A study of the bound states for square potential wells with position-dependent mass

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A square potential well with position-dependent mass is studied for bound states. Applying appropriate matching conditions, a transcendental equation is derived for the energy eigenvalues. Numerical results are presented graphically and the variation of the energy of the bound states are calculated as a function of the well-width and mass.

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I. INTRODUCTION

The concept of position-dependent mass comes from effective-mass approximation of many-body problem in condensed matter physics [1-8]. In recent times a good number of articles have been published in this field. The Schrödinger equation with position-dependent mass has been studied in the contexts of supersymmetry, shape-invariance, Lie algebra, point-canonical transformation, etc. It is well known that the kinetic energy operator in this case belongs to the two-parameter family [9]

\[ T(x) = \frac{1}{4} \left( m^\alpha p m^\beta p m^\gamma + m^\gamma p m^\beta p m^\alpha \right) , \] (1.1)

where \( m = m(x) \) and \( p = -i\hbar d/dx \), with the constraint

\[ \alpha + \beta + \gamma = -1. \] (1.2)

However, the correct values of the parameters \( \alpha, \beta, \gamma \) for a specific model is a long-standing debate [3-8]. For example, in the case of a potential step and barrier [8], as well as the discrete spectrum [9], are different compared to the constant-mass problem.

In this article we are going to study the following physical problem: the potential energy has the form of a well, both in symmetric as well as asymmetric form, and the kinetic energy is given by [1] with a mass function \( m(x) \) which has different constant values inside and outside the well. This problem has also interest from the point of view of applications in carbon nanotubes and quantum dots, as can be seen in [20, 21]. Our purpose is first to find an ordering of the kinetic energy term appropriate to this problem, and then, to study in full detail the bound states of this model and to compare the results with the conventional constant-mass case.

Several problems which resemble our model have been considered previously in the literature. For example, the scattering states of a potential step or barrier were studied in [8, 22]. Other special square well potentials were analysed in [22], and the bound states for some finite and infinite wells were studied using other kinetic energy operator and matching conditions in [8]. However, our approach is different from the very beginning because we propose an ordering for kinetic term based on a specific argument for the matching conditions. This ordering is also used in [24] for studying connection rules for effective-mass wave functions across an abrupt heterojunction.

The structure of this article is as follows. Sec. II is devoted to fix the ordering in the kinetic term. In Sec. III a transcendental equation determining the energy values for the bound states in the case of a potential energy well is derived. The numerical results are shown graphically and discussed in Sec. IV. Finally, Section V contains the conclusions of our work.

II. MATCHING CONDITIONS AT THE DISCONTINUITIES OF THE MASS AND POTENTIAL FUNCTION

The Hamiltonian operator for the position-dependent mass problem is given by

\[ H = T(x) + V(x) \] (2.1)

where \( T(x) \) is the operator defined in [1] and \( V(x) \) denotes the potential term. The one-dimensional time-independent Schrödinger equation for the stationary
states is

\[ H \psi(x) = E \psi(x). \]  \tag{2.2}

Substituting \( m' \) and \( m'' \) into Eq. (2.2) and taking units such that \( \hbar^2 = 2 \), we get the Schrödinger equation for the generalized kinetic energy operator

\[ \frac{d^2 \psi}{dx^2} - \frac{m'}{m} \frac{d \psi}{dx} + \left[ \frac{1}{2} \left( \nu \frac{m''}{m} - \eta \frac{m'}{m^2} \right) + m(E - V) \right] \psi = 0 \]  \tag{2.3}

where

\[ \eta = \alpha(\gamma + 2) - \gamma(\alpha + 2), \quad \nu = \alpha + \gamma, \]  \tag{2.4}

and \( m' = dm/dx \). If in Eq. (2.5) we make the following transformation

\[ \psi(x) = m(x)^{1/2} \theta(x) \]  \tag{2.5}

we can eliminate the first order derivative of \( \psi \) with respect to \( x \), to arrive at

\[ \frac{d^2 \theta}{dx^2} \left[ 1 + \nu \frac{m''}{2m} - \left( \frac{3}{4} - \frac{\eta}{2} \right) \frac{m'}{m^2} + m(E - V) \right] \theta = 0. \]  \tag{2.6}

Our aim is to generalize the usual matching conditions for the wave function \( \psi(x) \) suitable for this position-dependent mass problem. We will focus on the case of mass discontinuities.

A. Matching conditions

Now, let us assume that the mass \( m(x) \) has a finite discontinuity at \( x = a \) of the form

\[ m(x) = m_1(x) \Theta(-x + a) + m_2(x) \Theta(x - a) \]  \tag{2.7}

where \( m_1(x) \) and \( m_2(x) \) are smooth functions and the unit step function \( \Theta(x) \) is defined as

\[ \Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases} \]  \tag{2.8}

If we use Eq. (2.7) in Eq. (2.6), we see that it leads to strong discontinuities at \( x = a \) as well as some terms that require a careful interpretation. For instance, we should take into account that \( \Theta'(x) \equiv d\Theta(x)/dx = \delta(x) \), where \( \delta(x) \) denotes the Dirac delta distribution. In order to eliminate these problems in Eq. (2.6), we can choose

\[ 1 + \nu = 0, \quad \frac{3}{4} + \frac{\eta}{2} = 0, \]  \tag{2.9}

where \( \eta \) and \( \nu \) were given in Eq. (2.4). From these conditions, we obtain the values of the parameters \( \alpha = \gamma = -\frac{1}{2} \) and \( \beta = 0 \). With such values, the kinetic energy operator Eq. (2.6) takes the following simple form

\[ -\frac{d^2 \theta}{dx^2} + m(V - E) \theta = 0. \]  \tag{2.11}

Now, it is easy to get the matching conditions for \( \theta \) at \( x = a \). To do this, first we integrate Eq. (2.11) around the discontinuity point \( x = a \)

\[ \theta'(a + h) - \theta'(a - h) = \int_{a-h}^{a+h} m(x)(V(x) - E) \phi(x) \, dx. \]  \tag{2.12}

In the interval \((a-h, a+h)\), the functions \( m(x) \) and \( V(x) \) have finite discontinuities at \( x = a \) and \( \phi(x) \) is bounded. Therefore, when \( h \) goes to zero, the integral at the r.h.s. of Eq. (2.12) tends to zero. This means that \( \phi'(x) \) (and also \( \phi(x) \)) will be continuous at \( x = a \). In conclusion, using the transformation Eq. (2.5) we have arrived at the following matching conditions: the wave function \( \psi(x) \) is such that the two functions \( \psi(x)/\sqrt{m(x)} \) and \( (\psi(x)/\sqrt{m(x)})' \) are continuous at \( x = a \). Mathematically it may be expressed as

\[ \left. \frac{\psi(x)}{\sqrt{m(x)}} \right|_{x=a} = \left. \frac{\psi(x)}{\sqrt{m(x)}} \right|_{x=a+h} = \left. \frac{\psi(x)}{\sqrt{m(x)}} \right|_{x=a-h} = \left. \frac{\psi(x)}{\sqrt{m(x)}} \right|_{x=a}. \]  \tag{2.13}

where \( a \) is an interior point in the domain of the problem. It is straightforward to check that the above conditions are consistent with the definition of a time-independent inner product in the space of square integrable eigenfunctions \( \langle \psi(x), \phi(x) \rangle = \int \psi(x)^* \phi(x) \, dx \), as well as with the conservation of the current density

\[ j(x) = -i \left( \psi(x)^* \frac{1}{m(x)} \frac{d \psi(x)}{dx} - \frac{d \psi(x)^*}{dx} \frac{1}{m(x)} \psi(x) \right). \]  \tag{2.14}

It is clear that these matching conditions are consistent with the Hermitian character of the Hamiltonian Eq. (2.1) with \( \Theta(x) \). We should stress that the above mentioned boundary conditions indeed define a self-adjoint problem (this issue will be addressed in detail elsewhere).

III. A SQUARE POTENTIAL WELL AND A STEP MASS

A. Asymmetric well

Let us consider an asymmetric well of the form

\[ V(x) = \begin{cases} V_1, & x < -a \\ 0, & |x| < a \\ V_2, & a < x \end{cases} \]  \tag{3.1}
with the position-dependent mass
\[ m(x) = \begin{cases} m_1, & |x| > a \\ m_2, & |x| < a \end{cases} \]  
(3.2)

where \( m_1, m_2, V_1, \) and \( V_2 \) are constants such that \( V_2 \geq V_1, m_1, m_2 > 0, \) and \( m_1 \neq m_2. \) Next, we will study the bound states \( (0 < E < V_1 \leq V_2) \) for this problem using the matching condition obtained in the previous section.

The Schrödinger equation \( 2.3 \) for the wavefunction \( \psi(x) \) has the following form in each region
\[ \frac{d^2 \psi}{dx^2} - k_1^2 \psi = 0, \ k_1 = \sqrt{m_1(V_1 - E)}, \ x < -a, \]  
(3.3)
\[ \frac{d^2 \psi}{dx^2} + k_2^2 \psi = 0, \ k_2 = \sqrt{m_2 E}, \ |x| < a, \]  
(3.4)
\[ \frac{d^2 \psi}{dx^2} - k_3^2 \psi = 0, \ k_3 = \sqrt{m_1(V_2 - E)}, \ x > a. \]  
(3.5)

The physical solutions of these equations take the form
\[ \psi(x) = \begin{cases} A e^{k_1 x}, & x < -a \\ C \sin(k_2 x + \theta), & |x| < a \\ B e^{-k_3 x}, & x > a \end{cases} \]  
(3.6)

where \( A, B, C, \) and \( \theta \) are constants to be determined by the boundary and matching conditions. Using the continuity conditions \( 2.13 \) for this solution at \( x = -a, \) we obtain the following two equations
\[ A \left( \frac{m_2}{m_1} \right)^{1/2} e^{-k_1 a} = C \sin(-k_2 a + \theta) \]  
(3.7)
\[ A \left( \frac{m_2}{m_1} \right)^{1/2} k_1 e^{-k_1 a} = C k_2 \cos(-k_2 a + \theta) \]  
(3.8)

and at \( x = a, \) we get
\[ B \left( \frac{m_2}{m_1} \right)^{1/2} e^{-k_3 a} = C \sin(k_2 a + \theta) \]  
(3.9)
\[ B \left( \frac{m_2}{m_1} \right)^{1/2} k_3 e^{-k_3 a} = C k_2 \cos(k_2 a + \theta). \]  
(3.10)

From these four equations, we find
\[ k_1 = k_2 \cot(-k_2 a + \theta), \quad k_3 = -k_2 \cot(k_2 a + \theta) \]  
(3.11)

or
\[ \sin(-k_2 a + \theta) = \frac{k_2}{\sqrt{m_1 V_1 - k_2^2 (\frac{m_1}{m_2} - 1)}} \]  
(3.12)
\[ \sin(k_2 a + \theta) = \frac{k_2}{\sqrt{m_1 V_2 - k_2^2 (\frac{m_1}{m_2} - 1)}} \]  
(3.13)

Now, if we eliminate \( \theta \) from \( 3.12 \) and \( 3.13, \) we get the transcendental equation
\[ 2k_2 a = n\pi - \sin^{-1} \frac{k_2}{\sqrt{m_1 V_1 - k_2^2 (\frac{m_1}{m_2} - 1)}} - \sin^{-1} \frac{k_2}{\sqrt{m_1 V_2 - k_2^2 (\frac{m_1}{m_2} - 1)}}, \]  
(3.14)

where inside the well, the momentum \( k_2 \) of the bound states is obtained from the values \( n = 1, 2, 3, \ldots, \) and the range of the inverse sine is taken between 0 and \( \frac{\pi}{2}. \)

Since \( E = (k_2)^2/m_2, \) the roots of this equation also give the energy values of the bound states.

As the maximum value that \( k_2 \) could take is \( \sqrt{m_2 V_1}, \) from Eq. \( 3.11, \) we get an inequality for the number of bound states
\[ 2a \sqrt{m_2 V_1} > \left( n - \frac{1}{2} \right) \pi - \sin^{-1} \sqrt{\frac{m_2 V_1}{m_1 \Delta V}}, \]  
(3.15)

with \( \Delta V = V_2 - V_1 \geq 0. \) This means that the total number of bound states \( N \) will be the highest \( n \) satisfying this inequality. When we consider \( 3.15 \) as an equation for \( N = 1, 2, \ldots, \)
\[ 2a \sqrt{m_2 V_1} = \left( N - \frac{1}{2} \right) \pi - \sin^{-1} \sqrt{\frac{m_2 V_1}{m_1 \Delta V}}, \]  
(3.16)

we say that the parameters of the well are “critical”, in the sense that by modifying slightly their values we will have one bound state less or one bound state more.

From \( 3.10, \) for \( N = 1 \) we see that the first bound state of the asymmetric square well will appear when the following condition is satisfied:
\[ \sin^{-1} \frac{\sqrt{m_1 V_1}}{\sqrt{m_1 V_1 + m_1 \Delta V}} = \frac{\pi}{2} - 2a \sqrt{m_2 V_1}. \]  
(3.17)

Therefore, we can say that for \( V_1 \neq V_2, \) there are always some values of the parameters of the well that do not allow for bound states, as it is also the case for the conventional constant-mass problem.

The influence of \( m_1 \) (the mass outside the well) on the number of bound states is not so important. Let us call \( f(m_1) \) the function on the l.h.s. of \( 3.17, \) then
\[ \lim_{m_1 \to 0} f(m_1) - \lim_{m_1 \to \infty} f(m_1) = \frac{\pi}{2}. \]  
(3.18)

This means that as we increase \( m_1 \) the spectrum of bound states either will remain the same or will have one value less. This is in sharp contradistinction to the influence of \( m_2, \) that can change any number of levels in the discrete spectrum.

The conventional constant-mass case is obtained by taking \( m_1 = m_2 = m \) in Eq. \( 3.14 \) to get the well known formula \( 20 \)
\[ 2k_2 a = n\pi - \sin^{-1} \frac{k_2}{\sqrt{m V_2}} - \sin^{-1} \frac{k_2}{\sqrt{m V_1}}, \]  
(3.19)

where \( n = 1, 2, 3, \ldots. \) The inequality for the number of bound states is obtained now from \( 3.16 \) if we put \( m_1 = m_2 = m: \)
\[ 2a \sqrt{m V_1} > \left( n - \frac{1}{2} \right) \pi - \sin^{-1} \sqrt{\frac{V_1}{V_2}}. \]  
(3.20)
However, we must stress that in the position-dependent mass case the critical values given by formula (3.16) for the number of bound states depend on both $m_1$ and $m_2$, in particular, as $m_2 \to 0$, we see from (3.17) that no bound states will remain in the well.

### B. Symmetric well

If $V_1 = V_2 = V$, from (3.11), we get the energy equations corresponding to even and odd eigenfunctions by replacing $\theta = \pi/2$ and $\theta = 0$, respectively

$$\frac{k_1}{k_2} = \tan k_2 a, \quad \frac{k_2}{k_1} = -\tan k_2 a. \quad (3.21)$$

In this case, we can also write for both even and odd solutions the transcendental Eq. (3.14), using $k_2 = \sqrt{m_2 E}$, in the following way

$$2k_2 a = n\pi - 2\sin^{-1}\frac{k_2}{\sqrt{k_2^2 + m_1(V - E)}}, \quad (3.22)$$

where $n = 1, 2, 3, \ldots$. Here, the argument of the inverse sine is always less than 1 for $V - E > 0$, and therefore the formula is well defined. If we make $E = V$ in (3.22) the number of bound states $N$ is given by the highest $n$ satisfying the inequality

$$2a\sqrt{m_2 V} > (n - 1)\pi. \quad (3.23)$$

This means that there are always bound states for the symmetric well. Even more, once the depth $V$ and the width $2a$ of the well are fixed, the number of bound states does not depend on $m_1$, it depends only on the mass inside of the well ($m_2$). The relation (3.23) for the number of bound states coincides with that obtained also by Pastro et al using different matching conditions. However, the energy equations (3.21) – (3.22) are different from (3.16). In fact, when the inside mass is bigger (smaller) than the outside mass, then our energy spectrum is lower (upper) than the spectrum given in (3.16).

The critical values of the well (which determine when we have one bound state more) are obtained from

$$2a\sqrt{m_2 V} = (N - 1)\pi. \quad (3.24)$$

Thus the critical values of $a$ are linear in the number $N - 1$ of bound states, while the critical values $m_2$ grow as the square of $(N - 1)$. In conclusion, the important parameter here is the mass $m_2$ inside the well, while the mass outside ($m_1$) plays a secondary role.

The number of bound states for the conventional constant-mass symmetric well are given also by (3.22) replacing $m_2 \to m$. However, the energy of these bound states is defined through (3.22) by choosing $m_1 = m_2 = m$

$$k_2 a = \frac{n}{2} \pi - \sin^{-1}\frac{k_2}{\sqrt{mV}}. \quad (3.25)$$

Hence the values of the energies will be different from the position-dependent mass.

### IV. NUMERICAL RESULTS AND DISCUSSION

In this section we will discuss some numerical results and graphics obtained from the formulas of the previous sections, paying attention to the consequences of mass variation.

Consider the situation of a particle of mass $m_1$ in a square well potential, where we have altered the conditions inside the well to produce a different effective mass $m_2$. We want to study the effects that this change of mass will produce on the bound states.

#### A. Features of the asymmetric well

The main characteristics of the asymmetric well may be summarized as follows:

1. If $V_1 < V_2$, it can be seen from formula (3.15) that the number of bound states depends linearly on the width $2a$ of the asymmetric well as shown in Fig. 1.

![Fig. 1: Plot of the energy values and the number of the bound states depending on the width $2a$ of the asymmetric well.](image)

where we have plotted three situations:

(a) the usual constant-mass case, $m_1 = m_2 = 1$,
(b) $m_1 = 1, m_2 = 2$, that is the case where the mass inside is bigger than outside the well,
(c) $m_1 = 1, m_2 = 0.5$, that corresponds to a lighter mass inside the well.

Thus, the effect of $m_2$ on the bound states is quite strong for any value of $a$, as can be seen in Fig. 1. When $m_2$ is decreasing, the number of bound states also decrease, while each energy level is higher. In Table 1 it is shown the effect of these three values of $m_2$ on the first critical values of the width $2a$.

2. In Fig. 2 we plotted the bound state energies as we change only the inside mass $m_2$ for $m_1 = 1$ and...
TABLE I: The critical values of $a$ obtained from Eq. (3.10), determine the width where a new bound state appears in the well.

| $m_1$ | $m_2$ | $a^{(1)}$ | $a^{(2)}$ | $a^{(3)}$ | $a^{(4)}$ | $a^{(5)}$ | $a^{(6)}$ |
|-------|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1     | 1     | 0.2176    | 1.3283    | 2.4390    | 3.5498    | 4.6605    | 5.7712    |
| 1     | 0.5   | 0.3927    | 1.9635    | 3.5343    | 5.1051    | 6.6759    | 8.2469    |

FIG. 2: Plot of the energy values and the number of the bound states depending on the mass $m_2$ when the other parameters are fixed as: $a = 1$, $V_1 = V_2 = 2$, $m_1 = 1$ (solid lines), and $m_1 = 10$ (dashed lines).

$m_1 = 10$ (leaving the other parameter fixed). We see that the number of bound states is almost proportional to the square root of $m_2$ due to (3.10), while the energy value of each bound state decreases with $m_2$. The influence of $V_1$ is similar as that of $m_2$.

3. In the same figure, we can see that the influence of $m_1$ (the mass outside the well) on the number of bound states is not so important. Table II shows the influence of $m_1$ on the first critical energy values of $m_2$. The parameter $V_2$ has similar qualitative effects on the energy values and the number of the bound states as the parameter $m_1$.

B. Features of the symmetric well

In the symmetric well the importance of the mass $m_2$ inside the well is even stronger than in the asymmetric well. The main characteristics of the symmetric well are the following:

1. The number of bound states depends linearly on $a$, the square root of the $m_2$ and $V$, as in the asymmetric well, but it is independent of $m_1$.

2. The dependence on $m_2$ is shown in Fig. 3. A detail is given in Fig. 4. As a consequence, the critical values of $m_2$ are the same, independently of the values of $m_1$.

3. The energy values given by (3.22) are only slightly affected by the variation of $m_1$, the mass outside the well. This is shown in Fig. 3 for the values $m_1 = 1$, $m_1 = 10$ and $m_1 = m_2 = m$. A detail of this plot is shown in Fig. 4 where the energy levels of the case $m_1 = 1$ coincide with the conventional constant-mass case ($m_1 = m_2 = m$) at the point $m_2 = 1$. Clearly, the energy levels of the case $m_1 = 10$ will also coincide with those for constant-mass case $m_1 = m_2 = m$ at the point $m_2 = 10$ (see Fig. 6).

V. CONCLUSIONS

In this article we have studied a potential well both in symmetric and asymmetric form, with different constant mass inside and outside the well. We have proposed specific values for the ordering parameters in the kinetic term based on the simple argument that strong singularities in the effective-mass Schrödinger equation should be avoided. However, this choice is not unique: for instance, the symmetric well has been considered in [8] with a kinetic term proposed in [9]. Similar to the conventional
FIG. 4: Plot of the energy values and the number of the bound states depending on the mass $m_2$ when the other parameters are fixed as: $a = 1$, $V_1 = V_2 = 2$, $m_1 = 1$ (solid lines), $m_1 = 10$ (dashed lines), and $m_1 = m_2 = m$ (dotted lines).

constant-mass case we have obtained a transcendental equation for bound state energies. We have shown our numerical results for different values of the parameters. Many interesting differences from conventional constant-mass situation have been pointed out. In particular, the bound states are controlled mainly by the mass inside the well, while the mass outside, in general acts simply as a tuning of the specific values of the energies in the spectrum. The experiments have also shown that the energy level spacing is very sensitive to the effective mass inside the well, while the effects of the other parameters are not so important [20]. Finally, we have remarked the influence of the matching conditions, related to the kinetic term, on the discrete spectrum by comparing our results with those of [9].

We have also determined some critical values of the well, that is the values of the potential and mass functions giving rise to the new bound states in the well. These critical values are important in the study of the scattering states, because they fix the conditions where the transmission coefficients reach the maximum values.

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