The One Dimensional Infinite Square Well with Variable Mass

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Abstract

We introduce a numerical method to obtain approximate eigenvalues for some problems of Sturm-Liouville type. As an application, we consider an infinite square well in one dimension in which the mass is a function of the position. Two situations are studied, one in which the mass is a differentiable function of the position depending on a parameter $b$. In the second one the mass is constant except for a discontinuity at some point. When the parameter $b$ goes to infinity, the function of the mass converges to the situation described in the second case. One shows that the energy levels vary very slowly with $b$ and that in the limit as $b$ goes to infinity, we recover the energy levels for the second situation.
Mathematics Subject Classification: 81-08, 81Q10

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1 Introduction

In this paper, we introduce a method to evaluate eigenvalues for the some problems of Sturm-Liouville type. As this method should be valid in order to obtain the energy levels of some Schrödinger equations whose solutions should fulfil given boundary conditions, we were looking for an explicit example of application. One of the fields of research in physics which has recently received some attention is the study of quantum systems with variable mass[6]. Situations combining a one dimensional system with a mass jump at one point plus a point potential at the same point have been already studied by our group[3, 8, 4]. However, our principal aim in these case was looking for solvable or quasi solvable systems with resonances and the systems under the study did not have bound states. The simple system having a purely discrete spectrum capable to bear a non constant mass seems to be the one dimensional infinite square well. This is the reason why we have chosen this example in our discussion along the present paper.

As is well know, the Hamiltonian of the one dimensional infinite square well has the form (with $\hbar = 1$)

$$H = -\frac{1}{2m} \frac{d^2}{dx^2} + V(x), \text{ with } V(x) = \begin{cases} \infty & \text{if } x < -c \\ 0 & \text{if } -c < x < c \\ \infty & \text{if } x > c \end{cases}.$$  \hspace{1cm} (1)

In passing, we comment that this Hamiltonian is not self adjoint unless we fix some boundary conditions at the points $-c$ and $c$ for the wave functions in its domain. As a matter of fact, $H$ defined on its minimal domain has deficiency indices $(2, 2)$ so that its self adjoint extensions are determined by four independent real parameters. A study of these self adjoint extensions and their corresponding energy levels is available in the literature[7].

When we introduce a non constant mass a problem arises connected with the non commutation between the position and the momentum. In order to avoid it, one should replace the usual kinetic term in the Hamiltonian $K = p^2/(2m)$ by the following symmetric expression:

$$K = -\frac{1}{2} \left\{ m^\alpha(x) \frac{d}{dx} m^\beta(x) \frac{d}{dx} m^\alpha(x) \right\},$$  \hspace{1cm} (2)
Infinite square well with variable mass

with \(2\alpha + \beta = -1\). Thus, our Hamiltonian should be \(H = K + V(x)\) with
\(K\) as in (2) and \(V(x)\) as in (1).

However, this situation is too general and we should make one choice being
both simple and natural. The choice that looks more natural is probably
\(\alpha = 0, \beta = -1\). The connection of this choice with the conservation of Galilei
invariance was discussed by Levi-Leblond[11] and on this Galilei invariance is
already a basis to make it.

Assume first that the mass is a differentiable function \(m(x)\) of the posi-
tion. Then after a simple calculation, one shows that the time independent
Schrödinger equation \(H \varphi = E \varphi\) is given inside the interval \([-c, c]\) by
\[
\frac{1}{m(x)} \varphi''(x) - \frac{m'(x)}{m^2(x)} \varphi'(x) + 2E \varphi(x) = 0 \quad (3)
\]
and zero otherwise. Here, we may use the standard boundary condition at the
borders: \(\varphi(-c) = \varphi(c) = 0\) to obtain solutions of the eigenvalue problem.

A second possibility is the assumption of a constant mass except for a
discontinuity at some point, say \(a \in [-c, c]\) (we may take \(a = 0\), but also there
is no need for the interval to be \([-c, c]\), it may also be \([0, c]\) or any other). In
this case, along boundary conditions at the border, we should give matching
conditions at the point \(a\). Here, we use again \(\varphi(-c) = \varphi(c) = 0\). Then, we
need to fix the matching conditions at \(a\) (we henceforth assume that \(a = 0\) for
simplicity). In a previous paper[3], it was shown that the choice \(\alpha = 0, \beta = 1\)
along the additional condition
\[
\frac{1}{m_2} \varphi'(0+) - \frac{1}{m_2} \varphi'(0-) = 0, \quad (4)
\]
where \(\varphi'(0+)\) and \(\varphi'(0-)\) are the right and left limits of the wave function
\(\varphi(x)\) at the origin, gives the following expression for the kinetic term \(K\):
\[
K = \begin{cases} 
-\frac{1}{2m_1} & \text{if } x < 0 \\
-\frac{1}{2m_2} & \text{if } x > 0 
\end{cases} \quad (5)
\]

The problem of the self adjoint extensions of (5) was discussed earlier[12].
In order to fix a proper self adjoint choice for our Hamiltonian, in addition
to the boundary values at the borders we need to settle matching conditions
at the point at which we have the mass discontinuity. These conditions are
relations between the left and right limits of the function and its first derivative.
Then along (4), we can use the continuity of the wave function. The resulting
matching conditions can be written as
\[
\begin{pmatrix} \varphi(0+) \\ \varphi'(0+) \end{pmatrix} = T \begin{pmatrix} \varphi(0-) \\ \varphi'(0-) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{m_2}{m_1} \end{pmatrix} \begin{pmatrix} \varphi(0-) \\ \varphi'(0-) \end{pmatrix}. \quad (6)
\]
The self-adjointness of the Hamiltonian is determined by both, boundary and matching conditions. In particular, matching conditions are determined by the matrix $T$ in (6), which should verify the following relation:

$$M_1 = T^\dagger M_2 T, \quad M_i = \frac{1}{2m_i} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad i = 1, 2.$$ (7)

$T^\dagger$ denotes the adjoint matrix of $T$. The general solution of the Schrödinger equation under the above conditions is given by

$$\varphi(x) = A \sin(k_1(c + x))H(-x) + B \sin(k_2(c - x))H(x),$$ (8)

where $A$ and $B$ are constants, $H(x)$ is the Heaviside step function and

$$k_i = \sqrt{2m_i E}, \quad i = 1, 2.$$ (9)

Note that $\varphi(-c) = \varphi(c) = 0$ so that the required boundary conditions are satisfied. The given (6) matching conditions applied to (8) give:

$$A \sin(k_1 c) = B \sin(k_2 c) \implies B = A \frac{\sin(k_1 c)}{\sin(k_2 c)}$$ (10)

$$\frac{A k_1}{m_1} \cos(k_1 c) = \frac{B k_1}{m_2} \cos(k_2 c) \implies$$

$$\frac{k_1}{m_1} \cos(k_1 c) = \frac{k_1}{m_2} \frac{\sin(k_1 c)}{\sin(k_2 c)} \cos(k_2 c).$$ (11)

This and (9) give the following transcendental equation for $E$:

$$\sqrt{m_2} \tan[c \sqrt{2m_2 E}] = \sqrt{m_1} \tan[c \sqrt{2m_1 E}].$$ (12)

It is noteworthy that equation (12) gives the energy levels for any one dimensional infinite square well of width $2c$ with a jump of mass at the middle point and masses $m_1$ and $m_2$ (with jump $\Delta := m_2 - m_1$), because of this system is invariant under translation. Therefore, formula (12) given the energy levels is valid if the interval were $[0, 2c]$ instead $[-c, c]$, for instance. We shall take into account this fact in our explicit calculations.

This paper is organized as follows: In Section 2, we introduce the method for obtaining the energy levels and in Section 3, we compare our method to other methods. In Section 4, we apply our method to a situation in which the dependence of the mass with the position is differentiable. Furthermore, the function of mass depends on an additional parameter $b$ such that in the limit $b \to \infty$ we obtain the coordinate dependence of the mass given by $m(x) = m_1 H(-a) + m_2 H(x)$, i.e., a constant mass except for a discontinuity
at one point, say $a$. This is interesting as the energy levels for the continuous distribution of mass converge to the energy levels for the limit case.

\section{A Method for the Determination of the Eigenvalues}

Along the present section, we shall develop a method to solve numerically the equations that will arise in the problem described here. These equations are of the following type:

$$y''(x) = F_{\lambda}(x, y(x), y'(x)).$$  \hspace{1cm} (13)

This equation depends explicitly of the eigenvalue $\lambda$ to be determined, as is exactly the case of the (time independent) Schrödinger equation. Here, $x \in I \equiv [a, b]$. We assume that the following conditions hold:

$$c_1 y(a) + c_2 y'(a) = c_3, \quad d_1 y(b) + d_2 y'(b) = d_3,$$  \hspace{1cm} (14)

where the constants $c_k$ and $d_k$, $k = 1, 2, 3$ are known. Note that this problem is just a generalization of Sturm-Liouville.

A variety of methods for solving this problem ((13) with (14)) exist. One of the most efficient is the Differential Transformation Method (DTM)[9, 1, 14, 5, 15]. This method is beautiful, elegant and, in many cases, effective. However, its practical implementation requires numerical determination of roots, a calculation which is sometimes tedious, particularly in the case of non-linear equations.

We are introducing another method to solve numerically ordinary differential equations, which has been suggested to us by our experience in the use of the software Mathematica. A version of this method was designed to approximate periodic solutions [13].

We hereby describe the method and use it for the numerical study of the infinite square well with a variable mass.

Our method is based in the approximation of the solution $y(x)$ by means of Taylor polynomials whose order depends on the desired degree of accuracy. In order to perform the expansion on the finite Taylor series, we need to impose the condition that $F_{\lambda}(x, y, y')$, where $\lambda$ denotes a parameter, be analytic or at least differentiable up to the necessary order on the interval $[a, b]$. Contrary to the usual procedure in the DTM, we do not determine algebraically the coefficients in the Taylor polynomial, but instead we calculate them analytically, often with the help of a software for symbolic calculus.

The second difference between our method and the DTM can be explained as follows: when searching for solutions to ODE with given boundary conditions we often find periodic solutions which cannot be accurately approximated.
by a unique Taylor polynomial on the whole integration interval. When solving (13) subject to conditions (14), this problem has the following cure:

Let us divide the integration interval \([a, b]\) into \(m\) subintervals with the same length by taking the points \(x_k = a + kh\) with \(h = (b - a)/n, k = 1, 2, \ldots, m\). Here the number \(m\) of subintervals depends on the precision we want. Then, let us write (13) as the following system:

\[
y'(x) = z(x), \quad z'(x) = F_\lambda(x, y(x), y'(x)).
\]

(15)

Then on each interval \((x_k, x_{k+1})\), we approximate the functions \(y(x)\) and \(z(x)\) by respective Taylor polynomials as follows:

\[
y_n(x) = \sum_{j=0}^{n} \frac{1}{j!} y^{(j)}(x_k)(x - x_k)^j,
\]

\[
z_n(x) = \sum_{j=0}^{n} \frac{1}{j!} z^{(j)}(x_k)(x - x_k)^j,
\]

(16)

where we determine the derivatives \(y^{(j)}\) and \(z^{(j)}\) by means of (15), i.e., \(y^{(1)}(x) = z(x), y^{(2)}(x) = F_\lambda(x, y(x), z(x)), y^{(3)}(x) = \partial F_\lambda/\partial x + z \partial F_\lambda/\partial y + F_\lambda \partial F_\lambda/\partial z\) and so on up to the desired derivative. Similarly, we obtain the successive derivatives of \(z(x)\).

Then, starting with the first equation in (15), we obtain the initial values to obtain \(y_n(x)\) and \(z_n(x)\) on the interval \([x_0, x_1]\), which are parameterized by the eigenvalue \(\lambda\). Then, we know the values \(y_n(x_1)\) and \(z_n(x_1)\) which allow us to construct \(y_n(x)\) and \(z_n(x)\) on the interval \([x_1, x_2]\) and so on.

After obtaining the approximation for the last interval, we note that the second equation in (13) gives us the condition \(d_1 y(x_m) + d_2 z(x_m) = d_3\) with \(x_m = b\), which gives an algebraic equation in \(\lambda\). Then, the roots of this equation are the eigenvalues we search for.

Once we have chosen one of these eigenvalues, the segmentary solutions are well defined. The values of \(n\) and \(m\) should be determined by practice depending on the desired accuracy.

For the above calculations we use the software Mathematica.

3 Comparison with the Results Obtained by other Authors

Along the present section, we compare our results to the results obtained by the DTM method as introduced in some papers[9, 1]. Take for instance a
problem considered by Chao Kuang Chen and Shing Huei Ho[9], the differential equation with boundary conditions given by

\[ y''(x) + \lambda x^2 y(x) = 0, \quad y(0) = y(1) = 0. \]  

(17)

Here, the solution is given by

\[ y(x) = \frac{\Gamma(1/4)}{2 \times 2^{1/4} \lambda^{1/4} \sqrt{\pi}} \left( D_{-1/2} \left( (-1 + i) \frac{\lambda^{1/4}}{x} \right) - D_{-1/2} \left( (1 + i) \frac{\lambda^{1/4}}{x} \right) \right), \]  

(18)

where \( D_{\nu}(x) \) is the parabolic cylindric function\(^1\) of index \( \nu \) and \( \Gamma(x) \) is the Gamma function. Starting with (18) and the roots of the transcendental equation \( y(0) = 1 \), we obtain numerical values for the eigenvalues \( \lambda_{\text{exact}} \). Note that Taylor expansion of (18) on a neighborhood of zero has only the odd powers \( x^{4k-3} \) with \( k = 1, 2, \ldots \).

Now, let us go back to the method introduced in the previous section. Take the interval \([0, 1] \) and divide it into only one interval, so that \( m = 0 \). Then, let us determine the solutions of (17) for different values of \( n \). First of all, let us determine the the smallest eigenvalue. Its “exact” value is 30.9333. Then, we obtain

\[
\begin{array}{cccccc}
 n & 13 & 17 & 21 & 25 & 29 \\
 \lambda_n & 30.2370 & 30.9921 & 30.9303 & 30.9335 & 30.9333 \\
 \Delta y & - & 0.75 & -0.062 & 0.0032 & -0.0002 \\
 \epsilon_r, \% & 2 & 2 \times 10^{-1} & 1 \times 10^{-2} & 5 \times 10^{-4} & 1 \times 10^{-4} \\
\end{array}
\]

Table 1

Here, \( \Delta y \) denotes the differences \( \lambda_{17} - \lambda_{13} \), then, \( \lambda_{21} - \lambda_{17} \) and so on and \( \epsilon_r, \% \) is the modulus of the relative difference between \( \lambda_{\text{exact}} \) and the eigenvalue \( \lambda_n \) as given in the above table. These results are equivalent to those obtained by Chao Kuang Chen and Shing Huei Ho[9]. In order to implement our method, we have used Mathematica and the CPU times in a regular computer are less than a second. Since the exact solution is known, we can estimate the difference between solutions by means of the error parameter, here named as error for simplicity, defined as

\[ D_n = \int_0^1 \left( y_{\text{exact}}(x) - y_n(x) \right)^2 dx. \]  

(19)

\(^1\)This is a solution of the equation \( y'' + (\nu + 1/2 - x^2/4)y = 0 \), see [2].
For instance, for the first eigenvalue, according to Table 1, we obtain: $D_{13} = 2 \times 10^{-5}$ and $D_{12} = 4 \times 10^{-10}$. We see that this error is quite small.

Using (16), we can obtain the approximate eigenfunction for $n = 21$, which is

$$y = x - 1.54652 x^5 + 0.664364 x^9 - 0.131724 x^{13} + 0.0149789 x^{17} - 0.0011031 x^{21},$$

(20)

while the result obtained in the before mentioned paper[9] was:

$$y = x - 1.5465 x^5 + 0.664351 x^9 - 0.13172 x^{13} + 0.0149783 x^{17} - 0.00110305 x^{21}.$$  (21)

Here, the authors obtain $D_{21} = 5 \times 10^{-10}$ a result that our method slightly improves.

For the second eigenvalue, whose “exact” result is 139.530, we obtain:

<table>
<thead>
<tr>
<th>$n$</th>
<th>29</th>
<th>33</th>
<th>37</th>
<th>41</th>
<th>45</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_n$</td>
<td>141.889</td>
<td>139.315</td>
<td>139.549</td>
<td>139.529</td>
<td>139.530</td>
</tr>
<tr>
<td>$\Delta y$</td>
<td>–</td>
<td>–2.6</td>
<td>0.21</td>
<td>–0.02</td>
<td>0.001</td>
</tr>
<tr>
<td>$\epsilon_r,%$</td>
<td>$2 \times 10^{-2}$</td>
<td>$110^{-3}$</td>
<td>$110^{-4}$</td>
<td>$810^{-6}$</td>
<td>$110^{-6}$</td>
</tr>
</tbody>
</table>

Table 2

Here, the errors are given by $D_{29} = 1 \times 10^{-5}$ and $D_{45} = 2 \times 10^{-14}$.

Now, we want to estimate the third eigenvalue. In the DTM, we need to increase the degree $n$ of the polynomial. With our method, we can make use of the numbers $m$ and $n$ to obtain a sufficient accuracy for a bigger number of eigenvalues. For instance, if we take $m = 10$ and $n = 10$, we can obtain the values of the seven first eigenvalues of a reasonable precision. In the next table, we give the errors that our method shows in relation with the exact results for the seven first eigenvalues:

<table>
<thead>
<tr>
<th>eigenvalue</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon_r,%$</td>
<td>$2 \times 10^{-4}$</td>
<td>$7 \times 10^{-5}$</td>
<td>$2 \times 10^{-4}$</td>
<td>$3 \times 10^{-3}$</td>
<td>$2 \times 10^{-2}$</td>
<td>$1 \times 10^{-2}$</td>
<td>$6 \times 10^{-1}$</td>
</tr>
</tbody>
</table>

Table 3
Finally, we shall compare our method to the standard method of the determination of the eigenvalues by the method of the polynomial[10]. This is a numerical resolution of equation (15) by replacing the second derivative by an approximation by finite divided and centered differences. This generates a homogenous system of equations. The expansion of the determinant of the coefficient matrix produces a polynomial such that its real roots are the desired eigenvalues.

For the first eigenvalue, the method of the polynomial gives the following results:

\[
\begin{array}{ccc}
n & 200 & 500 & 1000 \\
\lambda & 30.9324 & 30.9332 & 30.9333 \\
\epsilon_r \% & 3 \times 10^{-3} & 5 \times 10^{-4} & 1 \times 10^{-4} \\
\end{array}
\]

Table 4

For the second eigenvalue, the method of the polynomial gives the following results:

\[
\begin{array}{ccc}
n & 200 & 500 & 1000 \\
\lambda & 139.510 & 139.527 & 139.529 \\
\epsilon_r \% & 1 \times 10^{-2} & 3 \times 10^{-2} & 5 \times 10^{-4} \\
\end{array}
\]

Table 5

From the results of Table 4 and Table 5, we conclude that in order to obtain the level of precision reached in the results given in Table 1 and Table 2, the polynomial method requires a large number of nodes than in the method proposed in Section 2. In addition, CPU times are significantly higher. Furthermore, if we want to find the eigenvalues next to the second, we need to add more nodes and consequently the CPU time.

As a conclusion, we have introduce an alternative to calculation to powerful methods such that, by using the software of symbolic calculus (we have used Mathematica), it shows a really simple implementation that can be even useful for a beginner. In addition, it has the advantage that the few former eigenvalues can be obtained with a Taylor polynomial of rather low degree and small CPU times.

4 Infinite Square Well with Variable Mass

Along this section, we shall apply the numerical formalism here introduced in the study of the energy levels of the infinite square well with a variable mass. We consider two possibilities:
i.) A mass jump as described in the Introduction. If the mass jump is located at the point \(a\), the mass function in terms of the position can be written, inside the interval with zero potential as

\[ m_{\infty}(x) = m_1 H(a-x) + m_2 H(x-a) = m_1 + (m_2 - m_1) H(x-a), \]

where \(H(\omega)\) is the Heaviside step function.

ii.) As a previous exercise, we shall approximate the mass jump by a differentiable mass function \(m_b(x)\), depending on a parameter \(b\), with the condition

\[ \lim_{b \to \infty} m_b(x) = m_{\infty}(x). \quad (22) \]

Thus, let us study first the Schrödinger equation (3) in which the well interval has been chosen to be \([0, 1]\) instead of \([-1/2, 1/2]\), \(c = 1\) for simplicity in our calculations. Note that the energy levels should be invariant under space translations, so that our results will be equally valid for any interval of width 1.

Now, we construct the function of mass \(m_b(x)\) as follows: Take the function

\[ g_b(x) := \frac{1}{1 + e^{-b(x-1/2)}}. \quad (23) \]

Observe that

\[
\begin{align*}
\text{if} & \quad x > 1/2 \quad \lim_{b \to \infty} g_b(x) \to 1 \\
\text{if} & \quad x = 1/2 \quad g_b(1/2) = 1/2 \\
\text{if} & \quad x < 1/2 \quad \lim_{b \to \infty} g_b(x) \to 0.
\end{align*}
\]

Therefore,

\[ \lim_{b \to \infty} \frac{1}{1 + e^{-b(x-1/2)}} = H(x - 1/2) \quad (25) \]

pointwise. Consequently, if we define

\[ m_b(x) := m_1 + \frac{m_2 - m_1}{1 + e^{-b(x-1/2)}} \quad (26) \]

then,

\[ \lim_{b \to \infty} m_b(x) = m_1 + (m_2 - m_1) H(x - 1/2) = m_{\infty}(x). \quad (27) \]

Now, take \(m_b(x)\) as defined in (26) and use it as a particular realization of \(m(x)\) in the Schrödinger equation (3). We intend to solve numerically this equation for given values of the parameters. Our first choice is \(m_1 = 1\), \(\Delta := m_2 - m_1 = 1\) and \(b = 10\). We have to use the boundary values of wave functions at the points 0 and 1. To be consistent with the comments in the Introduction, these boundary values should be \(\varphi(0) = \varphi(1) = 0\). Then, we determine the solutions using the method described in Sections 2 and 3.
Then, in order to initiate the iterative process as described in equation (16), let us take the initial values \( y(0) = \varphi(0) = 0 \) and \( z(0) = \varphi'(0) = 1 \) (observe that the value of the derivative \( \varphi'(0) \) can be somehow arbitrarily chosen as it affects to the norm of the wave function only). Following Section 2, results depend on two parameters: \( n \) the chosen degree of the polynomial and \( m \) the number of intervals which divide the integration domain (here \([0, 1]\)).

In the next table, we show as an example the values of the first \( E_1 \) and the fifth \( E_5 \) eigenvalues of the energy in terms of the parameters \( n \) and \( m \). The first column gives the values of \( n \) and the first row the values of \( m \).

Thus, for \( E_1 \), we have

<table>
<thead>
<tr>
<th>( n )</th>
<th>( m )</th>
<th>50</th>
<th>60</th>
<th>80</th>
<th>100</th>
<th>300</th>
<th>600</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>3.5540</td>
<td>3.5417</td>
<td>3.52712</td>
<td>3.51878</td>
<td>3.49804</td>
<td>3.49321</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>3.48446</td>
<td>3.48567</td>
<td>3.48690</td>
<td>3.48745</td>
<td>3.48837</td>
<td>3.48845</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>3.48841</td>
<td>3.48844</td>
<td>3.48847</td>
<td>3.48847</td>
<td>3.48848</td>
<td>3.48848</td>
</tr>
</tbody>
</table>

Table 6

For \( E_5 \) the values we have obtained are

<table>
<thead>
<tr>
<th>( n )</th>
<th>( m )</th>
<th>50</th>
<th>60</th>
<th>80</th>
<th>100</th>
<th>300</th>
<th>600</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>91.6682</td>
<td>89.3794</td>
<td>87.1101</td>
<td>86.0380</td>
<td>84.1501</td>
<td>83.8877</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>81.1658</td>
<td>81.8829</td>
<td>82.6441</td>
<td>83.0145</td>
<td>83.6271</td>
<td>83.6867</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>83.6004</td>
<td>83.6506</td>
<td>83.6860</td>
<td>83.6970</td>
<td>83.7064</td>
<td>83.7066</td>
</tr>
</tbody>
</table>

Table 7

In both tables, we can appreciate the convergence either if we fix \( n \) and increase \( m \) or viceversa. As one could have expected, the bigger \( n \) the smaller the number of \( m \) to achieve similar accuracy.

If we take the resulting values for \( n = 3 \) and \( m = 600 \) as reference values, then we may compare the percentual relative difference between the reference value and those obtained for \( m = 50 \). The results are given in the following table:

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_1 )</th>
<th>( E_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2 %</td>
<td>10%</td>
</tr>
<tr>
<td>2</td>
<td>0.1%</td>
<td>3%</td>
</tr>
<tr>
<td>3</td>
<td>0.001%</td>
<td>0.1%</td>
</tr>
</tbody>
</table>

Table 8
This shows that for the five first eigenvalues of the energy, at least, a good choice could be $n = 3$, $m = 50$. It is also interesting to remark that the approximation given by formula (28) below gives 6% for $E_1$ and 2% for $E_5$. This choice gives CPU times lower than two seconds in a computer AMD Athlon II X2 250 3.00 GHz, RAM 4 GB using Mathematica software.

4.1 Dependence of the mass on the parameter $b$.

Next, we analyze the behavior of the energy spectrum under changes on the values of the mass parameters. Take again $m_1 = 1$ and let us evaluate the ten first energy levels for different values on the difference $\Delta = m_2 - m_1$. We have moved $b$ along the interval $(0.05, 200)$ and along $(0.0, 3.0)$. The dependence of the energy levels does not depend significantly on $b$ within the considered interval. Contrarily, the variation of the energy levels with $\Delta$ behave according to the law

$$E_k \approx \frac{(k\pi)^2}{2 + \Delta}, \quad k = 1, 2, \ldots, 10,$$

with a relative error smaller than 8%.

In Figure 1, we show the value of the energy levels for different values of $\Delta$. The blue curve corresponds to $\Delta = 0$ (constant mass). Below, we plot the curves for $\Delta = 0.1, 1.0$ and 3.0. Curves obtained with formula (28) match with curves obtained numerically. This Figure remains essentially unaltered if we modify the values of $b$ from 0.05 to 50. Although the energy spectrum is discrete this continuous representation of the energy levels seem to be very explicative by itself.
4.2 Constant mass with jump at $x = 1/2$.

We discuss here the model of the infinite square well with a mass dependence on the position given by $m_\infty(x)$ as in (27). The equation we have to solve here is (12) with $c = 1/2$. Let us choose $m_1 = 1$. Then, the particular form of (12) becomes:

$$\sqrt{m_2} \tan \left[ \sqrt{m_2} \sqrt{\frac{E}{2}} \right] = \tan \left[ \sqrt{\frac{E}{2}} \right]$$

(29)

In the simple case in which we choose $m_2 = n^2$, i.e., the square of a natural number, this equation is explicitly solvable and gives:

$$E_k = 2(k\pi)^2, \quad k = 0, 1, 2, \ldots.$$ 

(30)

In addition, if we choose the mass jump $\Delta = m_2 - m_1$ to be smaller than three, the energy levels can be approximated quite reasonably by the following formula:

$$E_k^* = \frac{(k\pi)^2}{2 + \Delta}, \quad k = 0, 1, 2, \ldots.$$ 

(31)

Take, for instance $\Delta = 1$ ($m_2 = 2$) and compare the roots of (31) to the roots obtained from (29). We compare these results on Table 9, in which $E_r\%$ determines the percentual relative variation of $E_k^*$ with respect to $E_k$:

<table>
<thead>
<tr>
<th>$k$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>20</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_k$</td>
<td>3.5846</td>
<td>12.909</td>
<td>31.602</td>
<td>52.937</td>
<td>85.448</td>
<td>341.514</td>
<td>328.987</td>
<td>1362.00</td>
</tr>
<tr>
<td>$E_k^*$</td>
<td>3.290</td>
<td>13.159</td>
<td>29.609</td>
<td>52.638</td>
<td>82.247</td>
<td>328.99</td>
<td>740.22</td>
<td>1316.00</td>
</tr>
<tr>
<td>$E_r%$</td>
<td>8</td>
<td>2</td>
<td>6</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>4</td>
<td>3</td>
</tr>
</tbody>
</table>

Table 9

Another example is given in Table 10. Take the first eigenvalue of equation (29) as given by (31). This eigenvalue is $E_1^* = 3.5846$. Let us use the method described in Section 2 for the determination of the eigenvalue of (3) with mass dependence in the coordinate given by (26) and $\Delta = m_2 - m_1 = 1$. We use the integration parameters $n = 3$ and $m = 600$. On Table 10, we show the dependence of the value of the first energy level $E_1$ in terms of the parameter $b$ in (26). We also include the relative error, $\varepsilon_r\%$ defined above.

The results are:

<table>
<thead>
<tr>
<th>$b$</th>
<th>10</th>
<th>50</th>
<th>100</th>
<th>200</th>
<th>500</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1$</td>
<td>3.48847</td>
<td>3.57912</td>
<td>3.5835</td>
<td>3.58423</td>
<td>3.58460</td>
</tr>
<tr>
<td>$\varepsilon_r%$</td>
<td>3</td>
<td>2.10^{-1}</td>
<td>3.10^{-2}</td>
<td>1.10^{-2}</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 10

We note how close are the results obtained by our method to the empirical results given by formulas (29) and (31).

5 Concluding Remarks

We have proposed one method to obtain the energy levels of a given Hamiltonian with purely discrete spectrum. We have applied it to calculate the energy levels of the one dimensional infinite square well with variable mass. The mass is written as a function of position. We have considered two possibilities, one in which the mass is a continuous and even differentiable function of the position and in the other the mass is constant except for a jump at the middle of the well. In addition, the continuous function of mass depends on one parameter so that when this parameter goes to infinite the function of mass goes to the second case of constant mass with a jump. Our numerical calculations show that also the energy levels for the continuous mass case go to the energy levels for the mass jump case.

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References


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