Bound states in quantum systems with position dependent effective masses

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We study some simple one dimensional quantum mechanical systems characterized by a position dependent effective mass. We consider two systems with piecewise flat potential and mass, as well as a case with a smooth position dependence on these two quantities. These examples illustrate the influence that a non-constant effective mass has on the density of the (bound state) energy levels.

Keywords: Effective mass; quantum systems

En este trabajo se estudian algunos sistemas mecánico-cuánticos unidimensionales sencillos caracterizados por una masa efectiva dependiente de la posición. Se consideran dos sistemas donde el potencial y la masa efectiva se definen a intervalos tomando valores constantes diferentes, así como un caso en que estas dos magnitudes dependen suavemente de la posición. Los ejemplos analizados ilustran la influencia que una masa efectiva variable ejerce sobre la densidad de niveles de energía (de los estados ligados).

Descriptores: Masa efectiva; sistemas cuánticos

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1. Introduction

A quantum mechanical particle endowed with a position-dependent effective mass constitutes an interesting and useful model for the study of many physical problems. The effective mass approximation provides an important and widely used theory for the determination of the electronic properties of semiconductors [1] and quantum dots [2] (however, as is shown in Ref. 3, this approximation is valid only for systems with large coherence lengths, which is not the case of high Tc superconductors). Interest in this kind of approach is growing nowadays, stimulated by recent progress in crystal-growth techniques for the production of nonuniform semiconductor specimens. Much work has been done over the last years on the study of the solutions of the Schrödinger equation describing systems with non-constant mass. Some exactly soluble models with smooth potential and mass steps have been discovered [4, 5].

The concept of effective mass also plays an important role within the strictures of the energy density functional (EDF) approach to the quantum many body problem. The EDF formalism has yielded reasonable theoretical predictions of many experimental properties for several quantum many body systems. Within the EDF approach, the non-local terms of the associated potential can be often expressed as a position dependence on an appropriate effective mass $m^*(\mathbf{r})$. This formalism has been extensively used in nuclei [6], quantum liquids [7], ^{3}He clusters [8], and metal clusters [9]. The concomitant single particle wave functions and eigenenergies

comply with a Schrödinger equation of the form

$$\left[-\nabla \frac{\hbar^2}{2m^*(\mathbf{r})} \nabla + U(\mathbf{r}) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}). \qquad (1)$$

Besides its practical applications, the study of quantum mechanical systems with a position dependent mass also raises interesting conceptual problems of a fundamental nature. For example, Lévy-Leblond has recently discussed the quantum mechanical problem of a particle with position dependent mass in connection with the concept of instantaneous Galilean invariance [10]. The path integral approach to quantum mechanics for systems with nonconstant mass has also been studied [11].

The aims of the present work are: (a) to study, taking into account effects of a mass dependence on position, the bound states of some simple one dimensional systems usually discussed in elementary texts on quantum mechanics; and (b) to illustrate the effect on the density of bound state energy levels of a position dependent mass.

The paper is organized as follows. In Sect. 2 we provide a brief review of the Schrödinger equation for systems with position dependent effective mass. Sect. 3 deals with the eigenfunctions and eigenenergies of a finite potential well with different inside and outside masses. In Sect. 4 we consider an infinite potential well with a mass step. In Sect. 5 we compute numerically the eigenfunctions and energy eigenvalues corresponding to a particle with a Gaussian shaped x-dependent effective mass in an harmonic oscillator potential. Finally, some conclusions are drawn in Sect. 6.

2. Schrödinger equation with a position dependent effective mass

The one-dimensional time-independent Schrödinger equation associated with a particle endowed with a position dependent effective mass reads [4, 5, 10]

$$-\left[\frac{\hbar^2}{2m(x)}\right]\frac{d^2\Psi}{dx^2} - \frac{d}{dx}\left[\frac{\hbar^2}{2m(x)}\right]\frac{d\Psi}{dx}$$
$$+ V(x)\Psi(x) = E\Psi(x), \quad (2)$$

where $m(x)$ stands for the particle's effective mass, $V(x)$ denotes the potential, $\Psi(x)$ is the particle's wave function (wf) and $\hbar$ is Planck's constant. This equation can be cast as

$$\hat{H}\Psi = E\Psi, \quad (3)$$

where the Hamiltonian operator $\hat{H}$ is given by

$$\hat{H} = \hat{P}\left[\frac{1}{2m(x)}\right]\hat{P} + V(x). \quad (4)$$

The Schrödinger equation (2) can be derived from an energy variational principle akin to the standard one, that yields the wave equation for systems with constant mass. Let us consider the energy expectation value

$$\langle\hat{H}\rangle = \int dx\,\Psi(x)\left[-\frac{d}{dx}\frac{\hbar^2}{2m(x)}\frac{d}{dx} + V(x)\right]\Psi(x)$$
$$= \int dx\left[\frac{\hbar^2}{2m(x)}\left(\frac{d\Psi(x)}{dx}\right)^2 + V(x)\Psi^2(x)\right]. \quad (5)$$

It is easy to verify that the minimization of the mean energy $\langle\hat{H}\rangle$ under the normalization constraint $\langle\Psi|\Psi\rangle = 1$ leads to the differential equation (2). Actually, the Schrödinger equation (1) that appears in the EDF formalism is essentially obtained in the above fashion [12]. Furthermore, the variational principle will prove useful in order to understand some qualitative features of the energy eigenfunctions of systems with a position dependent mass.

An important technique used to deal with the Schrödinger equation (2) is based on the change of variables [12]

$$\Psi(x) = \sqrt{\frac{m(x)}{m}}\,u(x), \quad (6)$$

where m stands for "true" naked mass of the particle.

It is straightforward to verify that the function $u(x)$ complies with the differential equation

$$-\frac{\hbar^2}{2m}u'' + W(x, E)u(x) = Eu(x), \quad (7)$$

where

$$W(x, E) = \frac{m(x)}{m}\left[V(x) - \frac{m(x)}{2\hbar^2}\left(\frac{\hbar^2}{2m(x)}\right)'^2\right.$$
$$\left. + \frac{1}{2}\left(\frac{\hbar^2}{2m(x)}\right)''\right] + \left[1 - \frac{m(x)}{m}\right]E. \quad (8)$$

The differential equation (7) for $u(x)$ looks like the ordinary (*i.e.*, constant mass) time-independent Schrödinger equation, but with an *energy dependent potential function* $W(x, E)$. The potential W is usually referred to as the *local equivalent potential* (LEP).

The wave function connection rules across an abrupt interface (*i.e.*, a discontinuity in the effective mass) associated to the Schrödinger equation (2) are: *i*) the continuity of the wave function,

$$\Psi_- = \Psi_+; \quad (9)$$

and *ii*) the continuity of $\Psi'/m(x)$,

$$\left(\frac{1}{m(x)}\frac{d\Psi}{dx}\right)_- = \left(\frac{1}{m(x)}\frac{d\Psi}{dx}\right)_+, \quad (10)$$

where the subindexes $-$ and $+$ denote, respectively, the left and right hand sides of the mass discontinuity.

3. Finite potential well with different inside and outside masses

In this section we are going to compute the bound state eigenenergies of a finite potential well with an effective mass *inside* different from that *outside* the well. The corresponding potential $V(x)$ is given by

$$V(x) = 0, \quad |x| \le L/2,$$
$$V(x) = V, \quad |x| > L/2, \quad (11)$$

where L is the width of the well. The position dependent effective mass is (see Fig. 1a)

$$m(x) = m_1, \quad |x| \le L/2,$$
$$m(x) = m_2, \quad |x| > L/2. \quad (12)$$

The wave functions inside $[\Psi_1(x)]$ and outside $[\Psi_2(x)]$ the well verify, respectively, the differential equations

$$-\left(\frac{\hbar^2}{2m_1}\right)\Psi_1'' = E\Psi_1, \quad (13)$$

and

$$-\left(\frac{\hbar^2}{2m_2}\right)\Psi_2'' = (E - V)\Psi_2, \quad (14)$$

where E stands for the concomitant energy eigenvalue. Following the usual procedure we propose the forms

$$\Psi_1 = \sin kx \quad \text{(odd solutions)},$$
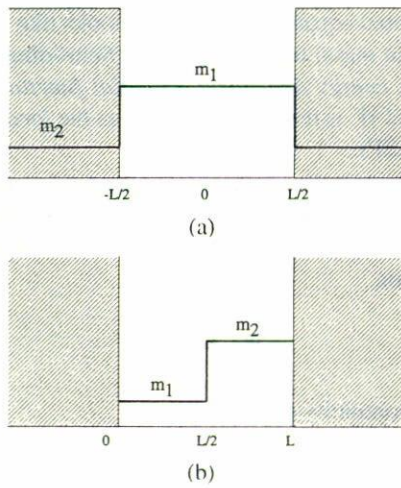$$\Psi_1 = \cos kx \quad \text{(even solutions)}, \quad (15)$$

FIGURE 1. (a) A square potential well of finite depht. The effective mass adopts the values m_1 inside the well and m_2 outside it. (b) An infinite potential well with a mass step. The effective mass is equal to m_1 (left side of the well) and to m_2 (right side of the well).

for the (unnormalized) wave function inside the well, the cos and sin solutions describing even and odd eigenfunctions, respectively. On the other hand, the wave function outside the well has the appearance

$$\Psi_2 = C \exp(-k'|x|). \tag{16}$$

Replacing the ansatzs (15) and (16) in Eqs. (13) and (14), we obtain, respectively,

$$k^2 = \frac{2m_1 E}{\hbar^2}, \tag{17}$$

and

$$k'^2 = \frac{2m_2(V - E)}{\hbar^2}. \tag{18}$$

These two equations immediately lead to

$$\frac{k}{k'} = \alpha \left(\frac{2m_1 V}{\hbar^2 k^2} - 1\right)^{-1/2}, \tag{19}$$

where

$$\alpha = \sqrt{\frac{m_1}{m_2}}. \tag{20}$$

The boundary conditions (9) and (10) at $x = +L/2$ are

$$\cos\left(\frac{kL}{2}\right) = C \exp\left(\frac{-k'L}{2}\right).$$

$$-\frac{k}{m_1}\sin\left(\frac{kL}{2}\right) = -\frac{Ck'}{m_2}\exp\left(\frac{-k'L}{2}\right) \tag{21}$$

for the even solutions, and

$$\sin\left(\frac{kL}{2}\right) = C \exp\left(\frac{-k'L}{2}\right),$$

$$\frac{k}{m_1}\cos\left(\frac{kL}{2}\right) = -\frac{Ck'}{m_2}\exp\left(\frac{-k'L}{2}\right) \tag{22}$$

for the odd ones. Equations (21) and (22) lead, respectively, to

$$\tan\left(\frac{kL}{2}\right) = \left(\frac{m_1}{m_2}\right)\left(\frac{k'}{k}\right), \quad \text{(even)} \tag{23}$$

and

$$\tan\left(\frac{kL}{2}\right) = -\left(\frac{m_2}{m_1}\right)\left(\frac{k}{k'}\right). \quad \text{(odd)} \tag{24}$$

which can be recast under the guise

$$\tan z = \alpha \frac{\sqrt{D^2\alpha^2 - z^2}}{z}, \tag{25}$$

and

$$\tan z = -\frac{z}{\alpha\sqrt{D^2\alpha^2 - z^2}}, \tag{26}$$

where

$$z = \frac{kL}{2}, \quad \text{and} \quad D^2 = \frac{m_2 V L^2}{2\hbar^2}. \tag{27}$$

It will prove convenient for our forthcoming discussion to express the masses $m_{1,2}$ in terms of a single variable m defined by

$$m_1 = \alpha^2 m, \quad \text{and} \quad m_2 = m. \tag{28}$$

The effective mass value m adopted by our particle when it is outside the well is regarded to coincide with the "true" mass of the particle. In other words, m is the mass of the particle when it can be regarded as a free particle that does not interact with its environment.

The solutions z of Eq. (25) provide the energy eigenvalues associated with the bound states of even parity, while the roots of Eq. (26) correspond to the eigenenergies of the bound states with odd parity. In the particular case of $\alpha = 1$ (i.e., $m_1 = m_2 = m$), Eqs. (25) and (26) reduce to the well-known transcendental equations determining the bound eigenvalues of a finite square well [13]. In Fig. 2 we depict the behavior, as a function of the parameter α, of the energy eigenvalues associated with the first five bound eigenstates of a finite well with $D = 7$. This value of D determines, in the case of $\alpha = 1$, a finite square well with five bound states. The number N of bound states is not constant for different values of α. It is determined by the integer part of $2\alpha D/\pi$, according to

$$N = 1 + \text{Int.}\left[\frac{2\alpha}{\pi}\left(\frac{mV L^2}{2\hbar^2}\right)^{1/2}\right]. \tag{29}$$

The above expression implies that for a small enough value of α there is only one bound state, regardless of the value of well parameter D. The number of bound states, for a given value of D, is an increasing function of α. The roots z of Eqs. (25) and (26) lie in the interval
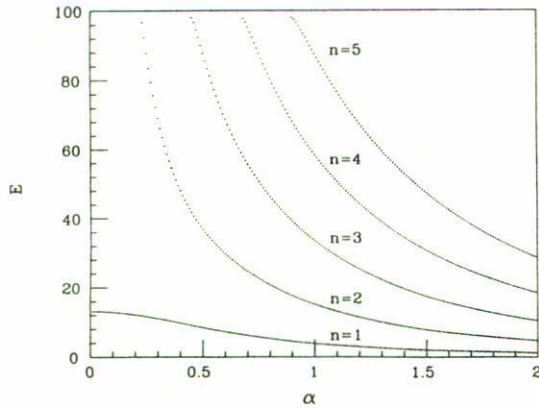
$$0 < z < \alpha D. \tag{30}$$

FIGURE 2. The first five energy eigenvalues of a finite square well with different "inside" and "outside" masses, as a function of the parameter α. We take $\hbar = m_2 = 1$ and $D = 7$ [see Eq. (27)]. The energy is given in units of $1/L^2$.

which means that the eigenenergies belong to the interval

$$0 < E_i < \frac{2\hbar^2 D^2}{mL^2} = V. \qquad (31)$$

In the case of constant mass this last equation simply means that the energy of a bound state must belong to $[0, V]$. However, the fact that these bounds on the energy spectra *do not depend on* α, while the number of bound states *increases with* α, has an interesting physical consequence: *the density of states is an increasing function of* α. More specifically, when the effective mass inside the well is lower than the effective mass outside ($\alpha < 1$), the density of states of the bound spectra is lower than the density of states associated with the constant mass situation. The oposite behavior occurs when the effective mass inside the well is larger than the mass outside. This effect on the density of states can be clearly appreciated in Fig. 2.

4. Infinite potential well with mass step

In this section we study the bound state eigenenergies of an infinite potential well in which an effective mass step exists: the value m_1 of the effective mass in the left side of the well ($x \in [0, L/2]$) differs form its right side counterpart m_2 ($x \in [L/2, L]$). The potential $V(x)$ is given by

$$V(x) = 0, \qquad 0 < x < L,$$
$$V(x) = \infty, \quad x < 0 \text{ or } x > L, \qquad (32)$$

where L is the width of the well. The position dependent effective mass is given by (see Fig. 1b)

$$m(x) = m_1, \qquad 0 < x < L/2,$$
$$m(x) = m_2, \quad L/2 < x < L. \qquad (33)$$

The wave functions $\Psi_1(x)$ (left side) and $\Psi_2(x)$ (right side) verify, respectively, the differential equations

$$-\left(\frac{\hbar^2}{2m_1}\right)\Psi_1'' = E\Psi_1, \qquad (34)$$

and

$$-\left(\frac{\hbar^2}{2m_2}\right)\Psi_2'' = E\Psi_2, \qquad (35)$$

where E stands for the concomitant energy eigenvalue and $\Psi_1(0) = \Psi_2(L) = 0$. Following the usual procedure we propose the ansatzs

$$\Psi_1(x) = \sin k_1 x, \qquad (36)$$

and

$$\Psi_2(x) = C \sin k_2 x + C' \cos k_2 x, \qquad (37)$$

for the (unnormalized) wave functions in each side of the well. The energy E is now given by

$$E = \frac{\hbar^2 k_1^2}{2m_1} = \frac{\hbar^2 k_2^2}{2m_2}, \qquad (38)$$

which implies that

$$k_2 = \sqrt{\frac{m_2}{m_1}} k_1. \qquad (39)$$

The connection conditions (9) and (10) at $x = L/2$ are now

$$\sin z = C \sin \gamma z + C' \cos \gamma z,$$
$$\gamma \cos z = C \cos \gamma z - C' \sin \gamma z, \qquad (40)$$

where $k_1 = k$, $z = Lk/2$, and $\gamma = \sqrt{m_2/m_1}$. The boundary condition on Ψ_2 at $x = L$ is

$$C \sin 2\gamma z + C' \cos 2\gamma z = 0. \qquad (41)$$

Solving for C' in the above equation and replacing in (40) we arrive at

$$\sin z = C (\sin \gamma z - \tan 2\gamma z \cos \gamma z), \qquad (42)$$

and

$$\cos z = \frac{C'}{\gamma} (\cos \gamma z + \tan 2\gamma z \sin \gamma z), \qquad (43)$$

whose ratio is

$$\tan z = \gamma \left(\frac{\sin \gamma z - \tan 2\gamma z \cos \gamma z}{\cos \gamma z + \tan 2\gamma z \sin \gamma z}\right)$$
$$= -\gamma \tan \gamma z. \qquad (44)$$

The roots z of this transcendental equation determine the bound state eigenenergies of the mass-step infinite well. We find, for all values of γ, an infinite number of roots and, correspondingly, an infinite number of bound states (as it happens, of course, in the $\gamma = 1$ instance that describes the well-known infinite well with constant mass). The eigenenergies are given by

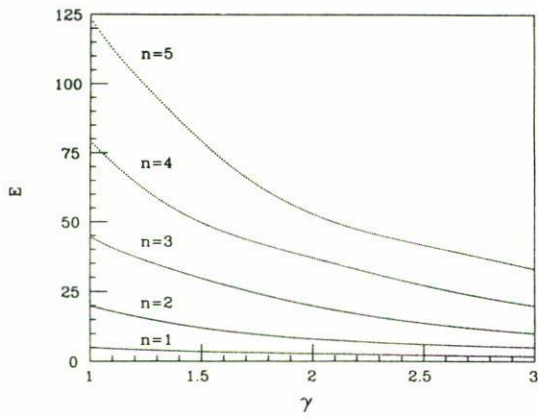$$E = \frac{2\hbar^2 z^2}{m_1 L^2}. \qquad (45)$$

FIGURE 3. The first five energy eigenvalues of an infinite square well with a mass step as a function of the parameter γ. We set $\hbar = m_1 = 1$. The energy is given in units of $1/L^2$.
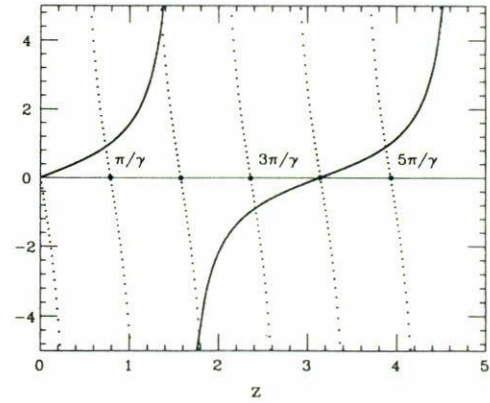

FIGURE 4. The intersections of the curves $\tan z$ and $-\gamma \tan \gamma z$, for $\gamma = 4$, yield the values of $z = kL/2$ that determine the eigenenergies of the infinite potential well with a mass step.

If z_1 is a solution of Eq. (44) for a given γ_1, then $z_2 = z_1/\gamma_1$ is a root of a similar equation but with a new value of γ given by $\gamma_2 = 1/\gamma_1$. This symmetry of Eq. (44) is just a consequence of the fact that interchanging the masses m_1 and m_2 we end up with essentially the same physical situation as the original one. More specifically, by interchanging the masses we obtain a mirror image of the original problem. It is clear from the above considerations that there is no loss of generality if we restrict our forthcoming discussion to values of γ larger than unity (that is, to mass steps where the left handside mass m_1 is smaller than the rigth hand side one m_2).

The behavior of the first five energy eigenvalues as a function of γ is depicted in Fig. 3. We can see that the density of states increases with γ.

The transcendental Eq. (44) can be solved exactly in the particular case of $\gamma = 2$. For such a value the equation verified by the variable z reduces itself to

$$\tan z(\tan^2 z - 5) = 0. \qquad (46)$$

The corresponding eigenvalues of the energy are

$$E_n^{(1)} = \frac{2\hbar^2(n+1)^2\pi^2}{m_1 L^2}, \qquad (n=1,2,\dots), \quad (47)$$

$$E_n^{(2)} = \frac{2\hbar^2(\arctan\sqrt{5}+n\pi)^2}{m_1 L^2}, \qquad (n=1,2,\dots), \quad (48)$$

and

$$E_n^{(3)} = \frac{2\hbar^2(\pi-\arctan\sqrt{5}+n\pi)^2}{m_1 L^2}, \qquad (n=1,2,\dots). \quad (49)$$

It is also instructive to consider the limiting situation of $\gamma \to \infty$. In that case, the roots of the transcendental Eq. (44) tend to (see Fig. 4)

$$z_n = \frac{n\pi}{\gamma}, \qquad (n=1,2,\dots), \qquad (50)$$

and the corresponding eigenenergies approach the limiting values

$$E_n = \frac{2\hbar^2}{m_1 L^2}\left(\frac{n\pi}{\gamma}\right)^2 = \frac{2\pi^2\hbar^2}{m_2 L^2}n^2, \qquad (n=1,2,\dots). \quad (51)$$

The above equation implies that, when m_2 is much larger than m_1, the energy eigenvalues of the system behave as if the particle had a constant mass equal to m_2 and were confined to an infinite well of lenght $L/2$. As far as the energy spectrum is concerned, "the larger mass wins". It is also worth considering the behavior, as $\gamma \to \infty$, of the coefficients C and C' appearing in the expresion for $\Psi_2(x)$. It is easy to see from Eqs. (42) and (43) that, in that limit,

$$C' \longrightarrow 0, \qquad (52)$$

and

$$C = (-1)^n\gamma. \qquad (53)$$

The above two equations imply that, for large values of γ,

$$\Psi_2^n(x) = (-1)^n\gamma \sin\frac{n\pi}{(L/2)}x. \qquad (54)$$

Summing up, when $m_2 \gg m_1$ the eigenstates of the system behave in such a way that

- The particle is almost completely confined to the part of the well where the effective mass adopts its largest value m_2.

- Within that part of the well where the mass value is m_2, the wave function looks like that of a particle of mass m_2 in a well of lenght $L/2$.

- The eigenenergies approach those of an infinite well of lenght $L/2$ with constant mass m_2.
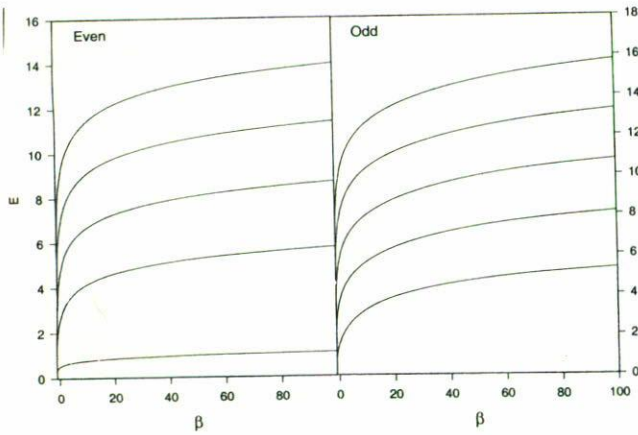
FIGURE 5. The first ten energy eigenvalues of the harmonic oscillator potential $x^2/2$ with a position dependent effective mass given by $m(x) = [1 + \beta \exp(-x^2)]^{-1}$, as a function of the parameter β.

FIGURE 6. (a) The effective mass $m(x)$ as a function of the coordinate x for $\beta = 20$ and the associated local equivalent potential for various even (continuous line) and odd (dashed line) eigenstates of the harmonic potential with effective mass. For comparison, the harmonic oscillator potential (dotted line) is also shown. (b) Same as Fig. 6a for $\beta = -1/2$.

5. An harmonic oscillator model with position dependent mass

In this section we consider a one dimensional harmonic potential (setting $\hbar^2/2m = 1/2$)

$$V(x) = \frac{x^2}{2}, \qquad (55)$$

along with an effective mass given by

$$\frac{\hbar^2}{2m(x)} = \frac{1}{2}(1 + \beta e^{-x^2}). \qquad (56)$$

We have that

$$\beta > 0 \Rightarrow m(x) < 1,$$

$$\beta < 0 \Rightarrow m(x) > 1. \qquad (57)$$

The Schrödinger equation (6) has been solved numerically by recourse to the Numerov standard numerical algorithm [14]. The corresponding first ten eigenvalues are depicted in Fig. 5 for $\beta \in (-1, 100]$. For clarity's sake the even and the odd states are displayed separatedly. Notice that the effect of a smooth position dependent effective mass on the energy levels is qualitatively the same as the one produced by a piece-wise flat effective mass. The level density is a monotonous decreasing function of the parameter β. As β increases, and the effective mass $m(x)$ decreases, the gap between the energy levels increases.

Since we now have both a smooth potential and a smooth mass it is instructive to consider the associated local equivalent potential (8). The LEPs corresponding to the first ten eigenstates and $\beta = 20$ are depicted in Fig. 6a. It is interesting to notice that the LEP becomes, in the case of excited states, a bistable potential. Moreover, the two concomitant potential wells become deeper as we consider greater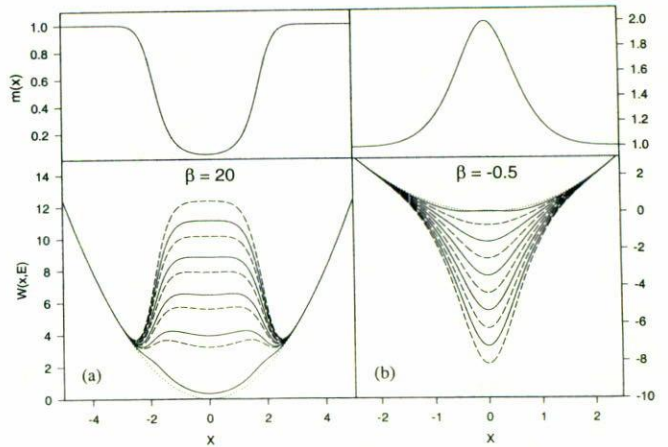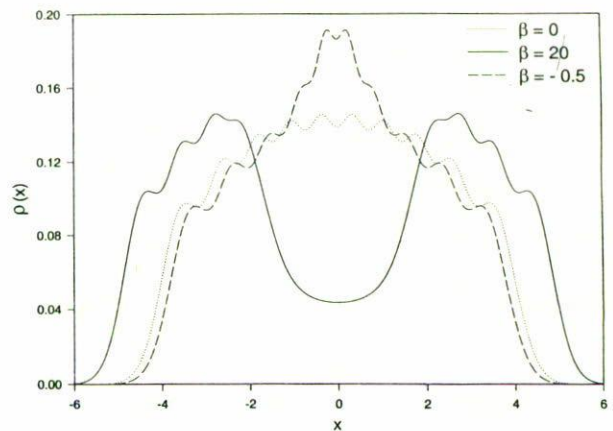 eigenenergies. As a consequence, the probability density associated with the eigenfunctions of the system will tend to be

FIGURE 7. The probability density function $\rho(x) = \sum_{i=1}^{10} |\Psi(x)|^2$ corresponding to ten particles occupying the first single particle states (one particle per level), computed for the same β values as in Fig. 6. Notice that $\beta = 0$ corresponds to the constant mass case.

small near $x = 0$. The neighbourhood of $x = 0$, where the effective mass adopts its lowest value, acts as a "repeller". This is clearly shown in Fig. 7, where we depict the probability density $\rho(x) = \sum_{i=1}^{10} |\Psi(x)|^2$ corresponding to ten particles occupying the first ten single particle states (one particle per level).

The LEPs for the first ten eigenstates and $\beta = -1/2$ are displayed in Fig. 6b. In this case the effective mass near $x = 0$ is larger than the one at $|x| \to \infty$, while the LEP function attains a deeper minimum near $x = 0$. As in the previous case, the effect due to the position dependent mass becomes more evident for highly excited states.

For both positive and negative values of the parameter β, the wave function tends to concentrate towards those places

in which the effective mass adopts its largest values (see Fig. 7). This behavior mimics that exhibited by the eigenstates of the infinite well with a mass step. The features exhibited by the eigenfunctions of systems with variable mass can be nicely interpreted in terms of the energy variational principle discussed in Sec.t II. By inspection of the mean energy (5) it is not hard to realize that, in order to minimize the kinetic energy contribution to $\langle \hat{H} \rangle$, the wave function must avoid those regions in which the effective mass adopts small values.

6. Conclusions

We have studied the bound states of three important one dimensional quantum systems with a position dependent effective mass. For two of the systems considered, *i.e.*, an infinite potential well with a mass step and a finite square well with different "inside" and "outside" masses, the energy eigenfunctions and eigenvalues can be obtained by solving an appropriate transcendental equation. Our third example, involving a smooth potential and a smooth effective mass, is solved by recourse to the numerical integration of the corresponding Schrödinger equation.

The concept of effective mass plays an important role in many applications of quantum mechanics. The examples analysed in the present work illustrate some aspects of the behavior of quantum systems with variable masses. We believe that our discussion shows that the quantum mechanics of systems with effective masses can be profitably discussed at the level of elementary quantum mechanics courses.

Acknowledgments

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