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Articles

Bound states in a semi-infinite square potential well

Estados ligados num poço de potencial quadrado semi-infinito

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The finite square potential well is a staple problem in introductory quantum mechanics. There is an extensive literature on the determination of the allowed energies, which requires the solution of a transcendental equation by numerical, graphical or approximate analytic methods. Here we investigate the less explored problem of a particle in a semi-infinite potential well. The energy eigenvalues, which are also determined by a transcendental equation, are found by a standard graphical method, and a simple rule that yields the number of stationary states is provided. Next a simplification of the aforementioned transcendental equation is attempted. During the process pitfalls are encountered and a purportedly simpler graphical treatment of the problem given in the solutions manual to a fine textbook is shown to be flawed. A more careful analysis brings forth the correct simplification, which is shown to be particularly suitable for finding highly accurate approximations to the energy levels. Finally, a class of exact solutions is produced, the associated normalized eigenfunctions are constructed and the probability of finding the particle inside the well is computed.
Keywords: Bound states, Semi-infinite potential well, Exact solutions, Quantum Mechanics.

O poço de potencial quadrado finito é um problema básico de mecânica quântica introdutória. Há uma extensa literatura sobre a determinação das energias permitidas, que requer a solução de uma equação transcendente por meio de métodos numéricos, gráficos ou de aproximações analíticas. Aqui investigamos o problema menos explorado de uma partícula num poço de potencial semi-infinito. Os autovalores da energia, que também são determinados por uma equação transcendente, são encontrados por um método gráfico padrão, e uma regra simples que dá o número de estados estacionários é fornecida. Em seguida, uma simplificação da referida equação transcendente é tentada. Durante o processo, armadilhas são encontradas e um supostamente mais simples tratamento gráfico do problema, dado no manual de soluções de um excelente livro-texto, mostra-se falho. Uma análise mais cuidadosa produz a simplificação correta, que se mostra particularmente apropriada para obter aproximações altamente precisas para os níveis de energia. Finalmente, uma classe de soluções exatas é apresentada, as autofunções normalizadas correspondentes são construídas e a probabilidade de encontrar a partícula dentro do poço é calculada.
Palavras-chave: Estados ligados, Poço de potencial semi-infinito, Soluções exatas, Mecânica Quântica.

1. Introduction

In modern physics or introductory quantum mechanics courses the time-independent Schrödinger equation is first applied to one-dimensional physical systems such as a particle in a potential well [1, 2]. These examples illustrate the quantization of energy and how the allowed energies arise from the imposition of appropriate boundary conditions on the wave function. The case of the infinite square well – or particle in a box – can be easily solved exactly, but for the less unrealistic finite potential well the allowed energies arise as solutions of a transcendental equation, which can be found only numerically [3], graphically [4–7] or by analytic approximation methods [8–15]. Given its apparent inexhaustibility, the recent appearence of a guide to the large literature on the finite square well problem is a good thing [16]. The finite square well has a wide range of practical applications, from the theory of alpha decay (square well coupled to Coulomb barrier) in nuclear physics [17] to lasers and condensed matter physics [18].

Here we turn our attention to the less studied problem of the semi-infinite square well [13, 19, 20]. Scattering states are excluded from the discussion, the focus is on bound states. This is usually a textbook problem – see Problems 6-23 on page 229 of [1] and 4.13 on page 270 of [19] – but it also finds application in condensed matter physics [21] and in modelling the nuclear potential [17]. Similarly to the finite well, the determination of the allowed energy levels for the semi-infinite well requires the solution of a transcendental equation.

In Section 2 the problem is stated and the transcendental equation whose solutions furnish the possible energies is derived. In Section 3 we discuss the standard graphical solution and supply an exact and practical way to determine the number of stationary states. Next, in Section 4, we address some attempts at simplification

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of the transcendental equation that yields the allowed energies. In this process, pitfalls are recognized and it is pointed out that the reasoning pursued in the solutions manual to Ref. [1] does not pass muster. The correct simplification is found and, in Section 5, it is shown to be especially apt for getting strikingly accurate approximations to the energy levels. Finally, in Section 6, a class of exact solutions for the energy is obtained. The associated wave functions are explicitly normalized and the probability of finding the particle inside the well is calculated. Section 7 is devoted to a few remarks of a general nature.

2. Semi-infinite Square Well in Quantum Mechanics

Consider a particle of mass m subject to the potential energy defined by

$$V(x) = \begin{cases} \infty & \text{if } x < 0 \\ 0 & \text{if } 0 \leq x \leq a \\ V_0 & \text{if } x > a \end{cases} . \tag{1}$$

This potential energy is depicted in Fig. 1. The positive constants a and V_0 characterize the well's width and depth, respectively. The particle is kept away from the region $x < 0$ by an infinitely high potential barrier.

There can be definite energy bound states, described by square integrable wave functions, only if the energy E is such that $0 < E < V_0$, which is assumed from now on.

The one-dimensional time-independent Schrödinger equation reads

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V)}{\hbar^2}\psi = 0. \tag{2}$$

Since the infinite potential barrier demands $\psi(x) = 0$ for $x < 0$, the boundary conditions on the physically acceptable solutions to equation (2) are

$$\psi(0) = 0; \qquad \psi, \psi' \text{ continuous at } x = a. \tag{3}$$

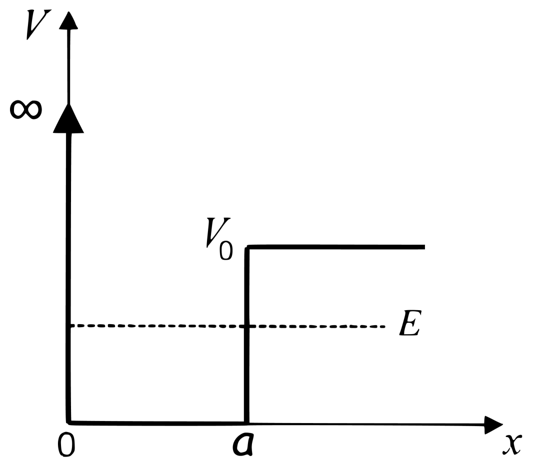

Figure 1: Semi-infinite potential energy square well. The particle is excluded from the region $x < 0$ by an impenetrable wall of infinitely high potential energy.

Because the potential energy is discontinuous at $x = a$, the time-independent Schrödinger equation must be set up separately for each of the regions $0 \leq x \leq a$ and $x > a$.

■ Inside the well ($0 \leq x \leq a$). Taking into account that $V = 0$, equation (2) becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \tag{4}$$

where

$$k = \frac{\sqrt{2mE}}{\hbar}. \tag{5}$$

The general solution to equation (4) is

$$\psi(x) = A\sin kx + C\cos kx, \tag{6}$$

where A and C are arbitrary constants. The condition $\psi(0) = 0$ yields $C = 0$. Therefore,

$$\psi(x) = A\sin kx \qquad\qquad (0 \leq x \leq a). \tag{7}$$

■ Outside the well ($x > a$). Given that $V = V_0 > E$, equation (2) takes the form

$$\frac{d^2\psi}{dx^2} - \tilde{k}^2\psi = 0 \tag{8}$$

where

$$\tilde{k} = \frac{\sqrt{2m(V_0 - E)}}{\hbar}. \tag{9}$$

The general solution to equation (8) is

$$\psi(x) = Be^{-\tilde{k}x} + De^{\tilde{k}x}, \tag{10}$$

where B and D are arbitrary constants. The positive exponential must be discarded because it grows without bound as $x \to \infty$ and would give rise to a non-normalizable wave function. Thus, one must set $D = 0$, which yields

$$\psi(x) = Be^{-\tilde{k}x} \qquad\qquad (x > a). \tag{11}$$

Continuity of ψ and ψ' at $x = a$ leads to

$$A\sin ka = Be^{-\tilde{k}a}, \tag{12}$$

$$Ak\cos ka = -B\tilde{k}e^{-\tilde{k}a}. \tag{13}$$

If $A = 0$, equation (12) implies that $B = 0$. This is unacceptable because it would give $\psi = 0$, meaning that the particle does not exist – it is nowhere to be found. Since $\sin ka$ and $\cos ka$ cannot be zero at the same time, it cannot be the case that $B = 0$ because this would imply $A = 0$. Finally, $\sin ka$ and $\cos ka$ must be both nonvanishing, otherwise one would have $B = 0$, which has just been seen to be inadmissible. Therefore, both

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sides of equations (12) and (13) are nonzero, and one can safely divide the second equation by the first to get

$$\tilde{k} = -k \cot ka. \qquad (14)$$

Since both k and $\tilde{k}$ depend on E, this transcendental equation determines the allowed energies.

It is worth noting that this is the same transcendental equation that gives the energies associated with the odd solutions to the time-independent Schrödinger equation for the finite square well when its middle point is chosen as the origin of the x-axis [2].

3. Graphical Determination of the Energy Levels

Except for certain especial values of V_0, exact solutions to the transcendental equation (14) are not known. Therefore, one must resort to numerical, graphical or approximate algebraic methods for solving it. From (5) and (9) it follows that

$$k^2 + \tilde{k}^2 = \frac{2mV_0}{\hbar^2}. \qquad (15)$$

It is useful to introduce the positive dimensionless quantities $z, \tilde{z}, z_0$ defined by

$$z = ka, \qquad \tilde{z} = \tilde{k}a, \qquad z_0 = \sqrt{\frac{2mV_0a^2}{\hbar^2}}, \qquad (16)$$

in terms of which equation (15) becomes

$$z^2 + \tilde{z}^2 = z_0^2, \qquad (17)$$

which represents a circle of radius z_0 with center at the origin of the $z\tilde{z}$-plane.

So, equation (14) can be written as

$$\sqrt{z_0^2 - z^2} = -z \cot z. \qquad (18)$$

Graphically, the allowed energies are determined from the z-values corresponding to the intersections of the first quadrant of the origin-centered circle of radius z_0 with the graph of the function $\tilde{z} = -z \cot z$ in the region $z > 0$ of the $z\tilde{z}$-plane. From equations (5) and (16), to each z_n that satisfies equation (18) there corresponds the allowed energy

$$E_n = \frac{\hbar^2 z_n^2}{2ma^2}. \qquad (19)$$

Note that $-z \cot z \leq 0$ for $z \in [0, \pi/2]$. Since necessarily $z < z_0$ and the left-hand side of (18) is positive, that equation has no solutions if

$$z_0 \leq \frac{\pi}{2}. \qquad (20)$$

According to (16), this means that there are no bound states as long as

$$V_0 a^2 \leq \frac{\pi^2\hbar^2}{8m}. \qquad (21)$$

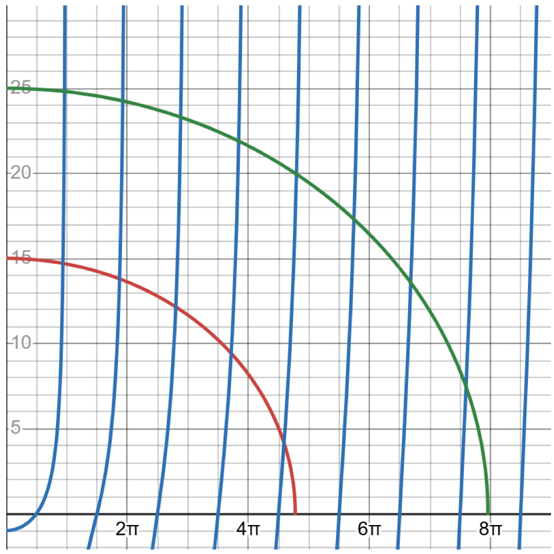

Figure 2: Graphs of the function $\tilde{z} = -z \cot z$ and of the first quadrant of the circle $z^2 + \tilde{z}^2 = z_0^2$ for $z_0 = 15$ and $z_0 = 25$. The circular arcs are slightly distorted because the horizontal and vertical scales are not quite the same. Values of z are on the horizontal axis while those of $\tilde{z}$ are on the vertical axis. The value of z for each intersection of the two graphs is a solution to equation (18). For $z_0 = 15$ there are 5 solutions, whereas for $z_0 = 25$ there are 8 solutions. The number of solutions is equal to the positive integer N that satisfies inequalities (22).

If the well is too shallow or too narrow there are no bound states. This distiguishes the semi-infinite well from the finite one, for which there is always at least one bound state.

The graphical solution[1] to equation (18) is given in Fig. 2 for $z_0 = 15$ and $z_0 = 25$. There are five solutions for $z_0 = 15$ and eight solutions for $z_0 = 25$. The function $z \mapsto \cot z$ vanishes at $z = (2n-1)\frac{\pi}{2}$ where $n = 1, 2, 3, \ldots$. Figure 2 makes it clear that there is only one intersection of the graphs between two consecutive zeroes of $\cot z$, that is, in each interval $(2n-1)\frac{\pi}{2} < z < (2n+1)\frac{\pi}{2}$. Thus, the number of bound states is given by the number that counts the last intersection, namely the positive integer N such that $(2N-1)\frac{\pi}{2} < z_0 < (2N+1)\frac{\pi}{2}$, which is equivalent to

$$2N - 1 < \frac{2z_0}{\pi} < 2N + 1. \qquad (22)$$

Except for the form, these inequalities for determination of the number of bound states appear in [19] and [20]. For $z_0 = 15$ we have $2z_0/\pi = 9.55$ with $9 < 9.55 < 11$, which gives $N = 5$; if $z_0 = 25$ we have $2z_0/\pi = 15.9$ with $15 < 15.9 < 17$, which yields $N = 8$. These results are born out by Fig. 2. Note that if $z_0 \leq \pi/2$ then $2z_0/\pi \leq 1$ and no positive integer N satisfies inequalities (22), a confirmation that in this case no bound state exists.[2]

[1] All graphical and numerical computations have been performed at https://www.desmos.com/?lang=en.

[2] If $z_0 = m\pi/2$ with $m > 1$ an odd integer, then z_0 is a zero of $\cot z$ and the last intersection occurs at $z = z_0$. This solution must

For the record, we give below the numerical values up to five decimal places of the solutions to equation (18) for the two values of z_0 considered in Fig. 2.

The five solutions $z_1, \ldots, z_5$ for $z_0 = 15$:

2.94404; 5.88035; 8.79801; 11.67442; 14.41691.

The eight solutions $z_1, \ldots, z_8$ for $z_0 = 25$:

3.02048; 6.03920; 9.05419; 12.06285; 15.06139; 18.04326; 20.99429; 23.86449.

4. Simplifying the Search for the Energy Eigenvalues

The transcendental equation for the energy levels can be simplified as follows. Upon multiplying equation (14) by the well's width a one gets

$$\tilde{z} = -z \cot z. \tag{23}$$

Combining this with equation (17) and taking into account that $1+\cot^2 z = \csc^2 z = 1/\sin^2 z$, one arrives at

$$z^2 = z_0^2 \sin^2 z. \tag{24}$$

This seems to lead to

$$z = z_0 \sin z, \tag{25}$$

which is far simpler than (18) and gives the energy eigenvalues in terms of the intersections of the straight line through the origin $\tilde{z} = z/z_0$ with the graph of the sine function $\tilde{z} = \sin z$. This is how the problem is treated in [22]. Accordingly, since $z > \sin z$ for all $z > 0$, there is no bound state if $z_0 \le 1$, which is equivalent to $V_0 a^2 \le \dfrac{\hbar^2}{2m}$. Unfortunately, this disagrees with (21) and leads to the incorrect prediction of bound states that actually do not exist.

Figure 3 shows the graphical solutions to equation (25) for $z_0 = 15$ and $z_0 = 25$. For $z_0 = 15$ there are 5 intersections, the same number shown in Fig. 2. However, the second and fourth intersections are not solutions to the transcendental equation (18) because they correspond to values of z for which $\cot z > 0$. Only the first, third and fifth intersections provide true energy levels. For $z_0 = 25$ there are 7 intersections, one less than the number of intersections in Fig. 2. The second, fourth and sixth intersections are spurious solutions to the transcendental equation (18) because they correspond to values of z such that $\cot z > 0$. Only the first, third, fifth and seventh intersections provide true energy levels. It is clear, therefore, that (25) is not the correct equation for the determination of the energy levels, and also it does not give rise to the correct condition (21) for the nonexistence of bound states.

be discarded because $z = z_0$ implies $\tilde{z} = 0$, which is unacceptable. In this case, the number N of bound states is still given by (22) as long as $2z_0/\pi$ is replaced with the even number $m - 1$.

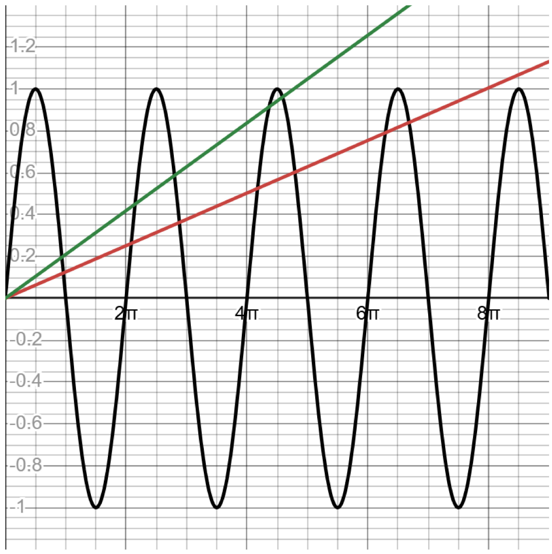

Figure 3: Graphical solutions of equation (25) for $z_0 = 15$ (steeper straight line) and $z_0 = 25$ (less slanted straight line).

4.1. Another simplification attempt

Since $z > 0$, perhaps the correct consequence to be derived from (24) is

$$z = z_0 |\sin z|. \tag{26}$$

According to Fig. 4, now there are nine intersections for $z_0 = 15$, four of which are spurious (the even-numbered ones). Similarly, there are fifteen intersections for $z_0 = 25$, seven of which are spurious (the even-numbered ones). The extraneous solutions are those such that $\cot z > 0$. Equation (26) gives the correct solutions and the correct number of solutions if it is supplemented with the condition $\cot z < 0$, entailing that z must lie in

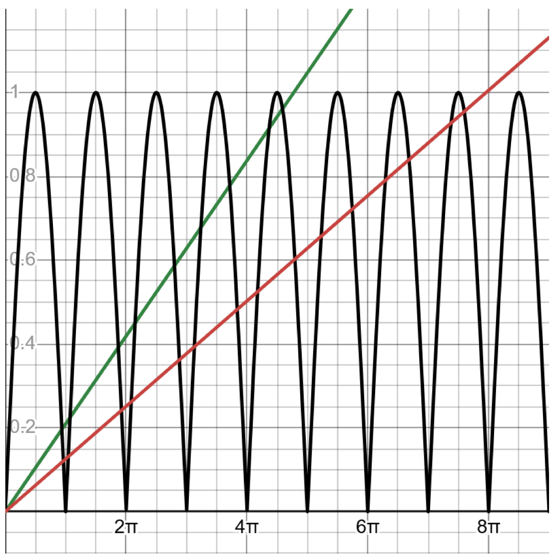

Figure 4: Solutions of equation (26) for $z_0 = 15$ and $z_0 = 25$. The steeper straight line corresponds to $z_0 = 15$.

the second or fourth quadrants. Nevertheless, it is not convenient for a graphical solution because it does not provide a bijective correspondence between intersections and energy levels.

4.2. Yet another simplification attempt

Maybe the right thing to do is to take the negative square root of equation (24) to obtain

$$z = -z_0 \sin z. \tag{27}$$

As shown in Fig. 5, there are only four intersections for $z_0 = 15$, two of which are spurious (the first and the third). Similarly, there are eight intersections for $z_0 = 25$, half of which are spurious (the odd-numbered ones). Once again, the extraneous solutions are those such that $\cot z > 0$. Equation (27) is incorrect because it does not give the right number of solutions, and even if supplemented with the condition $\cot z < 0$ it misses half of the solutions.

4.3. The correct simplification

Inserting (24) into (18) and taking into account that $\sqrt{x^2} = |x|$ one arrives at

$$z_0 |\cos z| = -z \cot z, \tag{28}$$

which is equivalent to

$$z = -z_0 \frac{\sin z \cos z}{|\cos z|}. \tag{29}$$

First of all, note that this equation does not admit solutions if $z_0 < \pi/2$ because both $\sin z > 0$ and $\cos z > 0$ for $0 < z < \pi/2$. Thus, it gives rise to the correct condition (21) that prevents the existence of

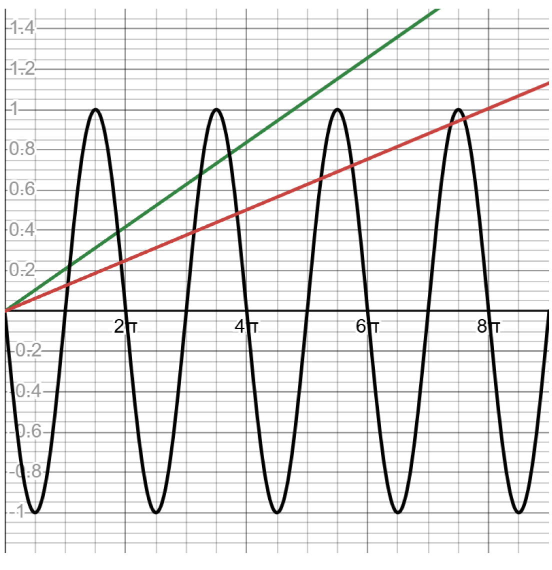

Figure 5: Solutions of equation (27) for $z_0 = 15$ and $z_0 = 25$. The steeper straight line corresponds to $z_0 = 15$.

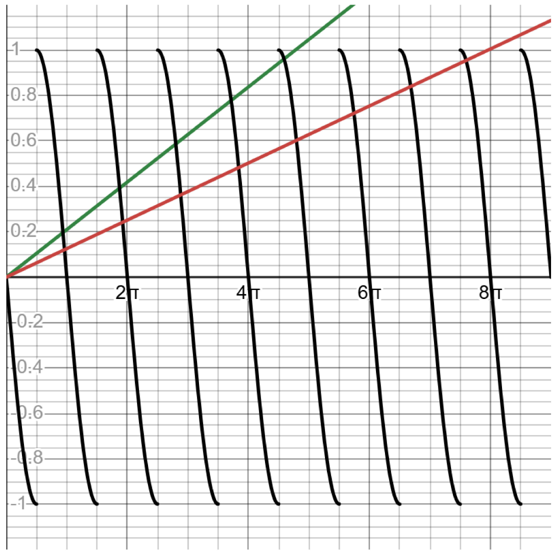

Figure 6: Graphical solutions of equation (29) for $z_0 = 15$ (steeper straight line) and $z_0 = 25$ (less slanted straight line).

bound states. Furthermore, this equation has solutions only if $\cos z$ and $\sin z$ have opposite signs, implying that $\cot z < 0$ as required by equation (18).

Figure 6 shows the graphical solutions to equation (29) for $z_0 = 15$ and $z_0 = 25$. The number of intersections and the corresponding values of z are the same as those displayed in Fig. 2. The discontinuities of the right-hand side of equation (29) at $z = m\pi/2$, m odd, naturally rule out the intersections at such z-values as valid solutions. As it turns out, however, the "simplified" form (29) of the transcendental equation (18) is not so much simpler after all. For the purpose of achieving graphical solutions, it may be preferable to stick to equation (18). Nevertheless, equation (29) turns out to be very expedient for finding extremely accurate approximations to the energy levels, as will be shown in the next section.

If z_0 is very large, the straight line $\tilde{z} = z/z_0$ is nearly coincident with the z-axis and Fig. 6 shows that the intersections occur almost exactly at $z_n = n\pi$, where n is a positive integer. Thus, as expected, in the limit $V_0 \to \infty$, which implies $z_0 \to \infty$ by (16), the system reduces to the particle in a box, which according to equation (19) has the well-known energy levels $E_n = \dfrac{n^2\pi^2\hbar^2}{2ma^2}$.

5. Approximate Energy Spectrum

Newton's method is a powerful iterative scheme for finding zeroes of functions. The strength of the method lies in its extraordinarily rapid rate of convergence [23, 24]. Suppose one is searching for a solution to $f(z) = 0$ in a certain interval (a, b). After guessing an initial approximate solution $z^{(0)} \in (a, b)$, under propitious conditions Newton's method engenders a convergent sequence $z^{(1)}, z^{(2)}, \dots$ of ever better approximations to the true solution which are iteratively given by

$$z^{(n+1)} = z^{(n)} - \frac{f(z^{(n)})}{f'(z^{(n)})}. \tag{30}$$

Owing to (29), the relevant function whose zeroes are to be found is

$$f(z) = z + z_0 \frac{\sin z \cos z}{|\cos z|}. \tag{31}$$

As we already know, the successive zeroes of this function belong to the intervals

$$(2m-1)\frac{\pi}{2} < z < m\pi, \qquad m = 1, 2, 3, \dots \tag{32}$$

with z in the second quadrant (for m odd) or in the fourth quadrant (for m even). Because $\cos z < 0$ if m is odd whereas $\cos z > 0$ if m is even, the appropriate function for the m-th interval is

$$f(z) = z + (-1)^m z_0 \sin z. \tag{33}$$

Therefore, the iterative procedure (30) takes the form

$$z^{(n+1)} = z^{(n)} - \frac{z^{(n)} + (-1)^m z_0 \sin z^{(n)}}{1 + (-1)^m z_0 \cos z^{(n)}}. \tag{34}$$

Note that $f'(z) = 1 + (-1)^m z_0 \cos z > 0$ and $f''(z) = -(-1)^m z_0 \sin z > 0$ regardless of whether m is odd or even. These are favorable conditions for the success of Newton's method [23, 24]. For each m, a reasonable initial guess is the midpoint of the corresponding interval, namely

$$z^{(0)} = (2m-1)\frac{\pi}{2} + \frac{\pi}{4} = (4m-1)\frac{\pi}{4}. \tag{35}$$

Example 1. Ground state in the case $z_0 = 15$. We have $m = 1$, $z^{(0)} = 3\pi/4 \approx 2.35619449$ and the iterative scheme

$$z^{(n+1)} = z^{(n)} - \frac{z^{(n)} - 15 \sin z^{(n)}}{1 - 15 \cos z^{(n)}}. \tag{36}$$

The first three iterations give

$$z^{(1)} \approx 3.0670319; \qquad z^{(2)} \approx 2.9448601; \qquad z^{(3)} \approx 2.9440409. \tag{37}$$

According to the results in Section 3, the second iterate is correct to three decimals and the third iterate is correct to six decimals.

Example 2. Third excited state (fourth energy level) in the case $z_0 = 25$. We have $m = 4$, $z^{(0)} = 15\pi/4 \approx 11.78097245$ and the iterative scheme

$$z^{(n+1)} = z^{(n)} - \frac{z^{(n)} + 25 \sin z^{(n)}}{1 + 25 \cos z^{(n)}}. \tag{38}$$

The first three iterations give

$$z^{(1)} \approx 12.0966808; \qquad z^{(2)} \approx 12.0631322; \qquad z^{(3)} \approx 12.0628480. \tag{39}$$

Upon rounding the numbers, the results in Section 3 show that the second iterate is correct to three decimals and the third iterate is correct to six decimals.

The convergence is very fast in both examples. The number of correct decimals is typically doubled at each iteration [23, 24]. The method is highly efficient for finding the energy not only of the ground state but also of the excited states.

6. A class of exact solutions

For certain values of V_0 there are exact solutions to (18) or (29) from which one can find the associated wave function.

By way of example, suppose

$$z = 2n\pi + \frac{3\pi}{4} = (8n+3)\frac{\pi}{4}, \qquad n = 0, 1, 2, \dots \tag{40}$$

are solutions to (29). Then, since $\cos z < 0$ and $\sin z = \sqrt{2}/2$,

$$z_0 = \sqrt{2}(8n+3)\frac{\pi}{4} \tag{41}$$

and also

$$\tilde{z} = \sqrt{z_0^2 - z^2} = (8n+3)\frac{\pi}{4} = z. \tag{42}$$

As a consequence, from (16),

$$V_0 = \frac{(8n+3)^2 \pi^2 \hbar^2}{16 m a^2} \tag{43}$$

whereas, from (19),

$$E = \frac{(8n+3)^2 \pi^2 \hbar^2}{32 m a^2} = \frac{V_0}{2}. \tag{44}$$

In order to avoid misunderstandings, let us emphasize that these energies *are not* energy levels associated with a *single* well depth V_0. For each n, equation (44) furnishes a *single* allowed energy for the *especific* V_0 given by equation (43).

And now for the wave function associated with the above energy. From equation (12) it follows that

$$B = e^{\tilde{k}a} A \sin z = e^{ka} \frac{A}{\sqrt{2}}, \tag{45}$$

where we have used $\tilde{k} = k$. Therefore, the wave function is

$$\psi(x) = A \begin{cases} \sin kx & \text{if } 0 \le x \le a \\ \dfrac{e^{-k(x-a)}}{\sqrt{2}} & \text{if } x > a \end{cases} \tag{46}$$

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where the normalization constant A can be taken as real and positive − of course the negative portion of the x-axis has been disregarded because $\psi = 0$ there. Normalization requires

$$A^{-2} = \int_0^a \sin^2 kx \, dx + \frac{1}{2}\int_a^\infty e^{-2k(x-a)}\, dx \equiv I_1 + I_2. \tag{47}$$

Taking into account that $k = z/a$, the first of the above integrals is easily computed as

$$\begin{aligned} I_1 &= \int_0^a \sin^2 \frac{zx}{a}\, dx \\ &= \frac{a}{z}\int_0^z \sin^2 u\, du = \frac{a}{z}\frac{2z - \sin 2z}{4} = \frac{a}{z}\frac{2z+1}{4}, \end{aligned} \tag{48}$$

where we have used

$$\sin 2z = \sin\left(4n\pi + \frac{3\pi}{2}\right) = \sin\frac{3\pi}{2} = -1. \tag{49}$$

As to the second integral in equation (47), we have

$$\begin{aligned} I_2 &= \frac{1}{2}\int_a^\infty e^{-2k(x-a)}\, dx \\ &= \frac{1}{2}\int_0^\infty e^{-2kx}\, dx = \frac{1}{2}\frac{1}{2k} = \frac{a}{4z}. \end{aligned} \tag{50}$$

Consequently, equation (47) yields

$$A^{-2} = I_1 + I_2 = \frac{a}{2}\frac{z+1}{z} \implies A = \sqrt{\frac{(8n+3)\pi}{(8n+3)\pi+4}\frac{2}{a}}, \tag{51}$$

where (40) has been used.

The probability of finding the particle inside the well is

$$\begin{aligned} P_n &= \int_0^a |\psi(x)|^2\, dx = A^2 \int_0^a \sin^2 kx\, dx \\ &= A^2 I_1 = \frac{2}{a}\frac{z}{z+1}\frac{a}{z}\frac{2z+1}{4} = \frac{4z+2}{4z+4}, \end{aligned} \tag{52}$$

where equations (48) and (51) have been used. With the help of equation (40) one finally gets

$$P_n = \frac{(8n+3)\pi + 2}{(8n+3)\pi + 4}. \tag{53}$$

Here are a few values of this probability:

$$\begin{gathered} P_0 \approx 0.851 = 85.1\%; \qquad P_{10} \approx 0.992 = 99.2\%; \\ P_{100} \approx 0.999 = 99.9\%. \end{gathered} \tag{54}$$

Although the value of the energy is always half the well depth, the probability of finding the particle within the well grows steadily as n increases. This probability is one in the limit $n \to \infty$, which is expected because by equation (43) this is exactly the limit of an infinitely deep well (particle in a box). One might think that the probability of finding the particle inside the well should be independent of n because it should depend only on the ratio E/V_0, which is $1/2$ for all n. This seems to be supported by the fact that the reflection and transmission coefficients for a step potential of height V_0 depend only on the ratio E/V_0 if the energy is larger than V_0 [25]. But the step potential problem contains no length scale and the reflection and transmission coefficients cannot depend even on the Planck constant because they are dimensionless magnitudes that can depend only on E/V_0, which is the sole dimensionless quantity that can be constructed. Dissimilarly, the probability of tunneling across a barrier of width a depends not only on the ratio E/V_0 but also on V_0, a, $\hbar$ and the particle's mass [25]. This is because V_0, a, $\hbar$ and m can be combined into the dimensionless quantity $mV_0a^2/\hbar^2$, and now there are two independent dimensionless quantities. The same behavior is expected in the present situation involving a potential well whose width a introduces a length scale in the problem. Indeed, if $V_0 \to \infty$ then, in virtue of equation (9), it is also the case that $\tilde{k} \to \infty$ even if E is arbitrarily close to V_0 while remaining less than V_0. As a consequence, equation (11) implies that the wave function vanishes outside the wall in this limit.

7. Conclusion

The semi-infinite potential well is an interesting theoretical model with practical applications to realistic physical systems. The allowed energies are determined by a transcendental equation, which has been graphically solved. Inequalities have been provided by means of which one easily finds the number of bound states in terms of the well's depth. The aforesaid transcendental equation can be simplified with the use of simple trigonometric identities. But we have shown that this must be done carefully lest false solutions be created and true solutions be missed. The simplified transcendental equation turns out to be particularly suited for obtaining remarkably accurate approximations to the energy levels. We have also exhibited a class of exact solutions for the energy whose associated wave functions have been exactly normalized. For these stationary states the exact probability of finding the particle inside the well has been calculated. All things considered, this is a nice problem for a modern physics or introductory quantum mechanics course.

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