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Application of a generalised function method to the infinitely deep square well problem

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Abstract: The Schrödinger equation for the eigenvalues of the infinitely deep square well potential is solved within the class of generalised functions. It is found that the ground state consists of a step function like eigenfunction with the eigenvalue zero.

Key words: Eigenvalue, eigenfunction, complete set, generalised function

1. Introduction

The basic problem of quantum mechanics is the solution of the eigenvalue equation

$$L_1 u_\lambda(x) = \lambda u_\lambda(x) \tag{1}$$

Here L_1 is a self-adjoint operator in one dimension of the type $L_1 = -\frac{d^2}{dx^2} + V(x)$, $\lambda = 2mE/\hbar^2$ is the eigenvalue with E the energy parameter, and m and $\hbar$ are particle mass and Planck constant, respectively. The function $V(x)$ is related to the potential $V_p(x)$ by $V(x) = 2mV_p(x)/\hbar^2$. Since equation (1) is of second order, there must be some data about the sought eigenfunction $u_\lambda(x)$ itself and about its derivative $u'_\lambda(x)$ on the system boundaries. Although the shape of $V(x)$ for the infinitely deep square well (IDSW) is very simple, satisfaction of boundary conditions (BCs) proved to be difficult [2]. The presently known solution, what I call the old one, uses ordinary functions, satisfies the BC for $u_\lambda(x)$, but does not satisfy the BC for $u'_\lambda(x)$. The old solution of IDSW problem is given in almost every physics book [5,6] on quantum mechanics and every mathematics book [1] on partial differential equations and boundary value problems. They, in fact, repeat a wrong result about the ground state energy that was found long time ago [7,8]. The earliest solution [8] dates back to 1929 and states that the ground state energy, or the lowest eigenvalue, is nonzero. This result causes a certain dissatisfaction among physicists; nevertheless, it continues to be accepted in the physics [4] and mathematics [3] literature, due to lack of a better solution.

This work resolves all the difficulties about the BCs by employing generalised functions [9]. Setting up suitable BCs needs special attention on the one hand and choosing the class of solution functions on the other. These two points deserve thorough discussion, which is done in section 2. Section 3 is for setting up the model and writing the differential equation for generalised functions. Section 4 is for obtaining the complete set of eigenfunctions and eigenvalues and finally section 5 is for discussing the results.

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2. Solution function class

The function $V(x)$ is shown schematically in Figure 1a. Mathematically it reads

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq L \\ \infty, & \text{otherwise} \end{cases} \tag{2}$$

Thus, equation (1) to be solved for $u_\lambda(x)$ is necessarily restricted to the allowed region, $0 \leq x \leq L$, and has the form

$$-\frac{d^2}{dx^2} u_\lambda(x) - \lambda u_\lambda(x) = 0 \tag{3}$$

together with suitable BCs about $u_\lambda(x)$, $u'_\lambda(x)$ at $x = 0$ and $x = L$. The solution of equation (3) may be sought in the form of a generalised function by writing

$$g_\lambda(x) = [H(x) - H(x - L)] u_\lambda(x). \tag{4}$$

Now we remove any restrictions on $u_\lambda(x)$, because the step function-like factor in square brackets takes care of it. This is why the schematic drawings in Figure 1b have been extended beyond $x = 0, L$. This, in turn, means that there are no BCs on $u_\lambda(x)$ except that we may use some symmetry arguments to be sensible. The wave function $u_\lambda(x)$ may be present inside the well region by any amount near the walls. Furthermore, the presence of $u_\lambda(x)$ outside the well is prevented by the square bracket term. If we can write an equation for $g_\lambda(x)$ and solve it, then it will carry the square bracket term and the eigenfunction $u_\lambda(x)$ in it. Since $g_\lambda(x)$ is a generalised function, the value of it at one point, like $x = 0$ or $x = L$, is not important [9]. Its integral effect over the range $0 \leq x \leq L$ is what is important.

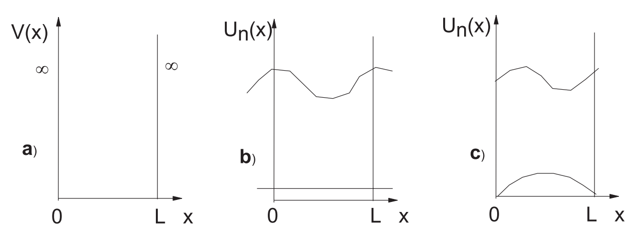

Figure 1. a) Square well, b) new eigenfunctions, c) old eigenfunctions.

In Figure 1c the first two eigenfunctions of the old solution are shown schematically to allow comparison.

3. Equation for generalised function

Obtaining the equation for $g_\lambda(x)$ is accomplished, as explained in [9] on page 371, by adding a generalised function $g_2(x)$ to the right-hand side of equation (3)

$$-\frac{d^2}{dx^2} g_\lambda(x) - \lambda g_\lambda(x) = g_2(x), -\infty < x < \infty. \tag{5}$$

To determine $g_2(x)$, let us take first and second derivatives of $-g_\lambda(x)$.

$$-g'_\lambda(x) = -[\delta(x) - \delta(x - L)] u_\lambda(x) - [H(x) - H(x - L)] u'_\lambda(x) \tag{6}$$

$$-g_\lambda''(x) = [-\delta'(x) + \delta'(x-L)]u_\lambda(x) + [-\delta(x)u_\lambda'(0) + \delta(x-L)u_\lambda'(L)]$$

$$-[\delta(x)u_\lambda'(0) - \delta(x-L)u_\lambda'(L)] - [H(x) - H(x-L)]u_\lambda''(x) \tag{7}$$

In the first square brackets in equation (7), we can use

$$-\delta'(x)u_\lambda(x) + \delta'(x-L)u_\lambda(x)$$

$$= -\{u_\lambda(0)\delta'(x) - u_\lambda'(0)\delta(x)\} + \{u_\lambda(L)\delta'(x-L) - u_\lambda'(L)\delta(x-L)\}. \tag{8}$$

This is due to the general relation [9],

$$g(x)\delta^{(k)}(x) = \sum_{j=0}^{k}(-1)^j g^{(j)}(0)\delta^{(k-j)}(x) \tag{9}$$

about the effect of the k th derivative of $\delta(x)$ on the function $g(x)$. Using the result (8), we can write equation (7) as

$$-g_\lambda''(x) = [-u_\lambda(0)\delta'(x) + u_\lambda(L)\delta'(x-L)]$$

$$+[-u_\lambda'(0)\delta(x) + u_\lambda'(L)\delta(x-L)] - [H(x) - H(x-L)]u_\lambda''(x). \tag{10}$$

If we put this into equation (5), and if we take $g_2(x)$ as the sum of first two square brackets in equation (10), we arrive at

$$-g_\lambda''(x) - \lambda g_\lambda(x) = [-u_\lambda(0)\delta'(x) + u_\lambda(L)\delta'(x-L)] + [-u_\lambda'(0)\delta(x) + u_\lambda'(L)\delta(x-L)]. \tag{11}$$

This looks like the inhomogeneous form of equation (3), only that both sides have been multiplied from the left by $[H(x) - H(x-L)] = 1$. This multiplying prefactor is present inherently on the left side in equation (11), while it is not shown on the right side. However, it does not matter anyway; we can put it if we wish. When the terms on the right are allowed to cancel, the corresponding terms on the left of equation (11) are equivalent to

$$[H(x) - H(x-L)]\{-u_\lambda''(x) - \lambda u_\lambda(x)\} = 0, \tag{12}$$

which is very similar to equation (3). Therefore, the solution of equation (11) may help us in finding $u_\lambda(x)$. Once we find $g_\lambda(x)$, it will carry the factor $[H(x) - H(x-L)]$ and dropping this factor we will have $u_\lambda(x)$ as the remaining terms.

Now giving some BCs about $u_\lambda(x)$ itself or its derivative $u_\lambda'(x)$ simplifies the right side of equation (11). For example, if we require

$$u_\lambda(0) = u_\lambda(L) \tag{13}$$

$$u_\lambda'(0) = u_\lambda'(L) = 0, \tag{14}$$

then the second square bracket on the right of equation (11) is dropped

$$-g_\lambda''(x) - \lambda g_\lambda(x) = -u_\lambda(0)\delta'(x) + u_\lambda(L)\delta'(x-L). \tag{15}$$

The interpretation of these BCs is as follows. The condition (13) reflects the symmetry of the two walls. Later on, we shall see that it is necessary for the occurrence of $[H(x) - H(x-L)]$ in the solution. If we take for example $u_\lambda(0) = -u_\lambda(L)$ we can again produce such a factor but this will be a different problem. The study of this different problem leads to odd integer values for n and gives a nonzero ground state energy. Hence, we are bound to use the condition (13). In equation (13) we are not giving a numerical value to $u_\lambda(x)$ because it can take any value on the walls as stated in section 2. The particle may be present inside the walls and may come as close as possible to them, like water in a glass, only that it cannot escape through. No current is allowed to pass through the walls as mentioned in the previous section. Equation (14) is also plausible because it expresses a way of preventing escape of flux through the walls. There may be other ways of doing this but this condition has been employed here and meaningful results have been found.

4. Eigenfunctions

Direct solution of equation (15) may be obtained by taking the Fourier transform of both sides with the parameter k_1

$$(k_1^2 - \lambda)G(\lambda, k_1) = -ik_1 u_\lambda(0) + ik_1 u_\lambda(0)e^{-ik_1 L}. \tag{16}$$

Then the inverse transform becomes

$$g_\lambda(x) = u_\lambda(0)\frac{1}{i2\pi}\int_{-\infty}^{\infty}\frac{e^{ik_1 x}}{k_1^2-\lambda}k_1 dk_1 - u_\lambda(0)\frac{1}{i2\pi}\int_{-\infty}^{\infty}\frac{e^{ik_1(x-L)}}{k_1^2-\lambda}k_1 dk_1. \tag{17}$$

There may also exist terms of the $C_1\delta(k_1-\sqrt{\lambda})$ and $C_2\delta(k_1+\sqrt{\lambda})$ types with C_1, C_2 arbitrary constants. They are dropped because they involve the solution of the homogeneous form of (16). To evaluate the two integrals

$$I_1(x) = \frac{1}{i2\pi}\int_{-\infty}^{\infty}\frac{e^{ik_1 x}}{k_1^2-\lambda}k_1 dk_1, \qquad I_2(x) = \frac{1}{i2\pi}\int_{-\infty}^{\infty}\frac{e^{ik_1(x-L)}}{k_1^2-\lambda}k_1 dk_1$$

we go to the complex z plane with $z = k_1 + ik_2$ and consider the real axis parts of the integrals $I_1(z), I_2(z)$ along two suitable contours C_1 and C_2. As usual, C_1 consists of a semicircle in the upper half plane for $x > 0$, and similarly C_2 is the same circle considered for $x - L > 0$. There are half contributions from the two residues at $z = \sqrt{\lambda}$, $z = -\sqrt{\lambda}$ and the result is

$$I_1 = \frac{1}{2}\frac{e^{-i\sqrt{\lambda}x}}{2} + \frac{1}{2}\frac{e^{i\sqrt{\lambda}x}}{2} \tag{18}$$

$$I_2 = \frac{1}{2}\frac{e^{-i\sqrt{\lambda}(x-L)}}{2} + \frac{1}{2}\frac{e^{i\sqrt{\lambda}(x-L)}}{2} \tag{19}$$

Using these in equation (17), we have

$$g_\lambda(x) = \frac{u_\lambda(0)}{2}\frac{1}{2}[e^{i\sqrt{\lambda}x} + e^{-i\sqrt{\lambda}x}]H(x) - \frac{u_\lambda(0)}{2}\frac{1}{2}[e^{i\sqrt{\lambda}x}e^{-i\sqrt{\lambda}L} + e^{-i\sqrt{\lambda}x}e^{i\sqrt{\lambda}L}]H(x-L). \tag{20}$$

If we have

$$\sqrt{\lambda}L = 2\pi n, \qquad n = 0, 1, .., \infty$$

the last square brackets become the same as the first ones

$$g_n(x) = [H(x) - H(x-L)]\frac{u_n(0)}{2}\cos\frac{n2\pi}{L}x, \qquad n = 0, 1.., \infty. \tag{21}$$

Since $\lambda = 2mE/\hbar^2 = n^2(2\pi)^2/L^2$, eigenenergies and eigenfunctions are given by

$$E_n = \frac{\hbar^2}{2m}\frac{(2\pi)^2}{L^2}n^2, \qquad n = 0, 1, 2, ..., \infty \tag{22}$$

$$g_0(x) = [H(x) - H(x-L)]\frac{u_0(0)}{2}, \qquad n = 0 \tag{23}$$

$$g_n(x) = [H(x) - H(x-L)]u_n(0)\cos\frac{n2\pi}{L}x, \qquad n = 1, 2, ..., \infty. \tag{24}$$

Validity of this solution can be checked by direct substitution to equation (15), together with taking into account equation (14). Each member of the eigenfunctions set need not be normalized to unity. It is only necessary that this set satisfies the completeness relation by a suitable choice of normalization constants.
The complete set of eigenfunctions of equation (3) are

$$u_n(x) = \sqrt{\frac{2}{L}}\cos\frac{n2\pi}{L}x, \qquad n = 0, \mp 1, \mp 2, ..., \mp\infty \tag{25}$$

and they satisfy the relation

$$\sum_{-\infty}^{\infty} u_n(x)u_n(x') = \frac{2}{L}\sum_{-\infty}^{\infty}\cos\frac{n2\pi}{L}x\cos\frac{n2\pi}{L}x' = \delta(x - x') + \delta(x + x'). \tag{26}$$

Here the second delta function is dropped since x, x' are positive. For comparison the old solutions using $u_n(0) = 0$, $u_n(L) = 0$ at the walls are

$$u_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x, \qquad n = 1, 2, ..., \infty \tag{27}$$

$$E_n = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}n^2, \qquad n = 1, 2, ..., \infty. \tag{28}$$

The derivatives, $u_n'(0) = (n\pi/L)(2/L)^{1/2}$, $u_n'(L) = (-1)^n(n\pi/L)(2/L)^{1/2}$, are neither equal nor continuous across the boundaries. This result has been subject to criticism [2].

5. Discussion and conclusions

In the old solution the lowest eigenenergy is nonzero. This causes great problems in our understanding of the real world. Depending on it, widespread comments exist stating the impossibility of a quantum particle's energy being zero. The new solution found the ground state energy as zero, which obeys the reality much better. Accordingly new interpretations of the subject may be expected to come. Spacing of subsequent energy levels also changed in the new solution, although the n^2 dependence remained the same.

It is wanted that particles do not escape through the walls. This requires flux density $j(x)$ to be zero on each of them. For real eigenfunctions, since $j(x) \sim u_n(x)u_n'(x)$, there are two ways of making $j = 0$. First $u_n(x)$ is zero on the walls, which is what the old solution uses, and second is $u_n'(0) = 0 = u_n'(L)$ as also given by equation (14), which is used in this work. In reference [4] they tried, using the first way, to place a linear eigenfunction of a triangle type inside the well but they did not succeed in obtaining an eigenvalue.

The use of generalised functions in the solution of differential equations has been described in [9] on page 371. This method has been applied to the solution of the IDSW problem for first time in this work and new eigenfunctions and eigenvalues have been found.

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