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Exact and approximate energy spectrum for the finite square well and related potentials

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We investigate the problem of a quantum particle in a one-dimensional finite square well. In the standard approach the allowed energies are determined implicitly as the solutions to a transcendental equation. We obtain the spectrum analytically as the solution to a pair of parametric equations and algebraically using a remarkably accurate approximation to the cosine function. The approach is also applied to a variety of other quantum wells. © *2006 American Association of Physics Teachers.*
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I. INTRODUCTION

The mathematics of quantum mechanics is usually introduced through physical systems described by one-dimensional potential wells.[1,2] These examples are used to show the emergence of quantized states as solutions of the Schrödinger equation subject to appropriate boundary conditions. Unfortunately, there are not many potentials for which the bound state energies can be expressed in closed form. The classic example is the infinite square well, but it is obviously artificial. In the more realistic case where the potential well is finite, the allowed energies as functions of the barrier height can be found by numerically solving a transcendental equation,[3] by graphical methods,[4–7] or by various approximation techniques.[8–12]

The finite quantum well is of great practical importance because it forms the basis for understanding low-dimensional structures such as quantum well devices.[13] Therefore, it is useful to explore other ways of representing the spectrum of allowed energies. In this paper we develop a method that allows us to obtain a closed-form solution for the exact energy spectrum for the finite quantum well by expressing a given bound state energy together with the barrier height in parametric form. The method leads to a simple but accurate approximation scheme involving the solution to a quadratic equation that leads to a closed-form algebraic expression for the nth allowed energy as a function of the well depth. (The accuracy can be improved by allowing cubic equations with results that are essentially indistinguishable from the exact values, but we will restrict our attention to quadratic approximations.) We also apply the method to the semi-infinite square well, the delta-function in an infinite square well,[14] and the double delta-function well.[15]

II. THE FINITE SQUARE WELL—EIGENVALUE EQUATIONS

We begin with the one-dimensional infinite square well

$$V_\infty(x) = \begin{cases} 0 & (-a \leq x \leq a), \\ \infty & (\text{otherwise}). \end{cases} \tag{1}$$

The (normalized) solutions to the (time-independent) Schrödinger equation are

$$\psi_n(x) = \begin{cases} \sqrt{1/a}\,\cos(k_n x) & (n = 1,3,5,\dots), \\ \sqrt{1/a}\,\sin(k_n x) & (n = 2,4,6,\dots), \end{cases} \tag{2}$$

where $k_n \equiv \sqrt{2mE_n}/\hbar$ is determined by the boundary conditions ($\psi = 0$ at $x = \pm a$). Specifically, $k_n = n\pi/2a$ and the allowed energies are

$$E_n = \frac{n^2 \pi^2 \hbar^2}{8ma^2} \quad (n = 1,2,3,\dots). \tag{3}$$

The finite square well

$$V(x) = \begin{cases} 0 & (-a \leq x \leq a), \\ V_0 & (\text{otherwise}), \end{cases} \tag{4}$$

is much more complicated.[16] The bound states are alternately even functions[17]

$$\psi_n(x) = \begin{cases} A_n e^{\kappa_n x} & (x \leq -a), \\ B_n \cos(k_n x) & (|x| \leq a)\ (n = 1,3,5,\dots), \\ A_n e^{-\kappa_n x} & (x \geq a), \end{cases} \tag{5}$$

and odd functions

$$\psi_n(x) = \begin{cases} -A_n e^{\kappa_n x} & (x \leq -a), \\ B_n \sin(k_n x) & (|x| \leq a)\ (n = 2,4,6,\dots), \\ A_n e^{-\kappa_n x} & (x \geq a), \end{cases} \tag{6}$$

where $\kappa_n \equiv \sqrt{2m(V_0 - E_n)}/\hbar$. The continuity of ψ at $\pm a$ forces

$$A_n = \begin{cases} e^{\kappa_n a} \cos(k_n a) B_n & (n = 1,3,5,\dots), \\ e^{\kappa_n a} \sin(k_n a) B_n & (n = 2,4,6,\dots). \end{cases} \tag{7}$$

(The remaining constant B_n is determined by normalization.) The continuity of ψ' at $\pm a$ imposes the constraints

$$\kappa_n = \begin{cases} k_n \tan(k_n a) & (n = 1,3,5,\dots), \\ -k_n \cot(k_n a) & (n = 2,4,6,\dots), \end{cases} \tag{8}$$

which, in turn, determine the allowed energies.

Equation (8) can be solved graphically. Let

$$z \equiv k_n a = \frac{a}{\hbar}\sqrt{2mE_n}, \quad z_0 \equiv \frac{a}{\hbar}\sqrt{2mV_0}, \tag{9}$$

where z is a dimensionless measure of the energy and z_0 is a dimensionless measure of the size of the well. In this notation Eq. (8) becomes
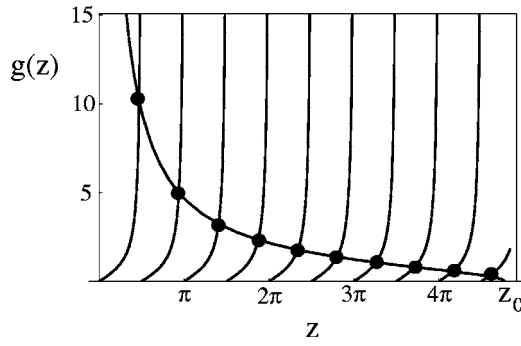
Fig. 1. Graphical solution of Eq. (10) for $z_0=15$. Here $g(z) = \{\sqrt{(z_0/z)^2-1}, \tan z, -\cot z\}$, and intersections (marked with bullets) indicate solutions.

$$\sqrt{(z_0/z)^2 - 1} = \begin{cases} \tan(z) & (n=1,3,5,\dots), \\ -\cot(z) & (n=2,4,6,\dots). \end{cases} \quad (10)$$

In Fig. 1 we plot both sides of Eq. (10) on the same graph for the case $z_0=15$; the points of intersection represent solutions (see Table I). Notice that the left side of Eq. (10) is zero at $z=z_0$. As the well becomes broader/deeper, more and more solutions occur, and the intersections approach $z=n\pi/2$, that is, $E_n \to n^2\pi^2\hbar^2/8ma^2$, reproducing the infinite square well result [Eq. (3)]. As the well becomes narrower/shallower, there are fewer and fewer solutions, and when $z_0 < \pi/2$, only a single bound state ($n=1$) survives.

It would be helpful if we could obtain an exact closed-form expression for the allowed energies, as functions of the well depth, but such an expression is out of the question. What about approximate formulas? In 1979 Garrett[8,18] proposed a method that amounts to treating the finite square well as an infinite well whose half-width a is augmented by the penetration depth of the exponential tail of the wave function, $1/\kappa_n$. Although the idea seems reasonable, the actual results are not very good. It gives very poor estimates for the energies and predicts the existence of unphysical bound states above the barrier. Our purpose is to present a parametric expression for the energy spectrum and a simple and surprisingly accurate formula for the bound state energies of the finite square well as functions of the well depth. We will also discuss similar approaches to some related potentials.

Table I. Numerical solution to Eq. (9) for $z_0=15$.

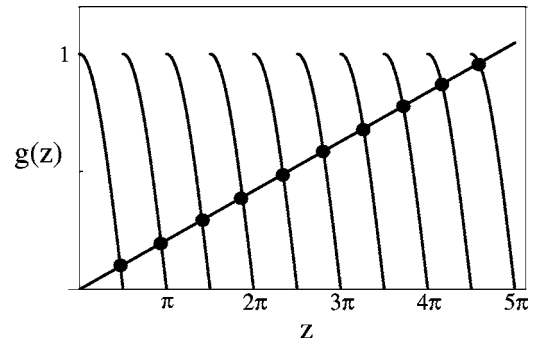| n	z	E_n/V_0
1	1.472 473	0.009 636
2	2.944 041	0.038 522
3	4.413 720	0.086 582
4	5.880 355	0.153 683
5	7.342 468	0.239 608
6	8.798 006	0.344 022
7	10.243 82	0.466 382
8	11.674 42	0.605 743
9	13.078 15	0.760 168
10	14.416 91	0.923 765

Fig. 2. Graphical solution of Eq. (12) for $z_0=15$. The slope of the straight line is $1/z_0$, and $g(z)$ is now the right side of Eq. (12).

III. EXACT AND APPROXIMATE ENERGIES OF THE FINITE SQUARE WELL

We rewrite Eq. (10) as

$$(z_0/z)^2 - 1 = \begin{cases} \tan^2(z) & (n=1,3,5,\dots), \\ \cot^2(z) & (n=2,4,6,\dots), \end{cases} \quad (11)$$

or

$$\frac{z}{z_0} = \begin{cases} |\cos z| & (n=1,3,5,\dots), \\ |\sin z| & (n=2,4,6,\dots), \end{cases} \quad (12)$$

where $n\pi/2-\pi/2 \leq z \leq n\pi/2$ (see Fig. 2). The eigenvalue equations in this form and their graphical representation have been the focus of previous work.[3,5,6] Equation (12) is equivalent to Eq. (10), but Eq. (12) is in a more convenient form. In particular, the ground state ($n=1$) is determined by the root of

$$z = z_0 \cos z \quad (13)$$

in the range $0 \leq z \leq \pi/2$ (the first intersection in Fig. 2).

We propose to solve Eq. (13) by approximating the cosine:

$$\cos x \approx f_s(x) \equiv \frac{1-(2x/\pi)^2}{(1+cx^2)^s} \quad (0 \leq x \leq \pi/2). \quad (14)$$

The numerator guarantees that $f_s(x)$ goes to zero at $x=\pi/2$. We shall use three values for the power in the denominator: $s=0$ (the parabolic approximation), $s=\frac{1}{2}$, and $s=1$. In the last two cases the parameter c in the denominator can be chosen so as to match the first two terms in the Taylor expansion of $\cos x$ at the origin,

$$c_1 = \begin{cases} 1-8/\pi^2 & (s=\frac{1}{2}), \\ \frac{1}{2}(1-8/\pi^2) & (s=1), \end{cases} \quad (15)$$

or by a least-squares fit

$$c_2 = \begin{cases} 0.212\,012\,6 & (s=\frac{1}{2}), \\ 0.101\,016\,4 & (s=1). \end{cases} \quad (16)$$

Either way, the approximation is excellent: for $s=\frac{1}{2}$ the maximum discrepancy is 0.68% using c_1 and 0.30% using c_2; for $s=1$ the maximum discrepancies are 0.41% and 0.17%, respectively. See Fig. 3 for a pictorial representation of these approximations. But the point of representing $\cos z$ in this way is that for $s=\frac{1}{2}$ Eq. (13) reduces to a quadratic for z^2, with the solution
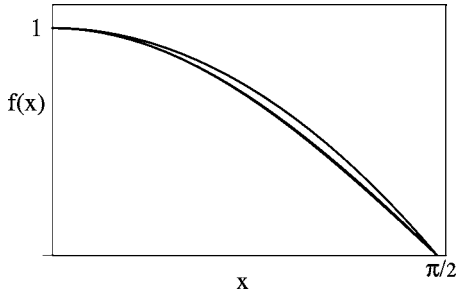
Fig. 3. Plot of $\cos(x)$ versus x (lower curve), together with the approximations f_s as defined by Eq. (14) using the parameters c_1 from Eq. (15). The upper curve is the parabolic approximation, f_0; the others are indistinguishable from $\cos(x)$, on this scale.

$$z^2 = \frac{1 + 8z_0^2/\pi^2 - \sqrt{1 + 4z_0^2[c + (2/\pi)^2]}}{2(16z_0^2/\pi^4 - c)}. \tag{17}$$

For example, if $z_0 = 15$, we obtain $z = 1.4761$ using c_1 and 1.4745 using c_2; the correct answer from Table I is 1.4725—errors of 0.24% and 0.14%, respectively.[19] In Fig. 4 we plot the ground state energy E_1 [which, apart from the scale factor in Eq. (9), is z^2] as a function of the well depth V_0 (which, with the same scale factor, is z_0^2). To the eye, the curves are indistinguishable.

The excited states can be obtained in much the same way if we first shift the intersection points in Fig. 2 to the left as illustrated for $n=2$ in Fig. 5:[20]

$$z_n = x_n + (n-1)\frac{\pi}{2} \quad (0 \le x_n \le \pi/2). \tag{18}$$

Now

$$y_n = \cos x_n = z_n \tan \theta_1 = z_n/z_0, \tag{19}$$

so

$$z_0 = \frac{x_n + (n-1)\pi/2}{\cos x_n}. \tag{20}$$

Equation (20) determines x_n (implicitly) as a function of z_0, and Eq. (18) then yields the nth allowed energy. If we treat x_n as a parameter, we can construct the graph of z_n [Eq. (18)] as a function of z_0 [Eq. (20)]. When x_n ranges from 0 to $\pi/2$, z_n goes from $(n-1)\pi/2$ to $n\pi/2$, and z_0 from $(n-1)\pi/2$ to infinity. If we express all energies in the terms of $\hbar^2/2ma^2$, then $z_n = \sqrt{E_n}$ and $z_0 = \sqrt{V_0}$. In this notation Eqs. (18) and (20) may be written in a more transparent way:
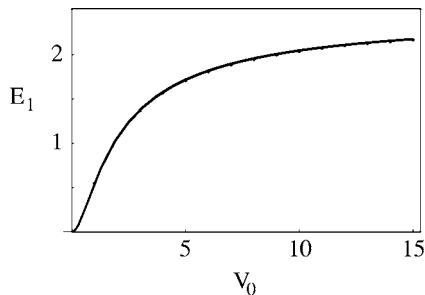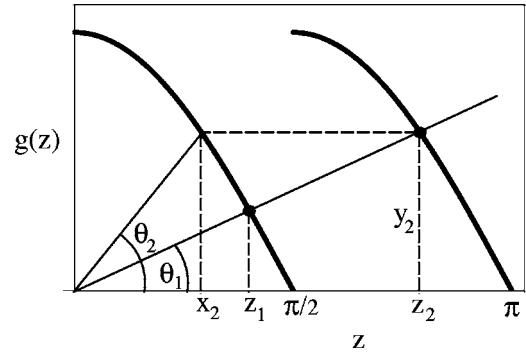

Fig. 5. Projecting the intersection points: z_n is the nth intersection (in Fig. 2), x_n is the corresponding point in the interval $[0, \pi/2]$.

$$\sqrt{E_n} = t + (n-1)\frac{\pi}{2}, \tag{21}$$

$$\sqrt{V_0} = \frac{t + (n-1)\pi/2}{\cos t}, \tag{22}$$

where t ranges from 0 to $\pi/2$. In Fig. 6 we plot $z_n = \sqrt{E_n}$ versus $1/z_0 = 1/\sqrt{V_0}$. Moving to the left means increasing the well depth, so more and more bound states appear; the nth state comes on line as $z_0 = \sqrt{V_0}$ hits $(n-1)\pi/2$.

To obtain a closed-form expression for the excited energies (as a function of the barrier height) we use the parabolic approximation[21]

$$\cos x \approx f_0(x) = 1 - (2x/\pi)^2, \tag{23}$$

which yields[22]

$$z_n \approx \frac{\pi}{8z_0}[4(n-1)z_0 - \pi + \sqrt{(4z_0 + \pi)^2 - 8\pi n z_0}]. \tag{24}$$

The graph of Eq. (22) is virtually indistinguishable from Fig. 6.

IV. RELATED POTENTIALS

We next apply the same strategy to three related potentials: the semi-infinite square well, the delta-function in an infinite square well,[14] and the double delta-function well.[15]

Fig. 4. Scaled ground state energy ($z^2 = 2ma^2E_n/\hbar^2$) as a function of scaled well depth (z_0^2). The exact solution (dots) and the two approximations, Eq. (17) with c_1 and c_2, are practically indistinguishable.
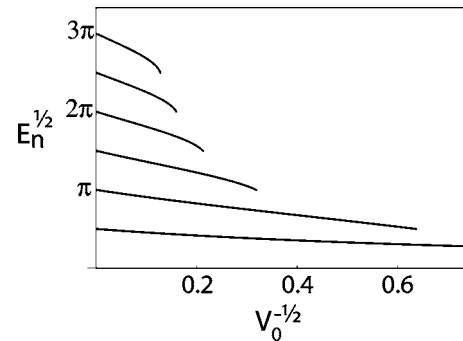

Fig. 6. Plot of z_n (scaled $\sqrt{E_n}$) vs. $1/z_0$ (scaled $1/\sqrt{V_0}$) for $n=1$, 2, 3, 4, 5, and 6. This plot shows the exact spectrum, obtained using Eqs. (21) and (22).
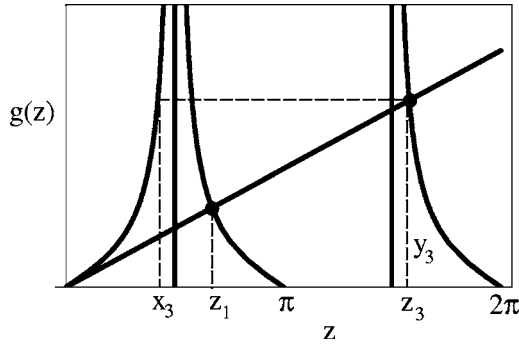
Fig. 7. Graphical solution of Eq. (30): We plot $g(z)=\{z/z_0, -\tan z\}$, and look for points of intersection. Also included is $\tan z$ on the interval $0 \leqslant z < \pi/2$ and the projection of y_3 onto it at x_3.

A. Semi-infinite square well

The potential

$$V(x) = \begin{cases} \infty & (x < 0), \\ 0 & (0 \leqslant x \leqslant a), \\ V_0 & (x \geqslant a), \end{cases} \qquad (25)$$

admits as bound states all the odd solutions to the finite square well in Eq. (6), because these are the solutions that go to zero at the origin. There is nothing new to be said about this case; we simply select the $n = 2, 4, 6, \ldots$ results from Sec. III.

B. Delta function in an infinite square well

Imagine introducing a delta-function barrier at the center of the infinite square well:

$$V(x) = \begin{cases} \alpha \delta(x) & (|x| < a), \\ \infty & (\text{otherwise}). \end{cases} \qquad (26)$$

The odd solutions [Eq. (2)] are not affected, because the wave function vanishes at the location of the spike:

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin(k_n x) \quad (n = 2, 4, 6, \ldots). \qquad (27)$$

The even solutions ($n = 1, 3, 5, \ldots$) can be written in the form

$$\psi_n(x) = \begin{cases} A \sin[k_n(a+x)] & (-a \leqslant x < 0), \\ A \sin[k_n(a-x)] & (0 < x \leqslant a). \end{cases} \qquad (28)$$

To express the wave function this way we have invoked continuity at $x = \pm a$ and 0; the delta function puts a kink in ψ at the origin[23]

$$-\frac{\hbar^2}{2m} \Delta \psi'(0) + \alpha \psi(0) = 0, \qquad (29)$$

or

$$\tan z = -z/z_0, \qquad (30)$$

where $z \equiv k_n a$ is a dimensionless measure of the energy, and $z_0 \equiv m a \alpha / \hbar^2$ is a measure of the strength of the delta function. In Fig. 7 we plot $-\tan z$ and z/z_0 and look for points of intersection.

For large n (small z_0) the solutions are just above $z = n\pi/2$, so $E_n = n^2 \pi^2 \hbar^2 / 8ma^2 (n = 1, 3, 5, \ldots)$, filling in the remainder of the infinite square well energies. For very large
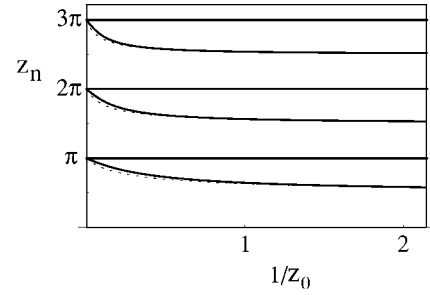

Fig. 8. The allowed energies for the delta-function barrier in an infinite square well; z_n in Eq. (31) is plotted against $1/z_0$ in Eq. (33) for $n = 1, 3$, and 5. The horizontal lines are the odd solutions for $n = 2, 4$, and 6. The dots represent the approximation, Eq. (35).

z_0, the solutions are just below $n\pi$, doubling the odd solutions; in this limit the barrier is impenetrable, the well separates into two (with half the width), and the energies are all doubly degenerate, because the particle could be in the left or the right half.

What we really want is E_n as a function of α, that is, z_n as a function of z_0. As before, we project z_n down to the first cell ($0 \leqslant x < \pi/2$):

$$z_n = (n+1)\frac{\pi}{2} - x_n. \qquad (31)$$

Now,

$$y_n = \tan x_n = z_n/z_0, \qquad (32)$$

so

$$z_0 = \frac{(n+1)\pi/2 - x_n}{\tan x_n}. \qquad (33)$$

We treat x_n as a parameter (which runs from 0 to $\pi/2$) and plot z_n [Eq. (31)] versus z_0^{-1} [Eq. (33)] in Fig. 8; for completeness, we also plot the odd solutions (which are constants).

We would prefer to have a closed-form expression for z_n (as a function of z_0), rather than an implicit formula, Eq. (30), or a parametric relation, Eqs. (31) and (33). Such a relation is not possible, but a fairly good approximation is afforded by the same procedure as before:[24]

$$\tan x \approx \frac{cx}{1 - (2x/\pi)}. \qquad (34)$$

A nonlinear curve fit gives $c = 0.450$. Using this value we find

$$z_n \approx \frac{\pi}{4}[n - cz_0 + \sqrt{(n + cz_0)^2 + 4cz_0}]. \qquad (35)$$

In Fig. 8 this approximation for $n = 1, 3$, and 5 is superimposed on the exact results.

C. Double delta-function potential

The double delta-function well,

$$V(x) = -\alpha[\delta(x+a) + \delta(x-a)], \qquad (36)$$

is sometimes used as a toy model for a diatomic ion such as H_2^+.[15] It has at least one bound (negative energy) state and at
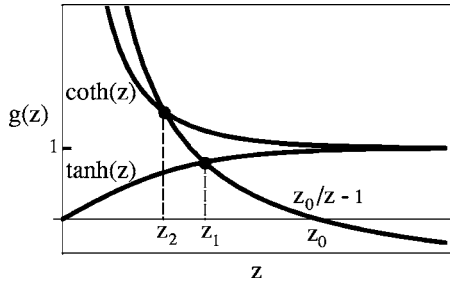
Fig. 9. Graphical solution of Eqs. (39) (z_1) and Eq. (42) (z_2). Here $g(z) = \{z_0/z - 1, \tanh z, \coth z\}$.

Fig. 10. Allowed energies (z_1, upper, and z_2, lower) for the double delta-function well, as functions of the strength of the well (z_0). The dots are the approximations Eqs. (46) and (50).

most two. The former is an even function; the latter (if it exists) is odd.

The even eigenfunction has the form

$$
\psi_1(x) = \begin{cases} Ae^{\kappa x} & (x \leqslant -a), \\ B\cosh(\kappa x) & (-a \leqslant x \leqslant a), \\ Ae^{-\kappa x} & (x \geqslant a), \end{cases} \tag{37}
$$

where $\kappa \equiv \sqrt{-2mE}/\hbar$. Continuity at $x = \pm a$ leads to $A = Be^{\kappa a}\cosh(\kappa a)$; the discontinuity in the derivative Eq. (29) yields

$$
\frac{\hbar^2 \kappa}{2m}[Ae^{-\kappa a} + B\sinh(\kappa a)] - \alpha Ae^{-\kappa a} = 0. \tag{38}
$$

We then obtain

$$
z(1 + \tanh z) = z_0, \tag{39}
$$

where $z \equiv \kappa a$ and $z_0 \equiv 2ma\alpha/\hbar^2$.

The odd eigenfunction has the form

$$
\psi_2(x) = \begin{cases} -Ae^{\kappa x} & (x \leqslant -a), \\ B\sinh(\kappa x) & (-a \leqslant x \leqslant a), \\ Ae^{-\kappa x} & (x \geqslant a). \end{cases} \tag{40}
$$

Continuity at $x = \pm a$ forces $A = Be^{\kappa a}\sinh(\kappa a)$; the discontinuity in the derivative yields

$$
\frac{\hbar^2 \kappa}{2m}[Ae^{-\kappa a} + B\cosh(\kappa a)] - \alpha Ae^{-\kappa a} = 0, \tag{41}
$$

and for this case we obtain

$$
z(1 + \coth z) = z_0. \tag{42}
$$

In Fig. 9 we plot $\tanh z$ and $z_0/z - 1$. There is exactly one intersection and hence just one even bound state. We also plot $\coth z$; depending on the value of z_0, there may or may not be an intersection.

To construct the graphs of z_1 and z_2 as functions of z_0, we treat z as a parameter, calculate z_0 using Eqs. (39) and (42), and plot the former as ordinate and the latter as abscissa (see Fig. 10).

The first excited state appears when $z_0 \geqslant 1$. For z_0 greater than about 5, $z_1 \approx z_2 \approx z_0/2$; in this regime the two wells are effectively separated, and the particle can either be in one or in the other, so the energy is doubly degenerate.

We would like closed-form expressions for $z_1(z_0)$ and $z_2(z_0)$. Note that
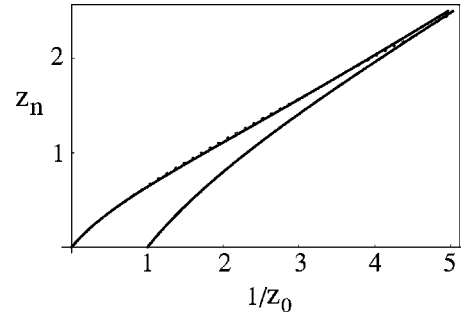
$$
1 + \coth z = 1 + \frac{e^z + e^{-z}}{e^z - e^{-z}} = \frac{2}{1 - e^{-2z}}, \tag{43}
$$

and thus Eq. (42) can be written in the form

$$
\frac{z}{z_0} = \frac{1}{2}(1 - e^{-2z}). \tag{44}
$$

Suppose we approximate the right-hand side of Eq. (44) as

$$
\frac{1}{2}(1 - e^{-2z}) \approx z\left[\frac{1 + az + bz^2}{1 + cz + dz^2}\right]. \tag{45}
$$

The best fit on the interval $0 \leqslant z \leqslant 5$ is[25] $a = 0.228$, $b = 0.010$, $c = 1.187$, and $d = 0.682$. We solve for z and denote the solution as z_2. The result is

$$
z_2 = \frac{az_0 - c + \sqrt{(az_0 - c)^2 + 4(z_0 - 1)(d - bz_0)}}{2(d - bz_0)}. \tag{46}
$$

For the ground state we note that

$$
1 + \tanh z = \frac{2}{1 + e^{-2z}}, \tag{47}
$$

and thus Eq. (39) reads

$$
\frac{z}{z_0} = 1 - \frac{1}{2}(1 - e^{-2z}). \tag{48}
$$

In this case we can adopt a two-parameter approximation[26]

$$
\frac{1}{2}(1 - e^{-2z}) \approx z\left[\frac{1 + az}{1 + cz}\right], \tag{49}
$$

where the best fit on the interval $0 \leqslant z \leqslant 5$ is $a = -0.0572$ and $c = 1.286$. Equation (39) yields

$$
z_1 = \frac{cz_0 - z_0 - 1 + \sqrt{(cz_0 - z_0 - 1)^2 + 4z_0(az_0 + c)}}{2(az_0 + c)}. \tag{50}
$$

In Fig. 10 we plot these approximate formulas for z_1 and z_2 superimposed on the exact results.

V. DISCUSSION AND CONCLUSION

We have developed a technique for calculating the complete energy spectrum for the finite square well and related problems. The eigenvalue equation for this family of potentials takes the form of a transcendental equation $z = z_0 g(z)$, where z is related to the energy of the system and z_0 is related to the strength of the well. Solving such equations by

graphical or numerical means is sometimes inadequate, and an analytical solution, even in approximate form, can be useful.

Our method recasts the transcendental equation as a pair of parametric equations. (If $g(z)$ is periodic, we exploit this feature to project the solution onto the interval $[0, \pi/2]$.) The parametric equations are plotted to show the nth allowed energy as a function of the well depth. We then approximate the sinusoidal or hyperbolic functions as ratios of polynomials (Padé approximants), converting the transcendental equations into quadratic equations, which we solve to obtain closed form expressions for the bound state energies. Although approximate, the results are surprisingly accurate (and can be made even more so if cubic equations are used).

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[1] D. J. Griffiths, *Introduction to Quantum Mechanics*, 2nd ed. (Prentice Hall, Englewood Cliffs, NJ, 2005).

[2] R. A. Serway, C. J. Moses, and C. A. Moyer, *Modern Physics*, 3rd ed. (Brooks Cole, Belmont, MA, 2005).

[3] R. D. Murphy and J. M. Phillips, "Bound-state eigenvalues of the square potential," Am. J. Phys. **44**, 574–576 (1976).

[4] P. H. Pitkanen, "Rectangular potential well in quantum mechanics," Am. J. Phys. **23**, 111–113 (1955).

[5] C. D. Cantrell, "Bound-state energies of a particle in a finite square well: An improved graphical solution," Am. J. Phys. **39**, 107–110 (1971).

[6] P. G. Guest, "Graphical solutions for the square well," Am. J. Phys. **40**, 1175–1176 (1972).

[7] J. V. Mallow, "Simple graphical solution for the finite square well with no change of variables," Am. J. Phys. **64**, 1072–1073 (1996).

[8] S. Garrett, "Bound state energies of a particle in a finite square well: A simple approximation," Am. J. Phys. **47**, 195–196 (1979).

[9] D. J. Searles and E. I. von Nagy-Felsobuki, "Numerical experiments in quantum physics: Finite-element method," Am. J. Phys. **56**, 444–448 (1988).

[10] B. I. Barker and G. E. Loup, "Approximating the finite well with an infinite well: Energies and eigenfuctions," Am. J. Phys. **59**, 1038–1042 (1991).

[11] D. L. Aronstein and C. R. Stroud, Jr., "General series solution for finite square-well energy levels for use in wave-packet studies," Am. J. Phys. **68**, 943–949 (2000).

[12] J.-F. Bloch, "A new approach to bound states in potential wells," Am. J. Phys. **69**, 1177–1181 (2001).

[13] R. M. Kolbas, "Man-made quantum wells: A new perspective on the finite square-well problem," Am. J. Phys. **52**, 431–437 (1984).

[14] I. R. Lapidus, "Particle in a square well with a δ-function perturbation," Am. J. Phys. **55**, 172–174 (1987).

[15] I. R. Lapidus, "One-dimensional hydrogen molecule revisited," Am. J. Phys. **50**, 453–456 (1982).

[16] Reference 1, Sec. 2.6.

[17] Awkwardly, the odd solutions ($\psi_n(-x) = -\psi_n(x)$) correspond to even indices and vice versa.

[18] This technique was used in Ref. 2, pp. 209–210.

[19] A particularly interesting example is $z_0 = \pi/4$ using c_1. In this case $z_1 = \pi/2\sqrt{3+\pi} = 0.633\,840$, and the exact answer is 0.633 159.

[20] A plot similar to Fig. 5 was used by Pitkanen[4] to analyze the bound-state solutions graphically.

[21] In this case $f_{1/2}$ yields a quartic equation for the energies, while f_1 leads to a cubic. Naturally, they provide more accurate results.

[22] For $z_0 = 15$ Eq. (22) yields 1.49 for $n=1$ and 14.44 for $n=10$; the correct values are 1.47 and 14.42, respectively (see Table I). For $z_0 = \pi/4$ the formula reduces to $z_n = (\pi/2)(n-2+\sqrt{4-2n})$, but in this case there are only two solutions: $z_1 = (\pi/2)(\sqrt{2}-1) = 0.6506$ (compare Ref. 15) and a spurious $z_2 = 0$.

[23] Reference 1, Eq. (2.125).

[24] The strategy is to nail down the two ends (0 and $\pi/2$). Equation (14) (using $s=1/2$ and c_1) yields a more accurate approximation, $\tan x \approx x\sqrt{1-(2/\pi)^4x^2}/[1-(2x/\pi)^2]$, but this approximation leads to a sixth-order polynomial equation for x_n. A reasonable compromise is given by $\tan x \approx x(1-cx^2)/[1-(2x/\pi)^2]$, which gives a cubic equation for x_n.

[25] For $z > 5$ we already know that $z_1 \approx z_2 \approx z_0/2$.

[26] Using the four-parameter fit, Eq. (45), leads to a cubic equation for z_1.