INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) L673–L678 doi:10.1088/0305-4470/38/42/L02

LETTER TO THE EDITOR

Analytical solution of the finite quantum square-well problem

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Received 3 August 2005, in final form 8 September 2005
Published 5 October 2005
Online at stacks.iop.org/JPhysA/38/L673

Abstract
The bounded positive- and negative-parity spectrum $E_n^{(\pm)}$ of the symmetric, one-dimensional, finite quantum square-well potential is computed exactly, explicitly and analytically in the form $E_n^{(\pm)} = f^{(\pm)}(n)$, where $f^{(\pm)}$ are known functions.

PACS number: 03.65.Ge

The finite square well is treated in all standard textbooks on introductory quantum mechanics (see, e.g. [1–8]). It is used as a simple 'model of departure' in many areas of physics. In atomic and molecular physics, it may be used as a model of an electron moving in the mean field of a linear molecule such as acetylene (H–C≡C–H) [2]. It also arises as the $l = 0$ partial wave radial equation for a spherically symmetric, finite square-well potential [1–7]. In nuclear physics, it is used as a simple model of the deuteron [7]. In solid-state physics, it is used to describe electrons bound to a thin sheet of conducting material [2]. The finite square well is also an excellent model for the computation of the resonance spectrum of flat microwave cavities loaded with dielectric inserts which were used recently to verify the existence of a ray-splitting correction to the Weyl formula [9].

Despite its importance in research and education, none of the textbooks states the analytical solution of the bounded spectrum of the one-dimensional square well. True, the spectral equation of the one-dimensional quantum square-well problem is a transcendental equation [2, 3]. This, however, does not preclude its explicit, analytical solution. Indeed, explicit solutions of the finite square-well problem were published by Siewert [10], Aronstein and Stroud [11], and Paul and Nkemzi [12].

Aronstein and Stroud [11] solved the spectral equation of the finite square well by a method known as *reversion of series* [13]. However, although an explicit formula for the general term of a reversed series exists [13], applying it to the series of Aronstein and Stroud is cumbersome. Accordingly, Aronstein and Stroud state only the first few terms of their series expansions explicitly.

Based on the work of Siewert [10], Paul and Nkemzi [12] cast the square-well problem into the form of a Riemann boundary problem [14] and arrive at an explicit integral representation of the bound-state energies of the finite square well. In principle, this representation can be used as the starting point of a systematic integral-free series representation, but only the first few terms were computed by Paul and Nkemzi [12]. An error in this expansion was corrected by Aronstein and Stroud [15].

The purpose of this letter is to present an integral-free, explicit solution of the one-dimensional, finite square-well potential in which all the terms in the series expansions are stated explicitly. Only elementary mathematics is used.

Starting point is the stationary Schrödinger equation for a quantum particle of mass m in the symmetric, finite, one-dimensional square-well potential [1–7]

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x), \tag{1}$$

where

$$V(x) = \begin{cases} 0, & \text{for} \quad |x| < a, \\ V_0, & \text{for} \quad |x| \geqslant a, \end{cases} \tag{2}$$

and $V_0 > 0, 2a > 0$ are the depth and width of the potential, respectively. The continuous spectrum $E > V_0$ of (1) is trivial [1–7]. We will not consider it any further in this letter. Instead we focus on the computation of explicit expressions for the bounded states of (1). Defining $\xi = ka, k = \sqrt{2mE/\hbar^2}, v_0 = \sqrt{2ma^2V_0/\hbar^2}$, the spectral equation for the bound states is

$$\tan(\xi) = p\xi^{-p}\left[v_0^2 - \xi^2\right]^{p/2}, \tag{3}$$

where $p = +1$ for the even solutions of (1) ($\psi(-x) = \psi(x)$, positive-parity states) and $p = -1$ for the odd solutions of (1) ($\psi(-x) = -\psi(x)$, negative-parity states). The total number of negative- and positive-parity bound states, respectively, is given by

$$N_B^{(p)} = \begin{cases} \left\lfloor \frac{1}{2} + \frac{v_0}{\pi} \right\rfloor, & \text{for} \quad p = -1, \\ \left\lfloor \frac{v_0}{\pi} \right\rfloor + 1, & \text{for} \quad p = +1, \end{cases} \tag{4}$$

where $\lfloor x \rfloor$ is the floor function defined here as the largest integer smaller than x. Examples: $\lfloor 2.37 \rfloor = 2$; $\lfloor 2 \rfloor = 1$.

In the following, we focus on the negative-parity spectrum to outline the method of solution of (3). From (3), we obtain the singularity-free spectral equation for negative-parity states:

$$\sqrt{v_0^2 - \xi^2}\,\sin(\xi) + \xi\cos(\xi) = 0. \tag{5}$$

The positive roots of (5) suffice to compute the negative-parity bound-state spectrum of (1). We denote them by $\xi_n^{(-)}, n = 1, 2, \ldots, N_B^{(-)}$. The nth root $\xi_n^{(-)}$, and only $\xi_n^{(-)}$, is found in the root interval $\left[(n - 1/2)\pi, b_n^{(-)}\right]$, where

$$b_n^{(-)} = \begin{cases} n\pi, & \text{if} \quad v_0 \geqslant n\pi, \\ v_0, & \text{if} \quad v_0 < n\pi. \end{cases} \tag{6}$$

Defining

$$g^{(-)}(\xi) = \xi + \arcsin(\xi/v_0), \tag{7}$$

equation (5) can be written in the equivalent form $\sin(g^{(-)}(\xi)) = 0$, from which we obtain the defining equation for $\xi_n^{(-)}$ [8, 16]

$$g^{(-)}(\xi) = n\pi, \qquad n = 1, 2, \ldots, N_B^{(-)}. \tag{8}$$

For given n, this equation has only a single root, namely $\xi_n^{(-)}$. Equation (8) is the key for computing the roots $\xi_n^{(-)}$ explicitly.

First we define the staircase function

$$\Theta^{(-)}(\xi) = -\frac{1}{2} + \frac{\xi}{\pi} + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\sin(2m\xi)}{m}, \tag{9}$$

which jumps by one unit whenever its argument ξ crosses a multiple of π. Then we define the function

$$\mathcal{N}^{(-)}(\xi) = \sum_{n=1}^{N_B^{(-)}} \theta\big(\xi - \xi_n^{(-)}\big), \tag{10}$$

where $\theta(x) = 0$ for $x < 0, \theta(x) = \frac{1}{2}$ for $x = 0$, and $\theta(x) = 1$ for $x > 0$. The function $\mathcal{N}^{(-)}(\xi)$ counts the number of roots $\xi_n^{(-)}$ of (5) smaller than ξ.

Since a root $\xi_n^{(-)}$ is encountered whenever $g^{(-)}(\xi)$ crosses a multiple of π, and since $\Theta^{(-)}(\xi)$ increases by one unit whenever its argument crosses a multiple of π, we can express the counting function $\mathcal{N}^{(-)}(\xi)$ explicitly with the help of $\Theta^{(-)}(\xi)$ according to

$$\begin{aligned}\mathcal{N}^{(-)}(\xi) &= \Theta^{(-)}(g^{(-)}(\xi))\\ &= -\frac{1}{2} + \frac{\xi}{\pi} + \frac{1}{\pi}\arcsin\left(\frac{\xi}{v_0}\right) + \frac{1}{\pi}\sum_{m=1}^{\infty}\frac{\sin[2m\xi + 2m\arcsin(\xi/v_0)]}{m}.\end{aligned} \tag{11}$$

Integrating $\mathcal{N}^{(-)}(\xi)$ over the nth root interval, we obtain

$$\int_{(n-1/2)\pi}^{b_n^{(-)}} \mathcal{N}^{(-)}(\xi)\,\mathrm{d}\xi = (n-1)\big[\xi_n^{(-)} - (n-1/2)\pi\big] + n\big[b_n^{(-)} - \xi_n^{(-)}\big]. \tag{12}$$

This expression can be solved for $\xi_n^{(-)}$ resulting in the following closed-form solution for $\xi_n^{(-)}$:

$$\xi_n^{(-)} = nb_n^{(-)} - (n-1)(n-1/2)\pi - \int_{(n-1/2)\pi}^{b_n^{(-)}} \Theta^{(-)}(\xi + \arcsin(\xi/v_0))\,\mathrm{d}\xi. \tag{13}$$

No knowledge of $\xi_n^{(-)}$ is needed to evaluate the right-hand side. Since all quantities on the right-hand side of (13) are known, (13) is an explicit solution of (5).

Using (11), we obtain the following explicit, exact, integral-free series solution for $\xi_n^{(-)}$:

$$\begin{aligned}\xi_n^{(-)} = &-\frac{b_n^{(-)2}}{2\pi} + \left(n+\frac{1}{2}\right)b_n^{(-)} - \frac{\pi}{2}\left(n-\frac{1}{2}\right)^2 - \frac{v_0}{\pi}\big[\varphi^{(-)}\big(b_n^{(-)}/v_0\big) - \varphi^{(-)}(\pi(n-1/2)/v_0)\big]\\ &- \frac{v_0}{\pi}\sum_{m=1}^{\infty}\frac{1}{m}\big[F_m\big(2mv_0; b_n^{(-)}/v_0\big) - F_m(2mv_0; \pi(n-1/2)/v_0)\big],\end{aligned} \tag{14}$$

where

$$\varphi^{(-)}(\xi) = \int \arcsin(\xi)\,\mathrm{d}\xi = \xi\arcsin(\xi) + \sqrt{1-\xi^2} \tag{15}$$

and

$$\begin{aligned}F_m(z;\xi) &= \int \sin[z\xi + 2m\arcsin(\xi)]\,\mathrm{d}\xi\\ &= -\frac{1}{2}\sum_{q=-\infty}^{\infty} J_q(z) \sum_{\mu=\pm 1}{}' \frac{\cos[(2m+\mu+q)\arcsin(\xi)]}{2m+\mu+q}.\end{aligned} \tag{16}$$

The prime on the summation symbol indicates that singular terms are not included in the sum. $J_q(z)$ are Bessel functions of the first kind [17]. The Bessel function series in (16) is essentially finite, since the Bessel functions cut off at $|q| \approx |z|$, i.e. the Bessel functions drop to zero faster than exponentially for $|q| > |z|$ [17]. Thus the convergence of (16) is guaranteed.

With the help of a partial integration, it is possible to show analytically that $|F_m(2mv_0; b) - F_m(2mv_0; a)| \leqslant h(v_0, a, b)/m$, where $0 \leqslant a, b \leqslant 1$ and $h(v_0, a, b) > 0$. Since the sum in (14) involves one additional factor of $1/m$, the sum in (14) converges absolutely.

Defining $\xi_{n,M}^{(-)}$ as the result obtained by including only the first M terms in the sum over m in (14), we can prove analytically that $\left|\xi_{n,M}^{(-)} - \xi_n^{(-)}\right| \leqslant C_n^{(-)}(v_0)\big/M$, where $C_n^{(-)}(v_0)$ is a positive constant. This result is a consequence of $|F_m(2mv_0; b) - F_m(2mv_0; a)| \sim 1/m$. It shows that $\xi_{n,M}^{(-)} \to \xi_n^{(-)}$ for $M \to \infty$. Numerical calculations indicate that the convergence of (14) is faster than suggested by the analytical result. In the cases we checked, we find $\left|\xi_{n,M}^{(-)} - \xi_n^{(-)}\right| \sim 1\big/M^2$, i.e. quadratic convergence. If true in general, it may be possible to improve the analytical estimate $\left|\xi_{n,M}^{(-)} - \xi_n^{(-)}\right| \leqslant C_n^{(-)}(v_0)\big/M$. However, this estimate is all we need in the context of this letter to prove that (14) converges. We mention that the numerical results do not invalidate the analytical estimate. In fact, the estimate $\left|\xi_{n,M}^{(-)} - \xi_n^{(-)}\right| \leqslant C_n^{(-)}(v_0)\big/M$ certainly covers a possibly faster convergence $\sim 1/M^2$.

With $\sum_{m=1}^{\infty} 1/(2m-1)^2 = \pi^2/8$ [17], it can be shown analytically that according to (14) $\xi_n^{(-)} \to n\pi$ for $v_0 \to \infty$. This is the correct result for the negative-parity solutions of the infinite square well and shows that (14) has the correct large-v_0 limit.

Derivation of (14) involves interchanging integration and summation in (13). We justify it in the following way. The series representation (11) of $\Theta^{(-)}(\xi + \arcsin(\xi/v_0)) = \Theta^{(-)}(g^{(-)}(\xi))$ in (13) converges uniformly in $\left[(n - 1/2)\pi, \xi_n^{(-)} - \epsilon\right]$ and $\left[\xi_n^{(-)} + \epsilon, b_n^{(-)}\right]$, where $\epsilon < \min\left\{b_n^{(-)} - \xi_n^{(-)}, \xi_n^{(-)} - (n-1/2)\pi\right\}$. In this case there is no problem interchanging integration and summation [18]. A problem may occur only in $\left[\xi_n^{(-)} - \epsilon, \xi_n^{(-)} + \epsilon\right]$, where $\Theta^{(-)}(g^{(-)}(\xi))$ jumps by one unit and is therefore not uniformly convergent. But since we can make ϵ as small as we like, and since $g^{(-)}(\xi)$ is a strictly monotonic function ($\mathrm{d}g^{(-)}(\xi)/\mathrm{d}\xi > 0$ for all ξ), we can linearize $g^{(-)}(\xi)$ in $\left[\xi_n^{(-)} - \epsilon, \xi_n^{(-)} + \epsilon\right]$, which turns the series representation (11) of $\Theta^{(-)}(g^{(-)}(\xi))$ into an ordinary Fourier sum. According to a theorem in [18] (appendix to chapter IX, pp 455–6), interchanging of integration and summation is always allowed for Fourier sums as long as the sum converges to a piecewise continuous function. Since $\Theta^{(-)}(g^{(-)}(\xi)) = \mathcal{N}^{(-)}(\xi)$ is piecewise constant, and therefore certainly piecewise continuous, the condition is fulfilled, the interchange is allowed and the proof is complete.

We now turn to the positive-parity states. From (3), we obtain the singularity-free spectral equation for the positive-parity states

$$\sqrt{v_0^2 - \xi^2}\cos(\xi) - \xi\sin(\xi) = 0. \tag{17}$$

Defining

$$g^{(+)}\xi = \xi - \arccos(\xi/v_0), \tag{18}$$

the spectral equation (17) can be written in the equivalent form $\sin(g^{(+)}(\xi)) = 0$, from which we obtain the defining equation [8, 16]

$$g^{(+)}(\xi) = n\pi, \qquad n = 0, 1, \ldots, N_B^{(+)} - 1 \tag{19}$$

for the roots $\xi_n^{(+)}$ of (17). The root $\xi_n^{(+)}$, and only $\xi_n^{(+)}$, is found in the root interval $\left[n\pi, b_n^{(+)}\right]$, where

$$b_n^{(+)} = \begin{cases} (n + 1/2)\pi, & \text{if} \quad v_0 \geqslant (n + 1/2)\pi, \\ v_0, & \text{if} \quad v_0 < (n + 1/2)\pi. \end{cases} \tag{20}$$

Defining the functions

$$\varphi^{(+)}(\xi) = \int \arccos(\xi)\,\mathrm{d}\xi = \xi \arccos(\xi) - \sqrt{1-\xi^2}, \tag{21}$$

$$K_\mu(q,m;\xi) = \begin{cases} \xi, & \text{if} \quad q-2m+\mu = 0, \\ \dfrac{\mathrm{e}^{\mathrm{i}[q-2m+\mu]\xi}}{\mathrm{i}[q-2m+\mu]}, & \text{if} \quad q-2m+\mu \neq 0, \end{cases} \tag{22}$$

and

$$\begin{aligned} G_m(z,\xi) &= \int \sin[z\xi - 2m\arccos(\xi)]\,\mathrm{d}\xi \\ &= -\frac{1}{2}\,\mathrm{Im} \sum_{q=-\infty}^{\infty} \mathrm{i}^{q-1} J_q(z) \sum_{\mu=\pm 1} \mu K_\mu(q,m;\arccos(\xi)), \end{aligned} \tag{23}$$

we obtain

$$\begin{aligned} \xi_n^{(+)} = &-\frac{b_n^{(+)2}}{2\pi} + \left(n+\frac{1}{2}\right) b_n^{(+)} - \frac{\pi}{2} n(n-1) + \frac{v_0}{\pi}\left[\varphi^{(+)}\left(b_n^{(+)}/v_0\right) - \varphi^{(+)}(n\pi/v_0)\right] \\ &- \frac{v_0}{\pi} \sum_{m=1}^{\infty} \frac{1}{m}\left[G_m\left(2mv_0, b_n^{(+)}/v_0\right) - G_m(2mv_0; n\pi/v_0)\right]. \end{aligned} \tag{24}$$

The convergence properties of $\xi_n^{(+)}$ in (24) are the same as those of $\xi_n^{(-)}$ in (14). In analogy to the negative-parity case, it can be shown analytically that in the limit of $v_0 \to \infty$ (24) predicts $\xi_n^{(+)} \to (n+1/2)\pi$, the correct result for the positive-parity states of an infinite square well.

Since $E_n^{(\pm)} = \hbar^2 \xi_n^{(\pm)2} / (2ma^2)$, formulae (14) and (24) accomplish the goal of computing the bound spectrum of the symmetric, finite square well explicitly in the form $E_n^{(\pm)} = f^{(\pm)}(n)$, where $f^{(\pm)}$ are known functions.

The solution method presented in this letter is based on a method first used in [19, 20] for the solution of a class of scaling quantum graphs [19–23]. Only above-barrier spectra are computed in [19–21]. Below-barrier spectra were recently computed for a scaling [24] and a nonscaling [25] step potential inside a box with infinitely high walls [19–21]. The results obtained in [24, 25] are not integral-free. Moreover it can be shown [26] that the methods used in [25] may lead to divergent results. Thus the solution of the square-well problem presented in this letter is the first time that a modified, convergent version of the algorithm of [19–21] is applied to a nonscaling potential with tunnelling and yields integral-free results. This step is significant, since it opens up the possibility of solving explicitly all quantum graphs, scaling or nonscaling, with or without tunnelling.

The solution method presented in this letter is not meant to provide the eigenvalues of the finite square-well potential with greater computational speed. It is an intellectual advance since it shows that the eigenvalues can be computed integral-free, analytically and explicitly in the form $E_n^{(\pm)} = f^{(\pm)}(n)$, where $f^{(\pm)}$ are the *same* functions for all n. This is surprising since the spectral equations (8) and (19) of the finite square-well potential are transcendental equations.

The method in [19–21] is based on the scattering matrix [22, 23]; the method in this letter is based entirely on the spectral equation. This feature has two advantages. (i) It makes the method more straightforward to use and (ii) it can be applied conveniently to a wide class of scaling and nonscaling potentials, with or without tunnelling, as soon as their spectral equations are known. This is a particularly appealing feature since for many potentials the spectral equation is known, but hard, or impossible, to solve explicitly with existing analytical tools. Here the method presented in this letter makes a difference.

In this letter, we presented an exact, explicit and analytical solution of the bound-state spectrum of the symmetric, one-dimensional, finite quantum square-well potential. The solutions (14) and (24) are characterized by the following features: (i) Only elementary mathematical methods (including Fourier series and Bessel functions) are used in their derivation, (ii) they are integral-free, (iii) all terms in the series expansions are stated explicitly and (iv) all series converge absolutely.

The method generalizes naturally to other types of one-dimensional potentials. Examples are quantum graphs [19–23], the δ-in-the-box potential [27], and piecewise constant potentials.

Acknowledgments

Financial support by NSF grant number PHY-9984075 is gratefully acknowledged.

References

[1] Schiff L I 1955 *Quantum Mechanics* (New York: McGraw-Hill)
[2] French A P and Taylor E F 1978 *An Introduction to Quantum Physics* (New York: W. W. Norton & Company, Inc.)
[3] Griffiths D J 1995 *Introduction to Quantum Mechanics* (Upper Saddle River, NJ: Prentice-Hall)
[4] Messiah A 1961 *Quantum Mechanics* (Amsterdam: North-Holland)
[5] Cohen-Tannoudji C, Diu B and Laloë F 1977 *Quantum Mechanics* (New York: Wiley)
[6] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* 3rd edn (Oxford: Pergamon)
[7] Park D 1992 *Introduction to the Quantum Theory* (New York: McGraw-Hill)
[8] Davydov A S 1966 *Quantum Mechanics* (Ann Arbor: NEO Press)
[9] Vaa C, Koch P M and Blümel R 2003 *Phys. Rev. Lett.* **90** 194102
[10] Siewert C E 1978 *J. Math. Phys.* **19** 434
[11] Aronstein D L and Stroud C R Jr 2000 *Am. J. Phys.* **68** 943
[12] Paul P and Nkemzi D 2000 *J. Math. Phys.* **41** 4551
[13] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* (New York: McGraw-Hill) pp 411–3
[14] Muskhelishvili N I 1953 *Singular Integral Equations* (Groningen: Noordhoff)
[15] Aronstein D L and Stroud C R Jr 2000 *J. Math. Phys.* **41** 8349
[16] Sprung D W L, Wu H and Martorell J 1992 *Eur. J. Phys.* **13** 21
[17] Gradshteyn I S and Ryzhik I M 1994 *Table of Integrals, Series, and Products* 5th edn ed A Jeffrey (Boston: Academic)
[18] Courant R 1937 *Differential and Integral Calculus* vol I 2nd edn (New York: Interscience)
[19] Dabaghian Yu, Jensen R V and Blümel R 2001 *JETP Lett.* **74** 235
[20] Blümel R, Dabaghian Yu and Jensen R V 2002 *Phys. Rev. Lett.* **88** 044101
[21] Dabaghian Yu and Blümel R 2004 *Phys. Rev.* E **70** 046206
[22] Kottos T and Smilansky U 1997 *Phys. Rev. Lett.* **79** 4794
[23] Kottos T and Smilansky U 1999 *Ann. Phys., NY* **274** 76
[24] Bhullar A S, Blümel R and Koch P M 2005 *J. Phys. A: Math. Gen.* **38** L563
[25] Dabaghian Yu and Jensen R 2005 *Eur. J. Phys.* **26** 423
[26] Blümel R 2005 *Eur. J. Phys.* submitted
[27] Lapidus I R 1987 *Am. J. Phys.* **55** 172