On a solution method for the bound energy states of a particle in a one-dimensional symmetric finite square well potential

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(Dated: March 25, 2019)

We present details of a new solution method for the bound energy states of a quantum particle in a one-dimensional symmetric finite square well potential. The solution is obtained in a clear way by introducing a simple method that relies on the use of two auxiliary functions. The approach is straightforward and leads to the well known even and odd-parity wave function solutions of the problem without having to do any a-priori assumptions about the nature or symmetry of the quantum states.

Keywords: Quantum mechanics; Bound energy states; Finite square well potential.

I. INTRODUCTION

Since its birth at the start of the twentieth century, quantum mechanics has evolved to become one of the most successful theories in science. Active development of modern quantum mechanical ideas have enabled scientists to calculate with very high precision various properties of systems at various length scales. Information technology relies on quantum theory and so does control of positions and energy levels of quantum states that emerge in a variety of systems and potentials. Studies of one-dimensional (1D), two-dimensional (2D), three-dimensional (3D) dynamic quantum wells, quantum dots, quantum localized lattices as well as nanosystems are also of great interest [1, 2]. The hydrogen atom, quantum oscillators, problems involving a quantum oscillator under the action of a periodic external potential, motion of a charged particle with spin in a constant or uniform periodic magnetic field and many others are some of the widely known problems that can be solved either analytically or numerically using various quantum theory methods [3–12].

For all these reasons, quantum mechanics is a very important part of any undergraduate physics curriculum. With time, undergraduate students are expected to become familiar with several quantum principles, they are taught a variety of calculation methods and learn how to apply these methods and techniques to solve simple quantum problems. One of such problems which is virtually found in all quantum textbooks in circulation is that of a particle in an infinite or finite 1D quantum well [13–17]. While the case of an infinite 1D quantum well is elementary, the solution of its finite counterpart is more demanding. In particular, the energy levels for the case of bound states are found by solving the resulting transcendental equations either numerically or graphically [18–21]. Obtaining even parity and odd parity wave function solutions generally involves algebraic manipulations of systems of equations for sets of arbitrary constants that may confuse some undergraduate students like those that are not very advanced on the topic of linear homogeneous/nonhomogeneous systems of equations (matrices, determinants, etc.). Therefore, finding simple solutions is not only relevant from a pedagogical point of view, but also important to engage better the audience.

The problem at hand is that of a particle subject to a 1D symmetric finite square (or rectangular) well potential of the form:

$$V(x) = \begin{cases} -V_0 \quad ; \quad -a \le x \le +a \\ \\ 0 \quad ; \quad \text{elsewhere} \ , \end{cases} \tag{1}$$

where $V_0 > 0$ is the depth of the well and $a > 0$ is its range. Note that we have chosen the origin of the x-axis at the center of the well so that the potential is an even function of x and symmetric about $x = 0$. For the bound states we require $-V_0 < E < 0$. The discrete bound energy eigenfunctions are found by solving the stationary Schrödinger equation in each region of constant potential separately. There are three such regions of space labeled as region I ($-\infty < x \le -a$), region II ($-a \le x \le +a$) and region III ($+a \le x < +\infty$). We denote the corresponding wave functions in each of the three regions as $\Phi_I(x)$, $\Phi_{II}(x)$ and $\Phi_{III}(x)$. As shown in Appendix. A a general acceptable quantum solution of the stationary Schrödinger's equation (which goes to zero as $|x| \to \infty$) has the form:

$$\begin{cases} \Phi_I(x) = A \, \exp(k' \, x) \quad ; \quad -\infty < x \le -a \\ \\ \Phi_{II}(x) = B_1 \, \sin(k \, x) + B_2 \, \cos(k \, x) \quad ; \quad -a \le x \le +a \\ \\ \Phi_{III}(x) = C \, \exp(-k' \, x) \quad ; \quad +a \le x < +\infty \ , \end{cases} \tag{2}$$

where A, B_1, B_2 and C are constants to be determined. We write all the formulas throughout the paper without simplifications. With other words, we do not use atomic units which are another familiar choice in the field [12].

Standard analysis and the usual boundary conditions for the corresponding wave functions in each of the three

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regions lead to a system of four equations for the four undetermined constants. At this juncture, some textbooks approach the problem as solving a system of homogeneous equations for four unknown constants [16]. To this effect, they work with systems of equations in matrix form (where the right-hand side column vector is zero) and then argue that non-trivial solutions are obtained only if the determinant of the coefficient matrix is zero [16, 17]. Some other textbooks get involved into complicated algebraic transformations by appealing to symmetry conditions [13]. Among the few notable exceptions is Ref.[3] where one does not even choose the 1D finite square well potential to have a symmetric form about $x = 0$ - see pg. 63 and Fig. 1 of Ref.[3].

These lines of discussion may confuse few students and it is fair to say that sometimes the transformations involved leading to the final result are rather complicated, for instance, see pgs. 280-282 of Ref.[16]. Therefore, in order to simplify the solution of the problem while keeping utmost clarity, in this work we provide a new method to solve this problem. We believe that this method is very clear to understand and leads to the known results in a way that students and teachers may find appealing. This method involves the use of two auxiliary functions that have unique properties.

II. NEW SOLUTION METHOD

The solution method that we introduce avoids some of the mathematical hurdles previously mentioned. The approach is also quite conventional therefore it requires only some basic knowledge of algebra and/or algebraic manipulations. Therefore, all the steps should be easy to follow even from the perspective of undergraduate students with limited mathematical background. The first step of the approach is to express three of the undetermined constants mentioned earlier in terms of the remaining one (chosen to be nonzero) while the second step is to introduce two auxiliary functions that lead to the final result written in a very simple compact form. To this effect, we use the first three equations in Eq.(A8) of Appendix. A to express the constants B_1, B_2, C in terms of A. The expressions for the constants B_1, B_2 and C in terms of $A \neq 0$ are given, respectively, in Eq.(A10), Eq.(A11) and Eq.(A12) of Appendix. A. The form of these expressions is highly suggestive. At this point, we introduce the following two auxiliary functions:

$$F(k, k') = \sin(k\,a) - \frac{k'}{k}\cos(k\,a) \tag{3}$$

and

$$G(k, k') = \cos(k\,a) + \frac{k'}{k}\sin(k\,a)\ . \tag{4}$$

A detailed description of the major properties of these two functions is provided in Appendix. B. These two auxiliary functions help us to write the expressions for the constants B_1, B_2 and C in a compact form as:

$$\begin{cases} B_1 = -A\,\exp(-k'a)\,F(k, k') \\ B_2 = A\,\exp(-k'a)\,G(k, k') \\ C = A\Big[-\sin(k\,a)\,F(k, k') + \cos(k\,a)\,G(k, k')\Big]\ . \end{cases} \tag{5}$$

Note that the last equation, namely the fourth equation in Eq.(A8), has not been used yet:

$$k\,[B_1\cos(k\,a) - B_2\sin(k\,a)] = -k'\,C\,\exp(-k'a)\ . \tag{6}$$

By substituting the values of B_1, B_2 and C from Eq.(5) into Eq.(6) one obtains the following neat, simple and very compact result:

$$2\,k\,F(k, k')\,G(k, k') = 0\ . \tag{7}$$

As explained in Appendix. B, the two auxiliary functions $F(k, k')$ and $G(k, k')$ have the remarkable property that they cannot be simultaneosly zero. This means that Eq.(7) is satisfied for two separate situations

$$F(k, k') = 0 \tag{8}$$

or

$$G(k, k') = 0\ . \tag{9}$$

This conclusion leads quite naturally to the well-known two sets of solutions (with even and odd parity wave functions) for the bound states of a particle in a 1D symmetric finite well potential.

III. EVEN AND ODD PARITY SOLUTIONS

The even and odd parity wave function solutions for the bound states of a particle in a 1D symmetric finite quantum square well potential are well known. However, for the sake of completeness, we report briefly below some key results. Obviously, we skip most of the details which are readily available in the literature.

A. Even parity solutions

The even parity solutions correspond to $F(k, k') = 0$ where $G(k, k') \neq 0$. This means that:

$$k\,\tan(k\,a) = k'\ . \tag{10}$$

By using Eq.(5) in conjuction with Eq.(B5) one has:

$$\begin{cases} B_1 = 0 \\ B_2 = A\,\exp(-k'a)\,G(k, k') \\ C = A\ . \end{cases} \tag{11}$$

As a result the even-parity wave function, $\Phi_e(x)$ becomes:

$$\Phi_e(x) = \begin{cases} A\,\exp(k'\,x) \quad ; \quad -\infty < x \le -a \\ A\,\exp(-k'\,a)\,G(k,k')\,\cos(k\,x) \;\; ; \;\; -a \le x \le +a \\ A\,\exp(-k'\,x) \quad ; \quad +a \le x < +\infty \;. \end{cases} \tag{12}$$

If one multiplies $\Phi_e(x)$ in Eq.(12) with $\exp(k'a)\cos(k\,a)$ and uses the property in Eq.(B5) one obtains:

$$\Phi_e(x) = \begin{cases} A\,\cos(k\,a)\,\exp[k'\,(x+a)] \quad ; \quad -\infty < x \le -a \\ A\,\cos(k\,x) \quad ; \quad -a \le x \le +a \\ A\,\cos(k\,a)\,\exp[-k'\,(x-a)] \quad ; \quad +a \le x < +\infty \;, \end{cases} \tag{13}$$

where the new wave function $\Phi_e(x)$ in Eq.(13) incorporates the irrelevant multiplication factor, $\exp(k'a)\cos(k\,a)$. The constant A is determined from the overall normalization of the wave function.

B. Odd parity solutions

The odd parity solutions correspond to $G(k,k') = 0$ where $F(k,k') \neq 0$. This means that:

$$k\,\cot(k\,a) = -k' \;. \tag{14}$$

By using Eq.(5) in conjuction with Eq.(B6) one has:

$$\begin{cases} B_1 = -A\,\exp(-k'a)\,F(k,k') \\ B_2 = 0 \\ C = -A \;. \end{cases} \tag{15}$$

Thus, the odd-parity wave function, $\Phi_o(x)$ becomes:

$$\Phi_o(x) = \begin{cases} A\,\exp(k'\,x) \quad ; \quad -\infty < x \le -a \\ -A\,\exp(-k'\,a)\,F(k,k')\,\sin(k\,x) \quad ; \quad -a \le x \le +a \\ -A\,\exp(-k'\,x) \quad ; \quad +a \le x < +\infty \;, \end{cases} \tag{16}$$

If one multiplies $\Phi_o(x)$ in Eq.(16) with $\exp(k'a)\sin(k\,a)$ and uses Eq.(B6) one has:

$$\Phi_o(x) = \begin{cases} A\,\sin(k\,a)\,\exp[k'\,(x+a)] \quad ; \quad -\infty < x \le -a \\ -A\,\sin(k\,x) \quad ; \quad -a \le x \le +a \\ -A\,\sin(k\,a)\,\exp[-k'\,(x-a)] \quad ; \quad +a \le x < +\infty \;, \end{cases} \tag{17}$$

where the new wave function in Eq.(17) incorporates the irrelevant multiplication factor, $\exp(k'a)\sin(k\,a)$.

C. Graphical solution for the energy

The energy of the bound state is calculated from the expressions in Eq.(A4) subject to the constraint:

$$k^2 + k'^2 = \frac{2\,m}{\hbar^2}\,V_0 \;. \tag{18}$$

In order to obtain more easily the allowed energies corresponding to even and odd parity solutions one introduces the following dimensionless variables:

$$\xi = k\,a > 0 \quad ; \quad \eta = k'\,a > 0 \quad ; \quad \gamma^2 = \frac{2\,m}{\hbar^2} V_0\,a^2 > 0 \tag{19}$$

As a result, the expression in Eq.(18) can be rewritten as:

$$\xi^2 + \eta^2 = \gamma^2 \;. \tag{20}$$

The energy values corresponding to even parity solutions are then obtained after solving the following transcendental equations:

$$\xi\,\tan(\xi) = \eta \quad ; \quad \xi^2 + \eta^2 = \gamma^2 \quad ; \quad \tan(\xi) > 0 \;. \tag{21}$$

On the other hand, for odd parity solutions one has:

$$\xi\,\cot(\xi) = -\eta \quad ; \quad \xi^2 + \eta^2 = \gamma^2 \quad ; \quad -\cot(\xi) > 0 \;. \tag{22}$$

The allowed bound state energies are related to k (and/or k') and may be expressed in terms of the new variables ξ and η. For instance, one may write the expression for the energy as:

$$E = -\frac{\hbar^2}{2\,m} k'^2 = -\frac{\hbar^2}{2\,m\,a^2}\,\eta^2 \quad ; \quad \eta = k'a \;. \tag{23}$$

Alternatively, one may choose to write:

$$V_0 = \frac{\hbar^2}{2\,m\,a^2}\,\gamma^2 \;, \tag{24}$$

and from there obtain

$$E = -V_0\,\left(\frac{\eta}{\gamma}\right)^2 \;. \tag{25}$$

Graphical solutions of the transcendental equations are widely available in the literature, for instance, see Ref.[22] for several such methods.

IV. CONCLUSIONS

In this work we considered the well known quantum mechanical problem of determining the bound energy states of a quantum particle in a 1D symmetric finite square well potential. The purpose of the study is to present a simple solution method to the problem that relies on the use of two auxiliary functions. The method adopted presents a new insight into the solution of this standard quantum mechanical problem. The key aspect of the approach is to highlight the important role that a special combination of trigonometric functions, denoted as the auxiliary functions $F(k,k')$ and $G(k,k')$, play in solving the problem at hand. The method allows one to elegantly separate the even and odd-parity wave function solutions of the problem by looking at each auxiliary function separately and show that one of the auxiliary functions (and one of them only) has to be equal to zero.

It is worthwhile pointing out that the method outlined in this work can be immediately generalized to a 1D asymmetric quantum well potential scenario, too. If the symmetric potential in Eq.(1) is changed to an asymmetric form so that $V(x) = V_1 \geq 0$ for $x \leq -a$ and $V(x) = 0$ for $x \geq +a$ then the approach to calculate the bound energy states (that correspond to $E < 0$) will lead to a compact equation involving the previously defined two auxiliary functions that is slightly different from Eq.(7). However, under these circumstance, the second argument of the two auxiliary functions (that was k' for the symmetric potential) will not be the same. Analogs in spirit to the procedure outlined in this work may be applied to even more complex problems such as computing the strong field Stark and Zeeman resonances (energies and widths) in atomic and molecular systems including DC and AC strong field effects, atomic, molecular and nuclear multiphoton resonances, different resonant effects in cooperative laser-electron nuclear processes and resonant effects in the interaction of strong electromagnetic pulses with solids, to mention a few [6–12].

Furthermore, this study also underscores the pedagogical value of the method from the perspective of undergraduate students taking an introductory quantum mechanics course. We believe that the results presented in this work would be useful to an audience of undergraduate and graduate students as well as instructors teaching quantum mechanics in an undergraduate physics environment.

Acknowledgements

This research was supported in part by National Science Foundation (NSF) Grant No. DMR-1705084.

APPENDIX A: WAVE FUNCTION

The stationary Schrödinger's equation reads:

$$\left[-\frac{\hbar^2}{2\,m}\frac{d^2}{dx^2} + V(x)\right]\Phi(x) = E\,\Phi(x)\ , \qquad \text{(A1)}$$

where m is the mass of the particle, $\hbar$ is the reduced Planck's constant and $\Phi(x)$ is the (unknown) wave function of the particle corresponding to energy, E. For convenience, one rewrites Eq.(A1) as:

$$\frac{d^2\Phi(x)}{dx^2} + \frac{2\,m}{\hbar^2}\Big[E - V(x)\Big]\Phi(x) = 0\ . \qquad \text{(A2)}$$

The above equation should be solved separately in three different regions of space: region I ($-\infty < x \leq -a$), region II ($-a \leq x \leq +a$) and region III ($+a \leq x < +\infty$). The differential equations written separately for each of the three regions read:

$$\begin{cases} \frac{d^2\Phi_I}{dx^2} - k'^2\,\Phi_I(x) = 0 \quad ; \quad -\infty < x \leq -a \\ \frac{d^2\Phi_{II}}{dx^2} + k^2\,\Phi_{II}(x) = 0 \quad ; \quad -a \leq x \leq +a \\ \frac{d^2\Phi_{III}}{dx^2} - k'^2\,\Phi_{III}(x) = 0 \quad ; \quad +a \leq x < +\infty\ , \end{cases} \qquad \text{(A3)}$$

where we have introduced two constants:

$$\frac{2\,m}{\hbar^2}E = -k'^2 \quad ; \quad \frac{2\,m}{\hbar^2}(E + V_0) = k^2\ . \qquad \text{(A4)}$$

It is implied that both k and k' are non-negative and real. A general acceptable quantum solution (which goes to zero as $|x| \to \infty$) has the form:

$$\begin{cases} \Phi_I(x) = A\,\exp(k'\,x) \quad ; \quad -\infty < x \leq -a \\ \Phi_{II}(x) = B_1\,\sin(k\,x) + B_2\,\cos(k\,x) \quad ; \quad -a \leq x \leq +a \\ \Phi_{III}(x) = C\,\exp(-k'\,x) \quad ; \quad +a \leq x < +\infty\ , \end{cases} \qquad \text{(A5)}$$

where A, B_1, B_2 and C are constants to be determined. It is also useful to calculate the first derivatives of the above wave functions:

$$\begin{cases} \frac{d\Phi_I(x)}{dx} = k'\,A\,\exp(k'\,x) \quad ; \quad -\infty < x \leq -a \\ \frac{d\Phi_{II}(x)}{dx} = k\Big[B_1\,\cos(k\,x) - B_2\,\sin(k\,x)\Big] \quad ; \quad -a \leq x \leq +a \\ \frac{d\Phi_{III}(x)}{dx} = -k'\,C\,\exp(-k'\,x) \quad ; \quad +a \leq x < +\infty\ . \end{cases} \qquad \text{(A6)}$$

Continuity conditions for the wave function and its first derivative at $x = -a$ and $x = +a$ require that:

$$\begin{cases} \Phi_I(x = -a^-) = \Phi_{II}(x = -a^+) \\ \frac{d\Phi_I}{dx}(x = -a^-) = \frac{d\Phi_{II}}{dx}(x = -a^+) \\ \Phi_{II}(x = +a^-) = \Phi_{III}(x = +a^+) \\ \frac{d\Phi_{II}}{dx}(x = +a^-) = \frac{d\Phi_{III}}{dx}(x = +a^+)\ . \end{cases} \qquad \text{(A7)}$$

The symbol $x = a^-$ indicates that x approaches a from the left ($x \to a^-$). This means that $f(x = a^-) = \lim_{x\to a^-} f(x)$ is the left-hand limit of $f(x)$ as x approaches a from the left. Likewise, $x = a^+$ indicates that x approaches a from the right ($x \to a^+$). Therefore, $f(x = a^+) = \lim_{x\to a^+} f(x)$ is the right-hand limit of $f(x)$ as x approaches a from the right. Application of the continuity conditions from Eq.(A7) leads to the following system of equations for the four unknown constants, A, B_1, B_2 and C:

$$\begin{cases} A\,\exp(-k'a) = -B_1\sin(k\,a) + B_2\cos(k\,a) \\ k'\,A\,\exp(-k'a) = k\Big[B_1\cos(k\,a) + B_2\sin(k\,a)\Big] \\ B_1\sin(k\,a) + B_2\cos(k\,a) = C\,\exp(-k'a) \\ k\Big[B_1\cos(k\,a) - B_2\sin(k\,a)\Big] = -k'\,C\,\exp(-k'a)\ . \end{cases} \tag{A8}$$

The four equations in Eq.(A8) determine four constants and the energy (for example, via the variable k). To obtain a system of equations that is not under-determined, one uses the normalization condition:

$$\int_{-\infty}^{+\infty} dx\,|\Phi(x)|^2 = 1\ . \tag{A9}$$

This provides the required additional fifth equation.

Since the wave function is nonzero in region I, the condition $\Phi_I(x) \neq 0$ implies that constant $A \neq 0$. The same arguments apply to constant C but cannot be generalized to B_1 and B_2. Therefore, a suitable approach is to express B_1, B_2 and C in terms of A (which is guaranteed to be nonzero). After some algebraic manipulations to the first three equations in Eq.(A8) we obtain the following expressions for B_1, B_2 and C in terms of A, respectively:

$$B_1 = -A\,\exp(-k'a)\Big[\sin(k\,a) - \frac{k'}{k}\cos(k\,a)\Big]\ , \tag{A10}$$

$$B_2 = A\,\exp(-k'a)\Big[\cos(k\,a) + \frac{k'}{k}\sin(k\,a)\Big]\ , \tag{A11}$$

and

$$C = A\left\{-\sin(k\,a)\left[\sin(k\,a) - \frac{k'}{k}\cos(k\,a)\right] + \cos(k\,a)\left[\cos(k\,a) + \frac{k'}{k}\sin(k\,a)\right]\right\}\ . \tag{A12}$$

Note that the fourth equation in Eq.(A8) has not been used in these transformations.

In a more traditional approach, use of the fourth equation in Eq.(A8) eventually leads to a transcendental equation involving k and k'. A typical treatment found in several books [16, 17] is to use all the equations in Eq.(A8) (including the fourth equation) to obtain a system of equations in matrix form for the four unknown constants, A, B_1, B_2 and C which in our case reads:

$$\begin{pmatrix} \exp(-k'a) & \sin(k\,a) & -\cos(k\,a) & 0 \\ k'\,\exp(-k'a) & -k\,\cos(k\,a) & -k\,\sin(k\,a) & 0 \\ 0 & \sin(k\,a) & \cos(k\,a) & -\exp(-k'a) \\ 0 & k\,\cos(k\,a) & -k\,\sin(k\,a) & k'\,\exp(-k'a) \end{pmatrix} \begin{pmatrix} A \\ B_1 \\ B_2 \\ C \end{pmatrix} = 0 \tag{A13}$$

The system of homogeneous equations in Eq.(A13) has either one solution, $A = B_1 = B_2 = C = 0$ or infinite solutions. The zero solution ($A = B_1 = B_2 = C = 0$) is the only solution if the determinant of the coefficient matrix is nonzero. However, since we are looking for a nonzero solution for the four unknown constants, we must require that the determinant of the coefficient matrix be zero. The normalization condition determines the specific values of constants A, B_1, B_2 and C from the infinite set of the solutions of Eq.(A13) for the case when the determinant of the coefficient matrix is zero.

APPENDIX B: AUXILIARY FUNCTIONS

Consider the following two auxiliary functions:

$$F(k,k') = \sin(k\,a) - \frac{k'}{k}\cos(k\,a) \tag{B1}$$

and

$$G(k,k') = \cos(k\,a) + \frac{k'}{k}\sin(k\,a)\ , \tag{B2}$$

where k, k' are non-negative and real parameters. The two functions $F(k,k')$ and $G(k,k')$ defined in Eq.(B1) and Eq.(B2) have the property that they cannot be simultaneosly zero. The proof od this statement is simple. If it is assumed that $F(k,k') = 0$ one obtains:

$$\tan(k\,a) = \frac{k'}{k}\ . \tag{B3}$$

If one assumes that simultaneously also $G(k,k')=0$ then one should have:

$$\tan(k\,a) = -\frac{k}{k'} \ . \tag{B4}$$

This means that if Eq.(B3) and Eq.(B4) are simultaneosly true, one should have $k'/k = -k/k'$, a result that eventually would lead to $k' = i\,k$ where $i=\sqrt{-1}$ is the imaginary unit number. However, this conclusion cannot be true since it is assumed that both k and k' are real. In short, if $F(k,k')=0$ then $G(k,k')\neq 0$ and, by the same token, if $G(k,k')=0$ then $F(k,k')\neq 0$. The two auxiliary functions have also the following interesting properties:

$$\cos(k\,a)\,G(k,k') = 1 \quad when \quad F(k,k')=0 \ , \tag{B5}$$

and

$$\sin(k\,a)\,F(k,k') = 1 \quad when \quad G(k,k')=0 \ . \tag{B6}$$

The proof of Eq.(B5) and Eq.(B6) is left to the reader as an exercise.

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