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A NEW ANALYTIC APPROXIMATION FOR THE ENERGY EIGENVALUES OF A FINITE SQUARE WELL

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Abstract. A new analytic approximation of the energy eigenvalues of the bound states of a particle in a square well is presented. It consists mainly in the approximation of the restrictions of functions $\sin x/x$, $\cos x/x$, on their intervals of monotony, with cubic polynomials. In this way, the solutions of the transcendental equations for the energy eigenvalues are simply expressed in terms of $\arcsin x$. The errors of this approximation is about 10^{-2} for the first odd level and decreases at about 10^{-4} at the next odd level. The results have applications in the physics of quantum wells, in the theory of revivals and of resonant cavities.

Key words: analytic approximation, quantum wells, square-well problem, transcendental equations.

1. INTRODUCTION

It is quite frustrating that even the simplest problems of quantum mechanics defy exact solutions; even if we can find an exact solution for the Schroedinger equation, the eigenvalue equations are, in general, transcendental equations, which can be solved only numerically. This is the case of the elementary problem of a particle moving in a finite square well potential, where the energy eigenvalues are the roots of transcendental equations, involving trigonometric functions.

Until the mid '80s, the square well problem was mainly of didactic 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 [1, 2]. But after the fabrication of quantum wells [3], the theoretical and experimental study of photon cavity systems [4–6], the experimental observation of revivals and super-revivals [7, 8] or the progress of the so-called "ghost orbit spectroscopy" [9], the square wells describe realistic physical systems or phenomena, and the need for an explicit solution exceeds the level of solving simple and relevant problems 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, see [10, 11].

A review of the main results obtained in the attempts of solving the energy eigenvalue equation for the bound states of a quantum particle moving in a finite square well is exposed in [12]. Among them, a special interest presents a simple approximation of the solution, given by Baker *et al.*, and an exact power series expansion, obtained by Aronstein and Stroud [13]. However, Barker's approximation is quite poor for the first energy levels, and the Aronstein - Stroud solution gives, instead of an expression valid for any value of the independent variable, only series expansions in the neighborhood of specific points.

In this paper, we shall present a new analytic approximation for the energy eigenstates of a square well, which has the advantage of being quite precise, and providing a simple expression of the roots, in terms of elementary functions. It is based on the approximation of the restrictions of the functions $\sin x/x$, $\cos x/x$ on their intervals of monotony, with three-order polynomials. This method improves the approach presented in [12], where a similar approximation has been worked out with second-degree polynomials.

The structure of this paper is the following: in Section 2, the problem of energy eigenvalues is outlined and the transcendental equations to be solved are introduced. The approached used in order to get a new approximations of the solutions is described and the main mathematical formulas to be used are indicated. In Section 3, this approach is worked out in detail, for the case of the second level of odd parity; after that, the general cases, both for even and odd states, are obtained. The solution for the first odd level is obtained separately. The last section is devoted to conclusions.

2. THE BOUND STATES OF A SQUARE WELL: A NEW APPROACH

Let us outline the problem of a quantum particle in a square well, mainly in order to define the notations. For a particle of mass m moving in a finite square well potential:

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

the eigenvalue equations for the energy of bound states (which have well defined parity – a consequence of the symmetry of the potential, see for instance [15] p.48) are equivalent to:

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

The roots correspond to the intersections of the functions $\sin x/x$, $\cos x/x$ with the line $y = \pm p$. 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 :

$$P = \frac{a}{2}\left(\frac{2mU}{\hbar^2}\right)^{1/2} = \frac{1}{p} \tag{3}$$

The alternation of signs, in (2), is connected to the parity of states and has, in fact, the following aspect. The extremum points of the function $\cos x/x$ are given by the roots r_{cn} of the equation:

$$\tan x = -\frac{1}{x} \tag{4}$$

where we denoted by r_{cn} the root close to $(n-1)\pi$. The eigenvalue equations for even states are:

$$x \in \left(0, \frac{\pi}{2}\right): \ \frac{\cos x}{x} = p; \ x \equiv \xi_1(p) \tag{5}$$

$$x \in \left(r_{c2}, \frac{3\pi}{2}\right): \ \frac{\cos x}{x} = -p; \ x \equiv \xi_2(p) \tag{6}$$

$$x \in \left(r_{c3}, \frac{5\pi}{2}\right): \ \frac{\cos x}{x} = p; \ x \equiv \xi_3(p) \tag{7}$$

and so on.

Similarly, the extremum points of the function $\sin x/x$ are the roots r_{sn} of the equation:

$$\tan x = x \tag{8}$$

where we denoted by r_{sn} the root close to $\left(n - \frac{1}{2}\right)\pi$. The eigenvalue equations for odd states are:

$$x \in (0, \pi): \ \frac{\sin x}{x} = p; \ x \equiv \zeta_1(p) \tag{9}$$

$$x \in (r_{s,2}, 2\pi): \ \frac{\sin x}{x} = -p; \ x \equiv \zeta_2(p) \tag{10}$$

$$x \in (r_{s,3}, 3\pi): \ \frac{\sin x}{x} = p; \ x \equiv \zeta_3(p) \tag{11}$$

and so on. Each of the equations (5) - (7), (9) - (11) has a unique solution, $\xi_1(p)$, $\xi_2(p)$, $\xi_3(p)$, respectively $\zeta_1(p)$, $\zeta_2(p)$, $\zeta_3(p)$. On the aforementioned intervals, the functions $\cos x/x$, $\sin x/x$ are monotonous, and can be inverted. The inverse functions are $\xi_1(p)$, $\xi_2(p)$, $\xi_3(p)$, respectively $\zeta_1(p)$, $\zeta_2(p)$, $\zeta_3(p)$.

Geometrically, we can obtain the inverse of a function $y = y(x)$, taking its symmetric with respect to the first bisectrix, *i.e.* by plotting the curve (y,x) instead of (x,y). Analytically, we shall approximate the restrictions of $\sin x/x$, $\cos x/x$ on the intervals defined in (5-7), (9-11), etc., with cubic polynomials:

$$y(x) = a_3x^3 + a_2x^2 + a_1x + a_0$$

Inverting this equation, *i.e.* writing $x = x(y)$, we find explicit approximate expressions for the functions ζ_i, ξ_i.

In the next section, we shall develop this approach. As using a simple expression for the roots of a cubic equation is essential for obtaining a convenient approximation, we shall mention here, following Glasser [16], that a trinomic cubic of the form:

$$x^3 - x + t = 0, \ \ t < \frac{2}{\sqrt{27}} \tag{12}$$

has the solutions:

$$x_1 = \frac{2}{\sqrt{3}} \sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}t\right)\right) \tag{13}$$

$$x_{2,3} = -\frac{1}{\sqrt{3}} \sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}t\right)\right) \pm \cos\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}t\right)\right) \tag{14}$$

3. ANALYTIC APPROXIMATIONS OF THE ROOTS OF THE TRANSCENDENTAL EQUATIONS

We shall find approximate analytic solutions for the roots ζ_i, ξ_i, following the method outlined in the previous section. We shall work out in detail a particular case, and we give finally the general results.

In fact, we shall evaluate ζ_2, so we shall invert the function $\sin x/x$ on the interval $(r_{s2}, 2\pi)$, where $r_{s2} = 4.493409457909064...$ is the root of the equation $\tan x = x$, close to $3\pi/2 \simeq 4.7124$. Shifting the x coordinate:

$$X = x - 2\pi \tag{15}$$

the cubic polynomial which approximate the restriction of $\sin x/x$ on the considered interval is:

$$y(X) = a_3 X^3 + a_2 X^2 + a_1 X \tag{16}$$

The curve has a zero in $x = 2\pi$. We shall ask $y(X)$ to have a minimum in the point $x = r_2$ or

$$X_{m2} = r_2 - 2\pi \tag{17}$$

with the value:

$$M_{s2} = \frac{\sin r_2}{r_2} = -0.217234... \tag{18}$$

We shall also ask that the derivative of $y(X)$ vanishes in X_{m2}, and has the same derivative as $\sin x/x$ in $X = 0$. So, from these equations:

$$y(X_{m2}) = M_{s2}, \;\; y'(X_{m2}) = 0, \quad y'(X_{m2}) = \frac{1}{2\pi} \tag{19}$$

we can obtain the coefficients of the polynomial (16):

$$a_3 = 2\frac{2M_{s2}}{X_{m2}^3} + \frac{a_1}{X_{m2}^2} = -\frac{2M_{s2}}{X_{m2}^3} + \frac{1}{2\pi X_{m2}^2} \tag{20}$$

$$a_2 = +\frac{3M_{s2}}{X_{m2}^2} - \frac{2a_1}{X_{m2}} = \frac{3M_{s2}}{X_{m2}^2} - \frac{1}{\pi X_{m2}} \tag{21}$$

$$a_1 = \frac{1}{2\pi} \tag{22}$$

In order to invert (16), we have to solve:

$$a_3 X^3 + a_2 X^2 + a_1 X - y = 0 \tag{23}$$

Dividing by a_3 and changing the variable to:

$$X = z - \frac{a_2}{3a_3} \tag{24}$$

we get:

$$z^3 + A_1 z + A_0 = 0 \tag{25}$$

with:

$$A_1 = \frac{a_1}{a_3} - \frac{1}{3}\frac{a_2^2}{a_3^2} < 0, \;\; A_0 = \frac{2}{27}\frac{a_2^3}{a_3^3} - \frac{y}{a_3} - \frac{a_1 a_2}{3a_3^2} \tag{26}$$

Using a change of scale:

$$z = au \tag{27}$$

the equation can be put in the standard trinomic form:

$$u^3 - u + \frac{A_0}{|A_1|^{3/2}} = 0 \tag{28}$$

if we choose:

$$a = |A_1|^{1/2} \tag{29}$$

Finally, with (12), (13), (29), (27), (24), (15), we get:

$$x(y) = 2\pi - \frac{a_2}{3a_3} + \frac{2}{\sqrt{3}} |A_1|^{1/2} \sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}\frac{A_0}{|A_1|^{3/2}}\right)\right), \quad M_{s2} < y < 0 \tag{30}$$

and:

$$\zeta_2(x) = 2\pi - \frac{a_2}{3a_3} + \frac{2}{\sqrt{3}} |A_1|^{1/2} \sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}\frac{A_0(x)}{|A_1|^{3/2}}\right)\right), \quad -m_2 < x < 0 \tag{31}$$

Numerically, this means:

$$\zeta_2(x = -p) = 5.9562 - 2.9257 \sin\left(\frac{1}{3}\arcsin(6.1213p - 0.32970)\right) \tag{32}$$

Formula (32) should be compared with Barker's result, eq. (13) of [13], for $n = 4$:

$$\alpha_4 = \frac{P}{P+1}\left(2\pi - \frac{(2\pi)^3}{6(P+1)^3}\right) \tag{33}$$

Putting $P = 1/p$, and taking into consideration as the precision of Barker's formula cover not more than cubic terms:

$$\alpha_4(p) = 2\pi - 2\pi p + 2\pi p^2 - p^3\left(2\pi + \frac{4}{3}\pi^3\right) \simeq \zeta_2(x = -p) \tag{34}$$

Simple numeric check shows that our formula has an error of 3.1871×10^{-4} for $p = 0.1$, while Barker's one - of -8.2582×10^{-4}; for $p = 0.2$, our error is 1.1618×10^{-3}, about 20 times smaller than Barker's one.

Following exactly the same way, we can obtain the formula for ζ_n, for arbitrary n. We need however to define appropriate symbols, generalizing the previous ones for a general index n.

As the zeros of the function $\sin x/x$ occurs in $x = n\pi$, it is convenient to write the approximation polynomial for the restriction of this function on the interval $\left(\left(n-\frac{1}{2}\right)\pi, n\pi\right)$ with respect to a shifted coordinate $X_{s,n}$:

$$X_{sn} = x - n\pi \tag{35}$$

The function has an extremum point in $x = r_{s,n}$, near $\left(n-\frac{1}{2}\right)\pi$; its value in this point is:

$$M_{sn} = \frac{\sin r_{s,n}}{r_{s,n}} \tag{36}$$

We shall denote the position of the extremum point on the shifted axis by

$$X_{sn,M} = r_{s,n} - n\pi \tag{37}$$

The cubic polynomial which approximates the restriction of the function $\sin x/x$ on the interval $\left(\left(n-\frac{1}{2}\right)\pi, n\pi\right)$ can be written, in the variable $X_{s,n}$, as:

$$y\left(X_{sn}\right) = a_{sn,3}X_{sn}^3 + a_{sn,2}X_{sn}^2 + a_{sn,1}X_{sn} \tag{38}$$

We find that:

$$a_{sn,3} = -\frac{2M_{sn}}{X_{sn,M}^3} + \frac{a_{sn,1}}{X_{sn,M}^2};\ a_{sn,2} = \frac{3M_{sn}}{X_{sn,M}^2} - \frac{2a_{sn,1}}{X_{sn,M}};\ a_{sn,1} = \frac{(-1)^n}{n\pi} \tag{39}$$

With the notations:

$$A_{sn,1} = \frac{a_{sn,1}}{a_{sn,3}} - \frac{1}{3}\frac{a_{sn,2}^2}{a_{sn,3}^2} < 0;\ \ A_{sn,0}\left(x\right) = \frac{2}{27}\frac{a_{sn,2}^3}{a_{sn,3}^3} - \frac{1}{3}\frac{a_{sn,1}a_{sn,2}}{a_{sn,3}^2} - \frac{x}{a_{sn,3}} \tag{40}$$

the inverse of the restriction of the function $\sin x/x$ on the interval $\left(\left(n-\frac{1}{2}\right)\pi, n\pi\right)$ is:

$$\zeta_n\left(x\right) = n\pi - \frac{a_{sn,2}}{3a_{sn,3}} + \frac{2}{\sqrt{3}}\left|A_{sn,1}\right|^{1/2}\sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}\frac{A_{sn,0}\left(x\right)}{\left|A_{sn,1}\right|^{3/2}}\right)\right) \tag{41}$$

$$n > 1,\ \text{odd}:\ 0 < x < M_{sn};\qquad n\ \text{even}:\ M_{sn} < x < 0. \tag{42}$$

Similarly, as the zeros of the function $\cos x/x$ occurs in $x = \left(n-\frac{1}{2}\right)\pi$, it is convenient to write the approximation polynomial for the restriction of this function on the interval $\left(n\pi, \left(n-\frac{1}{2}\right)\pi\right)$ with respect to a shifted coordinate

$$X_{cn} = x - \left(n - \frac{1}{2}\right)\pi \tag{43}$$

The function has an extremum point r_{cn}, in the neighborhood of $(n-1)\pi$. In this point, having the coordinate $X_{cn,M} = r_{cn} - \left(n - \frac{1}{2}\right)\pi$ on the shifted axis, the function takes the value:

$$M_{cn} = \frac{\cos r_{c,n}}{r_{c,n}} \tag{44}$$

The cubic polynomial which approximates the restriction of the function $\cos x/x$ on the interval $\left(n\pi, \left(n-\frac{1}{2}\right)\pi\right)$ can be written, in the variable $X_{c,n}$, as:

$$y\left(X_{cn}\right) = a_{cn,3}X_{cn}^3 + a_{cn,2}X_{cn}^2 + a_{cn,1}X_{cn} \tag{45}$$

Only the coefficient $a_{cn,1}$ takes a different value:

$$a_{cn,1} = \frac{(-1)^n}{\left(n-\frac{1}{2}\right)\pi} \tag{46}$$

The coefficients $a_{cn,3},\ a_{cn,2}$ can be obtained from (39), just replacing the index s with c; the same is true for $A_{cn,1},\ A_{cn,0}$, (see eq. (40)) which enter in the final formula:

$$\xi_n(x) = \left(n - \frac{1}{2}\right)\pi - \frac{a_{cn,2}}{3a_{cn,3}} + \frac{2}{\sqrt{3}}\left|A_{cn,1}\right|^{1/2}\sin\left(\frac{1}{3}\arcsin\left(\frac{\sqrt{27}}{2}\frac{A_{cn,0}(x)}{\left|A_{cn,1}\right|^{3/2}}\right)\right) \tag{47}$$

$$n > 1 \text{ odd} : 0 < x < M_{cn}; \quad n \text{ even} : M_{cn} < x < 0 \tag{48}$$

Even if the formulas (41), (47) may seem cumbersome, this impression is due mainly by the numerical coefficients; in fact, their aspect is quite simple, see (32). The main message of our results is that the energy eigenvalues of bound states in a square well are essentially proportional with:

$$\left(a + \sin\left(\frac{1}{3}\arcsin(b\cdot p + c)\right)\right)^2 \tag{49}$$

where a, b, c, d are numerical coefficients, dependent only of the quantum number n of the bound state, and $p = 1/P$, the potential strength. Let us remember that, if we approximate the monotonic parts of the functions $\sin x/x,\ \cos x/x$ with quadratic polynomials, instead of cubic ones, the same eigenvalues are essentially proportional to [12]:

$$\left(a + \sqrt{p+b}\right)^2 \tag{50}$$

Even if both approximations use only elementary functions, it is easy to see that the solutions obtained involving cubic polynomials are much more complicated that those generated by quadratic polynomials.

The root ξ_1 cannot be approximated with a polynomial, so it cannot be obtained using this approach. However, there are quite good approximations for this function (see for instance [12]). By contrary, the root ζ_1 can be calculated with our method, even if it cannot be obtained directly from (41). The result is:

$$\zeta_1(x) = \frac{\pi (1-x)^{1/2}}{2^{1/2}} \times \frac{1}{-\frac{1}{\sqrt{3}} \sin\left(\frac{1}{3}\arcsin\left(\frac{3^{3/2}}{2^{5/2}}(1-x)^{1/2}\right)\right) + \cos\left(\frac{1}{3}\arcsin\left(\frac{3^{3/2}}{2^{5/2}}(1-x)^{1/2}\right)\right)} \quad (51)$$

and the error is typically of order of some few percentages.

4. CONCLUSIONS

The transcendental equations for the energy eigenvalues of bound states of a quantum particle in a square well are solved approximately, using an approximation of the monotonous sectors of the functions $\sin x/x$, $\cos x/x$ with cubic polynomials. This method is an improvement of a previous approach, in which second order polynomials have been used. The solution is written in terms of simple combinations of elementary functions. The result is compared with the most popular approximation used till now, and one can see that the errors of our solution are sensibly smaller. An advantage of this approach is that it is obtained with very simple mathematics, mainly at high school level. However, the solution obtained in this way gives excellent results, especially for not very small quantum numbers, for all the values of the potential strength compatible with the respective root.

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