OPTOELECTRONICS AND ADVANCED MATERIALS – RAPID COMMUNICATIONS Vol. 6, No. 9-10, September - October 2012, p. 917 - 925

A new approximation for the quantum square well problem

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After a review of the results obtained in the quantum square well problem in the last six decades, Garrett's approach is reformulated in a consistent way, and Barker's solution is deduced using a simple method. A new analytic approximation for the roots of the transcendental equations for the energy eigenvalues is proposed, with applications to the study of quantum wells and resonant cavities.

(Received March 22, 2012; accepted September 20, 2012)

Keywords: Quantum square well, Resonant cavity, Normal modes, Transcendental equations

1. Introduction

One of the most elementary problems of quantum mechanics treats the movement of a particle of mass *m* in a square well potential:

$$V(x)=\begin{cases}-U, |x|<a/2\\ 0, elsewhere\end{cases} \tag{1}$$

The eigenvalue equations for the energy of states (which have well defined parity - a consequence of the symmetry of the potential, see for instance [1]) inside the well are equivalent to:

$$\frac{\sin\zeta(p)}{\zeta(p)}=\pm p, \frac{\cos\xi(p)}{\xi(p)}=\pm p \tag{2}$$

The roots correspond to the intersections of the functions $\frac{\sin x}{x},\frac{\cos x}{x}$ with the line $y=\pm p$; here, x is just the Cartesian coordinate of a point in a plane (xOy) and has nothing to do with the spatial variable x in (1). The number of roots depends on the value of *p*. To solve these equations means to find explicit expressions for $\zeta(p),\xi(p)$ - a highly non-trivial mathematical problem. The quantity p is the inverse of the potential strength *P*:

$$P=\frac{a}{2\hbar}(2mU)^{1/2}=\frac{1}{p}, p>0 \tag{3}$$

The alternance of signs, in (2), is connected to the parity of states and has, in fact, the following aspect:

$x\in\left(0,\frac{\pi}{2}\right)$: even states: $\frac{\cos x}{x}=p$; odd states: no solution. (4)

$x\in\left(\frac{\pi}{2},\pi\right)$: even states: no solution; odd states:

$$\frac{\sin x}{x}=p \tag{5}$$

$x\in\left(\pi,\frac{3\pi}{2}\right)$: even states: $\frac{\cos x}{x}=-p$; odd states: no solution. (6)

$x\in\left(\frac{3\pi}{2},2\pi\right)$: even states: no solution; odd states:

$$\frac{\sin x}{x}=-p \tag{7}$$

and so on.

In other words, the eigenvalues of the even states are given, for $x\in\left(0,\frac{\pi}{2}\right)$ by the roots $\xi_1(p)$ of $\frac{\cos x}{x}=p$ on this interval, and for $x\in\left(\pi,\frac{3\pi}{2}\right)$, by the roots $\xi_2(p)$ of $\frac{\cos x}{x}=-p$ on this interval, and so on (modulo 2π) (see Fig. 1). The eigenvalues of the odd states, for $x\in\left(\frac{\pi}{2},\pi\right)$ by the roots $\zeta_1(p)$ of $\frac{\sin x}{x}=p$ and for $x\in\left(\frac{3\pi}{2},2\pi\right)$, by the roots $\zeta_2(p)$ of $\frac{\sin x}{x}=-p$ etc. (see Fig. 2). The fact, that the same quantity is written as $\zeta_1(p)$ or $\xi_1(p)$ in (2) and *x* in (4-7), should not produce any confusion. Later on, when we shall be interested only in the mathematical aspects of inverting the functions (2), we shall write $\zeta_1(x)$ instead of $\zeta_1(p)$, considering that x is a generic variable, independent of the physical meaning of $p = \frac{1}{P}$, according to (3), and, evidently, having nothing to do with the coordinate x in (1).

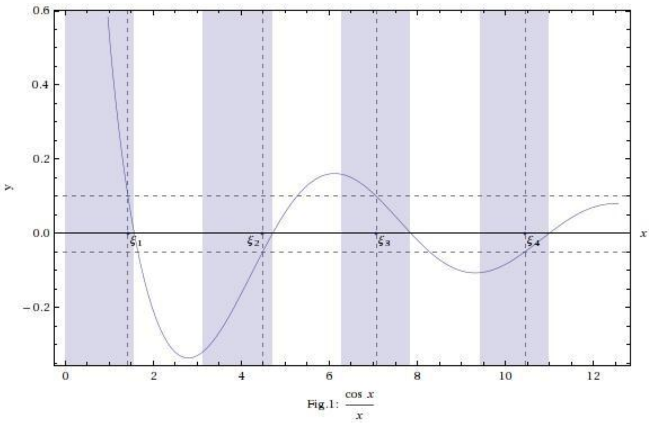

Fig. 1. The roots of the equation $\frac{\cos x}{x} = y$.

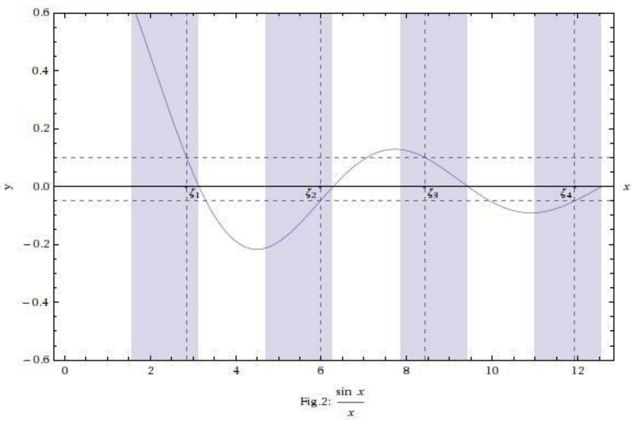

Fig. 2 The roots of the equation $\frac{\sin x}{x} = y$.

Until the mid '80s, the square well problem was of limited physical interest; its applications used to cover the oversimplified approach of some physical systems or phenomena, like electrons on a linear molecule, electrons just below the free surface of a metal, the Ramsauer-Townsed effect, the deuteron or alpha-particle emission from heavy nuclei ([2], [3]). But after the fabrication of quantum wires [4], the theoretical and experimental study of photon cavity systems [5], [6], [7], the experimental observation of revivals and super-revivals ([8], [9]) or the progress of the so-called "ghost orbit spectroscopy" [10], the square wells describe realistic physical systems or phenomena, and the need for an explicit solution exceeds the level of solving a simple problem of quantum mechanics. Another important application belongs to the domain of resonant cavities, where the frequency of normal modes are given by the same equations (2), see [11], [12].

In the last decade, refinement of experimental techniques made possible the realization of ultra-thin metallic films. Actually, as the size of a physical system is reduced to the nanometer range, electron confinement is expected to generate quantum well states; these states are very well described by the quantum mechanical 'particle in a box' model. In fact, the electron moving normal to the film surface can be considered a particle in a rectangular box. The case of a symmetric barrier describes only the electron states in a freestanding metallic thin film. However, in the realistic situation of a thin film grown on a substrate, the presence of this substrate produces an asymmetric potential barrier. However, such a potential has only the effect of "phase shifting" the physical properties of the freestanding film [13]. The rich physics of thin metallic films, as noticed by the pioneering papers [14] and [15], shows up an oscillatory behavior of the film stability [16], of lattice distortion [17] or work function, depending on the number of monolayers. So, by growing the thin films with atomic layer precision, it is possible to tune their work function, thus influencing the chemistry of the surface [18].

With few exceptions [19], [20], the physical properties of metallic ultra-thin films are obtained theoretically considering that the square well containing the electron can be approximated with an infinite one. This is of course a crude approximation, applicable only for films with a quite large numbers of monolayers ($n \geq 10$), but inacceptable for $n \sim 1$. In this last situation, it is necessary to use the solutions of the 'particle in a finite box' problem.

The main contribution of this paper is to propose solutions of the eigenvalue equations for the energy of a particle in a finite rectangular box, (2). A special attention will be paid to low order roots ξ_n, ζ_n, $n \sim 1$. Another contribution is the consistent use of Garrett's [21] iteration process, in order to associate, to a given square well, an infinite one, having approximately the same first n energy levels. Also, the results of Barker et al. [22] are re-obtained in a simple manner.

Some few words about conventions and notations are appropriate. Our choice, eq. (1), corresponds to a well having the top at $E = 0$, on the energy axis, so all the levels E_n are negative. Other popular choice is to have the bottom of the well at $E = 0$ so all the levels E_n are positive. It is adopted, of course, for infinite wells (the particle moving between rigid walls). Our paper contains a review of the previous work, where all these conventions have been used by various authors; in order to keep the notation simple, and to facilitate the direct access of the reader to references, we preferred to use the same symbol E_n, in all cases. We hope that this fact will not confuse the reader.

The structure of this paper is as follows. Section 2 is devoted to a detailed analysis of the previous work. It contains a critical discussion of the results already obtained, as well as, sometimes, suggestions concerning their possible improvements. In Section 3, we show how the levels of a finite square well can be obtained from those of an infinite one, using consistently the concept of characteristic depth, introduced by Garrett. In Section 4, we use a simple method to re-obtain the main results of Barker et al. [22]. Section 5 contains our main contribution, the parabolic approximation of the solution of equations (2). It is compared with other approximations proposed in literature, and with the exact solutions. Section 6 is devoted to conclusions.

2. Critical analysis of the previous work

In most textbooks, the energy eigenvalues of the problem (1) are obtained from the equation

$$\tan ka = \frac{\chi}{k} \tag{8}$$

for even states, and from

$$\cot ka = -\frac{\chi}{k} \tag{9}$$

for odd states, with:

$$E = -\frac{\hbar^2 \chi^2}{2m}, U = \frac{\hbar^2 k_0^2}{2m}, \chi^2 = k_0^2 - k^2 \tag{10}$$

In the early books of quantum mechanics ([23], [24]), these equations are solved graphically (if we refer specifically to these two textbooks - by two different methods). The first paper devoted to this problem is due, to the best of our knowledge, to P. H. Pitkanen [25], who writes (8, 9) in a simpler form, (2), allowing a simple visualization of solutions; a detailed discussion of the appropriate sign in (2) is also given. The second paper [26] (which does not cite [25], producing a delay in its citation by other authors) proposes again the replacement of eqs. (8,9) with (2) - which is in fact a repetition of Pitkanen's contribution -, notices that the equation for odd states is also the equation for the eigenvalues of a particle in a semi-infinite square well, i.e. with the potential:

$$U(x) = \begin{cases} \infty, x < 0 \\ -U, 0 < x < a, \\ 0, x > a \end{cases} \tag{11}$$

and introduces, for the bound states of this potential, the value of N_{onset} , defining the threshold value of the potential strength, allowing the occurrence of a new bound state. A first order approximation for the ground state of (9), in the limit of a deep well, is obtained, using the linear approximation of *sinx*.

An interesting graphical solution is proposed by Elmore [27] using polar coordinates, as intersections of the spiral of Archimedes $r = \theta$ with four circles of diameter $\theta_0 = \frac{2\pi a}{\lambda_0}$, with $\lambda_0 = \frac{h}{(2mV_0)^{1/2}}$ the de Broglie wavelength of a hypothetical zero-energy particle in the well. Another graphical construction, due to Guest [28], studying the intersection of the line $y = a^2 U$ with the branches of the curve $y = \frac{x}{|\sin x|}$, has the virtue of putting in value the striking resemblance of the bound states energies in a finite rectangular well with the modes of a metallic waveguide ([11], fig. (8.14)); in fact, the Sturm-Liouville problems are identical, for the eigenvalues of the frequencies in a waveguide and of the energy of a quantum particle in a rectangular well [12].

Murphy and Phillips [29] prefer to put the eigenvalue equation in the form:

$$y = \left|\arccos \frac{y}{\eta}\right|;\ \eta = \frac{\left(2mUa^2\right)^{1/2}}{\hbar} \tag{12}$$

and to solve it numerically, while Memory [30] applies the Newton-Raphson method to get the solution.

A completely different approach is proposed by Siewert [31]. Following a method of solving the Riemann problem developed previously [32], the author gives an explicit way of obtaining exact solutions for eqs. (3) and (4). Unfortunately, this approach needs the evaluation of some complicated integrals (task not yet accomplished by any author), so Siewert's solution is of limited use. Garrett [21] introduces an interesting concept in connection with the finite rectangular well: the characteristic depth δ :

$$\delta = \frac{\hbar}{(2m(U-E))^{1/2}} \tag{13}$$

defining the dimension of the region outside the well, where the wave function of a bound state can penetrate, decreasing exponentially. This concept is similar to the "skin depth" in electromagnetism [11] or to "viscous penetration depth" in fluids [33]. Garrett's suggestion is to introduce the value of the energy for the *n*-th bound state of the particle in the infinite well:

$$E_n^{(0)} = n^2 \frac{\pi^2 \hbar^2}{2ma^2}, n = 1,2,... \tag{14}$$

in eq. (13), and to use the value δ_n obtained in this way in order to define an effective width $a_n^{'} = a + 2\delta_n$ of another infinite well, with energies $E_n^{(1)}$ and to repeat the iteration. Finally, each energy level E_n of the finite well can be approximated to the *n*-th level of an infinite well of effective width $a + 2\delta_n^{'}$, with $\delta_n^{'}$ obtained in the second iteration, as just explained. Even if such an idea might be appealing, it is unclear how many iterations would produce a satisfactory solution. The consistent application of Garrett's idea, using an infinite number of iterations, is exposed in the Section 3 of the present paper.

Reed [34] introduces another simplification of the problem, replacing the two equations (2) with a unique one:

$$(K^2 - 2\xi^2)\sin(2\xi) + 2\xi\sqrt{K^2 - \xi^2}\cos(2\xi) = 0,$$

$$K^2 = \frac{2mV_0L^2}{\hbar^2} \quad (15)$$

although it is not necessarily evident the advantage of renouncing at two simpler, almost identical equations, for a more complicated one. Barker et al. [22] obtain the second term in the formula of an energy level of a deep well, in the form:

$$\alpha_n = \frac{P}{1+P}\left[\frac{n\pi}{2} - \frac{1}{6(1+P)^3}\left(\frac{n\pi}{2}\right)^3\right] \quad (16)$$

where P is defined in (3) and

$$\alpha = \left(\frac{2mE}{\hbar^2}\right)^{1/2}\frac{a}{2} \quad (17)$$

using essentially the cubic approximation for *sinx*. The authors stress the fact that the energy levels of a finite square well of width a and well strength P can be approximated as the first n levels of an infinite well of width $b = a\left(1+\frac{1}{P}\right)$ with n equal to the largest integer contained in $\left(\frac{2P}{\pi}+1\right)$.

Sprung et al. [35] put Reed's equation in the form (eq. (11) of his paper):

$$\theta = \frac{n\pi}{2(K+1)} + \frac{K}{K+1}(\theta - \sin\theta) \quad (18)$$

and solve it using an iteration method, suited to deep wells. The discussion of the solution is interesting, but the solution is quite cumbersome and difficult to use.

Aronstein and Stroud [36] solve Reed's equation, put in the form:

$$\alpha + \arcsin\frac{\alpha}{P} = \frac{n\pi}{2}, \alpha = \frac{\sqrt{2mE}}{\hbar}\frac{a}{2},$$

$$P = \frac{\sqrt{2mU}}{\hbar}\frac{a}{2} \quad (19)$$

obtaining a series expansion for the energy E eq. (17) of their paper), in powers of $\eta = \frac{n\pi}{2} - \arcsin(r) - \frac{r}{P}$, where $r = \frac{\alpha}{P}$ is the so-called height ratio (giving the position of the level in the well), with coefficients depending on r, consequently of α consequently on E. This E-dependence of the r.h.s. term is suppressed by giving to r numerical values, e.g. $r = 0$ for the well bottom. So, the authors are able to obtain accurate expressions for certain regions of the well, for instance $r = 0$ or $r = \frac{1}{2}$. Also, they give a remarkable physical interpretation of the quantization condition of the particle in the well. It is also interesting the valorization of their results in the study of revivals and super-revivals.

Paul and Nkemzi [37] use a variant of Burniston-Sewart method [32], [31] in order to express the solutions of the eigenenergy equations (3), (4). The result is given as an integral (eq. (26) of their paper), so its practical utility is limited from the very beginning; it is unclear if one can obtain from it a series expansion in the potential strength (denoted here by p). Even the large p limit gives an incorrect result. Aronstein and Stroud [38] complete the bibliographic omissions of Paul and Nkemzi [37] and notice an incorrect coefficient in their low-order expansion of the energy. Pickett and Millev [39] also develop an extension of the Siewert-Burniston approach [32], [31], again without any easy-to-use final formula. Blumel [40] obtains an original exact solution which, even integral-free, contains complicated series of functions.

Last but not the least, de Alcantara Bonfim and Griffith [41] solve the transcendental equations for the finite well and also for other simple potentials using unexpected (and excellent!) approximations, for instance:

$$\cos(x) \cong f_s(x) = \frac{1-\left(\frac{2x}{\pi}\right)^2}{(1+cx^2)^s}, 0 \le x \le 2\pi \quad (20)$$

For $s = 0$, or $s = \frac{1}{2}$

$\left(c_1 = 1 - \frac{8}{\pi^2}, c_2 = 0.2120126\right)$ of $s = 1$

$\left(c_1 = \frac{1}{2}\left(1 - \frac{8}{\pi^2}\right), c_2 = 0.1010164\right)$. Even if the ground state energy is obtained with high precision, for the other levels the situation is different, i.e. there is no series expansion for each level, with a given precision.

With the amazing development of the mathematical software, the exploration of simple quantum mechanical problems, like various rectangular square wells, becomes more and more accessible. An example is the excellent book of Van Wyk [42], where (inter alia) the semi-infinite square well ("the deuteron problem") and the finite square well are both discussed, however without mentioning that the first one is a particular case of the second.

3. Garrett's concept of "characteristic depth"

Garrett [21] was the first to approach the square well problem starting from a simple physical idea, in the attempt of obtaining the expressions of the energy levels. Considering that the main difference between the infinite square well and the finite one is the fact that, in the second case, the particle can penetrate the potential well, Garrett tries to associate, for a finite well, an infinite one, of somewhat larger length, having the same first n energy levels, as the finite well. Garrett proposes an iterative approach for obtaining the value of this "somewhat larger length".

Actually, Garrett's approach is as follows. A particle in an infinite well has the energy levels given by (14). The same particle, moving in a square well of finite depth *U* can penetrate the wells of this potential, on a distance of the order:

$$\delta_n^{(1)} = \frac{\hbar}{\left(2m\left(U - E_n^{(0)}\right)\right)^{1/2}} \tag{21}$$

So, it behaves as a particle moving in an impenetrable well of length $a + 2\delta_n^{(1)}$ and its energy can be written as:

$$E_n^{(1)} = n^2 \frac{\pi^2\hbar^2}{2m\left(a + 2\delta_n^{(1)}\right)^2} \tag{22}$$

which can be considered as a first correction to (14). With $E_n^{(1)}$ we can define a new characteristic depth

$$\delta_n^{(2)} = \frac{\hbar}{\sqrt{2m(U - E_n^{(1)})}} = \frac{\hbar\left(a + 2\delta_n^{(1)}\right)}{\sqrt{2mU\left(a + 2\delta_n^{(1)}\right)^2 - \pi^2\hbar^2 n^2}} \tag{23}$$

to produce, similar to (22), a second correction to (14). A consequent application of this idea should involve infinity of steps, the general one being:

$$\delta_n^{(p+1)} = \frac{\hbar}{\sqrt{2m(U - E_n^{(p)})}} = \frac{\hbar\left(a + 2\delta_n^{(p)}\right)}{\sqrt{2mU\left(a + 2\delta_n^{(p)}\right)^2 - \pi^2\hbar^2 n^2}} \tag{24}$$

Putting:

$$\lim_{p\to\infty} \delta_n^{(p)} = \Delta,\; y = \frac{2\Delta}{a} \tag{25}$$

we get the following equation for the characteristic depth, obtained after an infinite number of iterations:

$$4P^2y^4 + 8P^2y^3 + \left(4P^2 - \pi^2n^2 - 4\right)y^2 - 8y - 4 = 0 \tag{26}$$

where *P* is defined in (3).

As y<<1, we shall solve this equation in increasing orders of *y*. In the first order, the equation gives y=-1/2, so $\Delta = -\frac{a}{2}$, an unacceptable result, as Δ should be positive. The conclusion is that the first acceptable approximation starts at least at the second order:

$$\left(P^2 - \frac{\pi^2n^2}{4} - 1\right)y^2 - 2y - 1 = 0 \tag{27}$$

The root:

$$y \cong \frac{1}{P} + \frac{1}{P^2} \tag{28}$$

gives:

$$\Delta = \frac{a}{2}\left(\frac{1}{P} + \frac{1}{P^2}\right) \tag{29}$$

and a corrected value for the energy of the particle in a finite well:

$$E_n = n^2 \frac{\pi^2\hbar^2}{2m(a + 2\Delta)^2}$$

With α given by (17), we get:

$$E_n = n^2 \frac{\pi^2\hbar^2}{2ma^2}\left(\frac{P}{P + 1 + \frac{1}{P}}\right)^2$$

The term 1/P in the denominator gives a spurious precision, so it can be disregarded; the final result is:

$$E_n = \alpha_n^2 \frac{2\hbar^2}{ma^2} = n^2 \frac{\pi^2\hbar^2}{2ma^2}\left(\frac{P}{1+P}\right)^2 \tag{30}$$

We obtain the first term of Barker's formula (16), which means that the energy levels of a particle in a square well of length *a* and strength *P* can be approximated with the levels of an identical particle, in an infinite well of length $\left(1 + \frac{1}{P}\right)a$. This is one of the main conclusions of Barker's paper. As we have shown here, it can be obtained directly from Garrett's approach, applied in a consistent manner.

Let us mention that the result is valid if (see for instance (24)):

$$P^2 > \frac{\pi^2n^2}{4} + 1 \text{ or } U > E_n^{(0)}\left(1 + \frac{4}{\pi^2n^2}\right) \tag{31}$$

with $E_n^{(0)}$ - the *n*-th level of the infinite well, according to (14).

4. Barker's solution of the transcendental equations

Barker et al. [22] find an approximate solution of the transcendental equations (2) using a series expansion of the trigonometric functions. As their method is quite complicated, we shall re-obtain their main result in a simpler way.

We shall use the notations explained just after eq. (7). Let us first consider the equation:

$$\sin\zeta_{2n+1} = x\zeta_{2n+1} \tag{32}$$

Putting

$$\zeta_{2n+1} = (2n+1)\pi - \delta \tag{33}$$

we get, expanding the *sin* up to the third order:

$$\delta^3 - 6(x+1)\delta + 6(2n+1)\pi x = 0 \tag{34}$$

It is convenient to use, for the cubic equation, the form given (for instance) in [43]:

$$z^3 - z + t = 0 \tag{35}$$

Its solution which approaches 0 when $t \to 0$ is:

$$z = t + t^3 + ... \tag{36}$$

After simple calculations one obtains:

$$\delta = \frac{(2n+1)\pi x}{x+1} + \frac{(2n+1)^3\pi^3x^3}{6(x+1)^4} \tag{37}$$

and:

$$\zeta_{2n+1} = \frac{(2n+1)\pi x}{x+1} + \frac{(2n+1)^3\pi^3x^3}{6(x+1)^4},$$
$$-\frac{1}{\left(2n-\frac{1}{2}\right)\pi} < x < \frac{1}{\left(2n+\frac{1}{2}\right)\pi} \tag{38}$$

In exactly the same way, we get, for the solution of the equation:

$$\sin\zeta_{2n} = x\zeta_{2n} \tag{39}$$

the root:

$$\zeta_{2n}(x) = \frac{2n\pi}{1-x} + \frac{4n^3\pi^3x^3}{3\left(1-x^4\right)},$$

$$-\frac{1}{\left(2n-\frac{1}{2}\right)\pi} < x < \frac{1}{\left(2n+\frac{1}{2}\right)\pi} \tag{40}$$

Similarly, for the equation

$$\cos\xi_{2n} = x\xi_{2n} \tag{41}$$

we get:

$$\xi_{2n}(x) = \left(2n-\frac{1}{2}\right)\pi + \frac{\left(2n-\frac{1}{2}\right)\pi x}{1-x} + \frac{\left(2n-\frac{1}{2}\right)^3\pi^3x^3}{6(1-x)^4}$$
$$-\frac{1}{(2n-1)\pi} < x < \frac{1}{2n\pi} \tag{42}$$

For the odd index roots:

$$\xi_{2n+1}(x) = \left(2n+\frac{1}{2}\right)\pi + \frac{\left(2n+\frac{1}{2}\right)\pi x}{1+x} + \frac{\left(2n+\frac{1}{2}\right)^3\pi^3x^3}{6(1+x)^4}$$
$$-\frac{1}{2n\pi} < x < \frac{1}{(2n+1)\pi} \tag{43}$$

The difference between eqs. (38,40,42,43) and Barker's result (16,17) is due to the fact that Barker do not solve the eqs. (2) in their general form, similar to (32), i.e.

$$\frac{\sin x}{x} = y, \frac{\cos x}{x} = y \tag{44}$$

with $y \neq 0$, but in the variant used in the eigenvalue problem, (4-7).

As Barker's formulas are obtained from a 3[rd] order expansion in the small parameter, any higher order term gives a spurious precision. In fact the more appropriate form of (38)-(43) is the polynomial one. For instance, Barker's general formula should be written as:

$$\alpha_n = \frac{\pi n}{2} - \frac{\pi n}{2}p + \frac{\pi n}{2}p^2 - \frac{\pi n}{2}\left(1+\frac{\pi^2n^2}{24}\right)p^3 =$$
$$= \frac{\pi n}{2}\left[1 - p + p^2 - \left(1+\frac{\pi^2n^2}{24}\right)p^3\right] = \frac{\pi n}{2}f_n(p) \tag{45}$$

With

$$f_n(p) \sim O(1) \text{ for } p << 1.$$

5. The parabolic approximation

To solve the eigenvalue equation (2), or its more general form (44), with $y < 0$ or $y > 0$, means to invert the function $y(x)$ defined by (44), i.e. to obtain the function $x(y)$. Geometrically, the inverse of the function $y(x)$, represented as a curve with a generic point (x, y), is represented by its symmetric with respect to the first bisector. A generic point of the inverse function has the coordinates (y, x).

Of course, only monotonous functions can be inverted, so, "inverting the function $\sin x / x$" (for instance), means, in fact, to consider the restriction of this function on intervals defined by its neighbor extremum points, which are indeed monotonous functions, and to invert each of these functions. Our approach contains two approximations. Firstly we shall approximate the extremum points of the functions $\sin x/x$ (respectively $\cos x/x$) with $(2n \pm 1/2)\pi$ (respectively with $n\pi$). Rigorously speaking, the extremum points are located at the roots of the equation $\tan x = x$ (respectively $\tan x = -1/x$) and are slightly shifted to the left of the aforementioned values.

Secondly we shall replace the negative or positive parts of the $\sin x/x$ (respectively $\cos x/x$), restricted on their intervals of monotony, with segments of parabolas.

Recently, a similar approach for obtaining approximate solutions of the transcendental eq. (2) has been proposed, but using a cubic polynomial, instead of a quadratic one, and using exact extremum points [44]. The solutions are expressed in terms of arcsin functions, and are quite difficult to use in applications. This is why we propose here a simpler approximation. The loss in precision, due to this less accurate approximation, will be discussed.

Using the method just exposed, we find the parabolic approximation for the first root for the odd states equation, the following expression:

$$\zeta_1^{(1)}(x) = \pi\sqrt{1-x} \tag{46}$$

A better formula, at least for $x < 1$, is obtained from an approximation of the sin function:

$$\zeta_1^{(2)}(x) = \sqrt{6(1-x) + 1.8(1-x)^2}\ ,\ 1-p << 1 \tag{47}$$

Let us compare these solutions with the cubic approximation [44]:

$$\zeta_1^{(3)}(x) = \frac{\pi}{\sqrt{2}} \frac{\sqrt{1-x}}{-\frac{1}{\sqrt{3}}\sin\left(\frac{1}{3}\arcsin\left(\frac{3^{3/2}}{2^{5/2}}\sqrt{1-x}\right)\right) + \cos\left(\frac{1}{3}\arcsin\left(\frac{3^{3/2}}{2^{5/2}}\sqrt{1-x}\right)\right)} \tag{48}$$

with Barker's result:

$$\zeta_1^{(4)}(x) = \pi - \pi x + \pi x^2 - \pi\left(1 + \frac{\pi^2}{6}\right)x^3 \tag{49}$$

and with the exact formula, cut after the first four terms is:

$$\zeta_1^{(5)}(x) = \pi - \pi x + \pi x^2 - \pi\left(1 + \frac{\pi^2}{6}\right)x^3 + \pi\left(1 + \frac{2}{3}\pi^2\right)x^4 \tag{50}$$

In Fig. 3, the exact solution ζ_1 is obtained graphically, as a reflection with respect to the first bisector, together with the approximate solutions given by eqn. (46) – (50). The accuracy of the cubic approximation is remarkable. $\zeta_1^{(2)}$ is very good too, for "large" arguments $0.6 < x \le 1$, and better than the parabolic one, excepting small values of x $(x < 0.2)$. The series expansion near $x = 0$ of the exact solution diverges for moderate values of x, but for $x < 0.2$, even the series cut after four order terms, gives an excellent approximation. For practical purposes, it seems that Barker's solution is equally good.

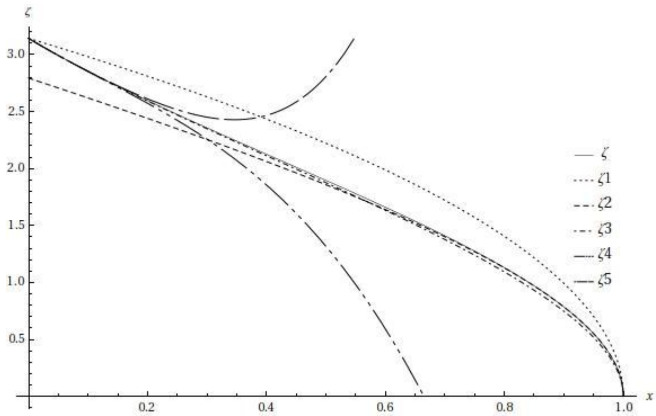

Fig. 3. The first root the equation $\frac{\sin x}{x} = y$: the exact solution and various approximations, eqn. (46) – (50).

Similar exercises show that, for larger n, the accuracy of the parabolic approximation increases (see Fig. 4), as well as the convergence of the exact solution, both for ζ_n and ξ_n. The higher order solutions ζ_n, $n > 1$, has a form analogous to (46):

$$\zeta_n = a_n + \sqrt{b_n + c_n x} \tag{51}$$

Where the numerical coefficients can be easily obtained, following the recipe given at the beginning of this section.

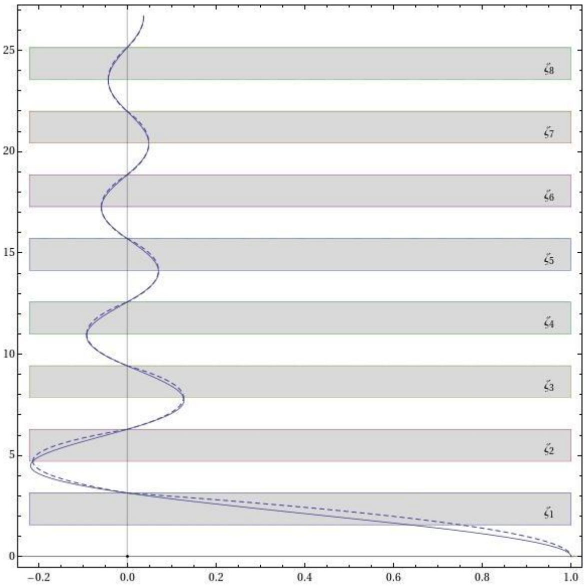

Fig. 4. The first 8 roots of the equation $\frac{\sin x}{x} = y$. *The continuous line corresponds to the exact solution, and the dotted line to the parabolic approximation.*

The situation of the first solution of the even equation in (2), ξ_1, is atypical, in the sense that it cannot be approximated by a polynomial. However the quadratic approximation of cos gives:

$$\xi_1^{(1)} = \frac{1}{x} - \frac{1}{2x^3}$$

Barker's formula is:

$$\xi_1^{(2)}(x) = \frac{\pi}{2} - \frac{\pi}{2}x + \frac{\pi}{2}x^2 - \frac{\pi}{2}\left(1 + \frac{\pi^2}{24}\right)x^3 \quad (52)$$

and the exact solution (series expansion near the origin), cut after the 5th order term, has the form:

$$\xi_1^{(3)}(x) = \frac{\pi}{2} - \frac{\pi}{2}x + \frac{\pi}{2}x^2 - \frac{\pi}{2}\left(1 + \frac{\pi^2}{24}\right)x^3 + \\ + \frac{\pi}{2}\left(1 + \frac{\pi^2}{6}\right)x^4 - \frac{\pi}{120}\left(60 + 25\pi^2 + \frac{9\pi^4}{32}\right)x^5 \quad (53)$$

The plot (Fig. 5) shows that, for $x > 1.5$, $\xi_1^{(1)}(x)$ is a good approximation, as $\xi_1^{(2)}(x)$ and $\xi_1^{(3)}(x)$ are, for $x < 0.3$; the exact solution is of little use (near $x = 0$), and it diverges more rapidly than Barker's approximation. However, for $0.5 < x < 1.5$, all the functions mentioned here are inappropriate; the only approach is to write a series expansion of the exact solution, similar to $\xi_1^{(3)}(x)$, not in the neighborhood of $x = 0$, but of the value $x_0 \in (0.5, 1.5)$, in which we are interested.

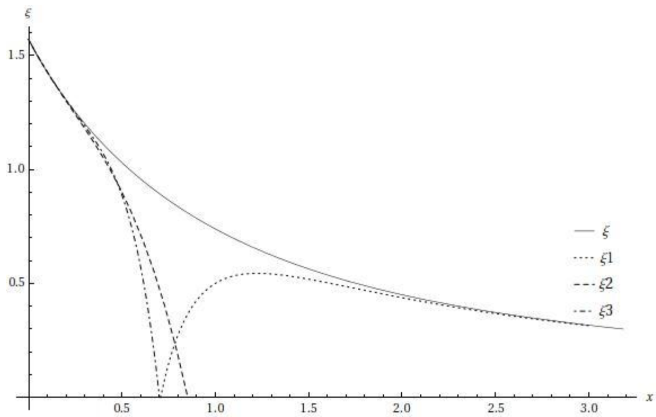

Fig. 5. The first root of the equation $\frac{\cos x}{x} = y$ *: the exact solution and various approximations.*

For $n > 1$, the solutions ξ_n have a form similar to (51), but with different values for the numerical constants.

The solution ξ_1 is however of special interest, as it gives the ground state energy for a symmetric square well. It is well known that an arbitrarily shallow well can "keep" a bound state, and its energy is crucial for the correct determination of the quantum well states in a metallic ultra-thin film [45].

Also, for a semi-infinite square well, ζ_1 gives the ground state energy, so the previous considerations are valid for films described by such a potential [13]. Our "parabolic approximation" has a reasonable accuracy for ζ_1, and a much better one, for ζ_n, with $n > 1$. So, they can be used to describe the physics of a large class of ultra-thin films.

Other applications of our results are the evaluation of the resonant modes of resonant cavities [11], [12].

6. Conclusions

The present paper is devoted to the presentation of a new approximate analytical solution for an elementary problem of quantum mechanics – the square well. In spite of its elementary character, its energy eigenvalue equation is equivalent to two very interesting transcendental equations; the explicit determination of their solution is a very challenging mathematical problem. In the absence of an easy-to-use exact solution, a simple analytical approximation for the energy eigenvalue equations is of real practical interest. In this paper, such an approximate solution is proposed. It is interesting not only for the investigation of physical systems and phenomena of modern nanophysics and nanophotonics, like quantum wells and interaction of femptosecond laser pulses with solids (revivals and super-revivals), but also for the analytic description of normal modes in resonant cavities. The applications in the physics of metallic ultra-thin films are also discussed.

Even if numerical results were available for such problems, the analytical approximations are important, as they make clear the physical aspects of the phenomena under investigation. Recently, similar approaches have been successfully applied in other fields of nanophysics [46], [47].

Acknowledgement

The financial support of ANCS (Romanian National Authority for Scientific Research), CNCS-UEFISCDI, project IDEI 2008 number 953, of the ANCS project PN 09 37 01 06 and of JINR Dubna - IFIN-HH Magurele-Bucharest project no. 01-3-1072-2009/2013 are kindly acknowledged.

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