end{aligned} \tag{43}$$

respectively, and the Fourier transform of equation (6) reads

$$-\left(p^2+1\right)\phi(p) - \mathrm{i}\gamma \int_0^p \phi(p')\, \mathrm{d}p' + \frac{\gamma}{2\pi} \int_0^{\infty} \frac{\psi(\zeta)}{\zeta}\, \mathrm{d}\zeta - \frac{1}{2\pi} \frac{\mathrm{d}\psi(0)}{\mathrm{d}\zeta} = 0. \tag{44}$$

The last two terms of the left-hand side of equation (44) are constants. Taking a variable transform $s = \mathrm{i}p$, we can easily prove that equation (44) reduces to equation (7) and the Fourier transform reduces to a Laplace transform. Then we arrive at the conclusions of section 2.

Equation (44) can also be solved directly. Deriving equation (44) with p, we obtain

$$-\left(p^2+1\right)\phi'(p) - 2p\phi(p) - \mathrm{i}\gamma\phi(p) = 0. \tag{45}$$

Its general solutions are

$$\phi(p) = \frac{A}{p^2+1} \mathrm{e}^{-\mathrm{i}\gamma \,\mathrm{Arctan}\, p} \tag{46}$$

where Arctan p is a multi-valued function, and

$$\mathrm{Arctan}\, p = \arctan p \pm k\pi \qquad (k = 0, 1, 2, \ldots) \tag{47}$$

$$-\tfrac{1}{2}\pi \leqslant \arctan p \leqslant \tfrac{1}{2}\pi. \tag{48}$$

Substituting equation (47) into equation (46),

$$\phi(p) = \frac{A}{p^2+1} \mathrm{e}^{-\mathrm{i}p\gamma \arctan p \pm \mathrm{i}\gamma k\pi}. \tag{49}$$

Since the wavefunction $\psi(\zeta)$ and $\phi(p)$ must be a single-valued function, we obtain

$$\gamma = 2n \qquad (n = 1, 2, 3, \ldots) \tag{50}$$

and the energy levels equation (19). Substituting equation (49) into equation (44), one can confirm equation (49) is the solution of equation (44) by a direct calculation.

In summary, employing the Laplace transform and using the series expansion method, we have found that the exact bound state solutions and the eigenenergies of the 1D Schrödinger equation with the potential $-Ze^2/x$. We have proven that the energy levels of the $-Ze^2/x$ potential are proportional to $1/n^2$, where n is an integer. The character of the bound states for the potential $-Ze^2/x$ is the same as that of $V_1(x)$ given by equation (1) because the value of the wavefunction at the origin point is zero for both cases. Since $\psi(\zeta) = 0$ for $\zeta \leqslant 0$, the Fourier transform will reduce to a Laplace transform directly. The basic reason for the incorrect solutions given by [15] is that they have not paid attention to the behaviour of wavefunction, i.e. $\psi(0) = 0$ and $\psi(\zeta) = 0$ when $\zeta \leqslant 0$.

Acknowledgments

This work was supported in part by the National Natural Science Foundation of China under contract no 19975010, and the Foundation of Education Department of China.

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