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Schrödinger Equation with Position-Dependent Mass: Staggered Mass Distributions

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***Abstract*—**The Point canonical transformation method is applied for solving the Schrödinger equation with position-dependent mass. This class of problem has been solved for continuous mass distributions. In this work, a staggered mass distribution for the case of a free particle in an infinite square well potential has been proposed. The continuity conditions as well as normalization for the wave function are also considered. The proposal can be used for dealing with other kind of staggered mass distributions in the Schrödinger equation with different quantum potentials.

***Keywords*—**Free particle, point canonical transformation method, position-dependent mass, staggered mass distribution.

I. Introduction

SOLVING the one-dimensional Schrödinger equation with position dependent mass has had applications in the description of physical systems such as semiconductors [1], superlattices [2], materials of non-uniform chemical composition [3], heterostructures [4], and abrupt heterojunctions [5]. Recently, the generalized point canonical transformation method [6] has been proposed to solve a Schrödinger-type equation, from an arbitrary second-order differential equation whose solution is known [7]. This methodology has allowed the study of different potentials in quantum mechanics [8] as well as other new potential [9] associated with the former one. Different schemes of solution [10] and generalized methods such as the supersymmetric theory [11], the Darboux transform [12], Hamiltonians with energy-dependent potentials [13], Schrödinger equation with effective mass [14] among others, have been also applied. In the first part of this work the point canonical transformation method [14] is briefly exposed. Then, the method is explained with an example where a continuous mass distribution is used. In this case, a harmonic oscillator potential is proposed to link both, the position-dependent mass distribution with its corresponding constant-mass problem. After that, in Section III, a step-type mass distribution is proposed. In this particular case, the mass is constant in some known interval, but it changes its value in a subsequent interval. Specific examples of staggered mass distributions are proposed for solving the Schrödinger equation with different quantum potentials, namely an infinite square well potential and a harmonic oscillator are used to show the usefulness of the proposed method.

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II. Exactly Solvable Schrödinger Equation with Position Dependent Mass

The one-dimensional Schrödinger equation with time-independent potential and position-dependent mass used in the literature [15], is expressed in the form

$$\left[-\frac{d}{dx}\left(\frac{\hbar^2}{2m(x)}\right)\frac{d}{dx}+V(x)\right]\psi_n(x)=E_n\psi_n(x) \quad (1)$$

E_n is the energy spectra, and $V(x)$ is the interaction potential. This equation can be written as

$$\left[-\frac{\hbar^2}{2m(x)}\frac{d^2}{dx^2}-\left(\frac{\hbar^2}{2m(x)}\right)'\frac{d}{dx}+V(x)\right]\psi_n(x)=E_n\psi_n(x) \quad (2)$$

With the aim of finding solution to (1), it is convenient to transform it into a problem of constant mass. To do that, the point canonical transformation method is used, namely, if $m(x)=m_0M(x)$ where m_0 is a constant mass, whereas $M(x)$ is a unitless function, the transformation

$$u=g(x)=\int^x\sqrt{M(t)}dt \quad (3)$$

such that $x=F(u)=g^{-1}(u)$, leads to the transformation of the differential operator

$$\frac{d}{dx}=\sqrt{M(F(u))}\frac{d}{du} \quad (4)$$

from where

$$\left(\frac{1}{M(x)}\right)'\frac{d}{dx}=\frac{d\,ln\left(\frac{1}{M(F(u))}\right)}{du}\frac{d}{du} \quad (5)$$

and

$$\left(\frac{1}{M(x)}\right)\frac{d^2}{dx^2}=\frac{d^2}{du^2}+\frac{d\,ln\sqrt{M(F(u))}}{du}\frac{d}{du} \quad (6)$$

thus (2) is written as

$$\left[\frac{d^2}{du^2}+2W(u)\frac{d}{du}+\frac{2m_0}{\hbar^2}\left(V\left(F(u)\right)-E\right)\right]\psi_n(F(u))=0 \quad (7)$$

where

$$W(u) = \frac{d}{du}\ln(M(F(u)))^{-\frac{1}{4}}\ . \quad (8)$$

Then, after applying the similarity transformation

$$\psi_n(F(u)) = \varphi_n(u)exp\left[-\int^u W(t)dt\right] \quad (9)$$

It is possible to write (1) as

$$-\frac{\hbar^2}{2m_0}\varphi_n''(u) + U(u)\varphi_n(u) = E_n\varphi_n(u), \quad (10)$$

which is a constant mass problem, where $U(u)$ is the potential

$$U(u) = V\big(F(u)\big) + \frac{\hbar^2}{2m_0}\big(\ W^2(u) + W'(u)\big) \quad (11)$$

Hence both potentials $V(x)$ and $U(u)$ are related to each other through the transformation (3)

$$V(x) = U\big(g(x)\big) - \frac{\hbar^2}{2m_0}\Big(\ W^2\big(g(x)\big) + W'\big(g(x)\big)\Big) \quad (12)$$

where in this case (8) is written as

$$W(g(x)) = \frac{1}{2}\frac{d}{dx}\left(\frac{1}{\sqrt{M(x)}}\right) \quad (13)$$

In short, the problem of variable mass and constant mass is isospectral because (1) and (10) have the same energy spectra. Additionally, from (9), the corresponding wave functions are related as

$$\psi_n(x) = \varphi_n(g(x))exp\left[-\int^{g(x)} W(t)dt\right] \quad (14)$$

or, by using (8) and (3)

$$\psi(x) = \varphi(g(x))\sqrt{g'(x)} \quad (15)$$

From this equation, it is possible to verify that if the solutions $\varphi_n(u)$ are normalized, then the wave functions $\psi_n(x)$ will be also normalized, in fact

$$\int|\psi(x)|^2\,dx = \int|\varphi(g(x)|^2\,d\big(g(x)\big) = 1. \quad (16)$$

Finally, it has been possible to relate the solutions of the Schrödinger equation with position-dependent mass (1) to those solutions of standard (constant mass problem) Schrödinger equation (10).

As a simple example of application for the case of a mass varying continuously with the position, the potential of the Harmonic oscillator $U(u) = \beta^2u^2$ is considered in (10), which is a solvable problem in the context of the Schrodinger equation with constant mass. In fact, the wave function and the energy spectra are given as

$$\varphi_n(u) = N_n exp\left[-\frac{\beta u^2}{2}\right]H_n(\sqrt{\beta}u) \quad (17)$$

where $N_n = \sqrt{\frac{\sqrt{\beta}}{2^n n!\sqrt{\pi}}}$ is the normalization constant, H_n are the Hermite polynomials and $E_n = \beta(2n+1)$ is the corresponding energy spectra. To connect this problem with its corresponding one in the context of position-dependent mass, it is necessary to propose a mass distribution, in this case

$$m(x) = m_0(1+\gamma x)^{-2} \quad (18)$$

which has been used in the treatment of the generalized displacement operator under a position-dependent mass scheme [16]. According with the transformation (3)

$$u = g(x) = \frac{1}{\gamma}\ln(1+\gamma x)\,,\quad x\ \in\left(-\frac{1}{\gamma},\ \infty\right) \quad (19)$$

leading to

$$W(g(x)) = \frac{\gamma}{2}. \quad (20)$$

The corresponding potential given in (12) is

$$V(x) = \left(\frac{\beta}{\gamma}\ln(1+\gamma x)\right)^2 - \frac{\hbar^2\gamma^2}{8m_0} \quad (21)$$

with wave function given in (15) as

$$\psi_n(x) = N_n exp\left[-\frac{\beta\left(\frac{1}{\gamma}\ln(1+\gamma x)\right)^2 + ln(1+\gamma x)}{2}\right]H_n\left(\frac{\sqrt{\beta}}{\gamma}\ln(1+\gamma x)\right) \quad (22)$$

The results of this example are shown in Fig. 1 for the problem of a continuous mass distribution (18). In this case the harmonic oscillator potential is mapped into the interval $\left(-\frac{1}{\gamma},\ \infty\right)$. Regarding the wave functions, it is possible to see that they are no longer symmetrical. The reason why they are unsymmetrical is because the transformation $g(x)$ deforms the x-space where the Schrödinger equation is involved with the position-dependent mass. It is worth pointing out that when $\gamma \to 0$, the problem of constant mass is recovered, namely $m(x) \to m_0,\ V(x) \to \beta^2x^2,\ \psi_n(x) \to \varphi_n(x)$ as well as the interval $\left(-\frac{1}{\gamma},\ \infty\right) \to (-\infty,\ \infty)$

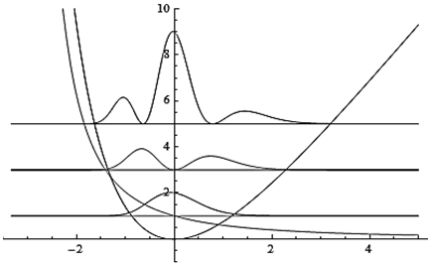

Fig. 1 Potential (21), the probability density $|\ \psi_n(x)\ |^2$, $n = 0, 1, 2$, the energy spectra $E_n = \beta(2n+1)$ and the mass distribution $m(x)$ given in (18) with parameters $\gamma = 0.3,\ \beta = 1$ and $\hbar = m_0 = 1$

III. The Problem of Staggered Mass

Despite the fact that the approach given in the previous section is applied to continuous mass distributions, the case of staggered masses, which deals with a constant mass in some defined interval [17], can be incorporated to the proposal described above. This kind of mass distributions is given as

$$m(x) = \begin{cases} m_1, & x \in (\alpha, \beta) \\ m_2, & x \in (\beta, \gamma) \end{cases} \tag{23}$$

where $m_1 \neq m_2$ are constant. In this case, the transformation (3) takes the general form

$$g(x) = \begin{cases} Ax + c, & x \in (\alpha, \beta) \\ Bx + d, & x \in (\beta, \gamma), \end{cases} \tag{24}$$

where the constants A, B, c and d are choosen on condition to have continuity for the transformation $g(x)$. Furthermore, from (13), the function $W(g(x)) = 0$ leads to

$$V(x) = U\big(g(x)\big) \tag{25}$$

Some specific examples of staggered masses are given next.

$$m(x) = \begin{cases} m_1 & |x| > x_0 \\ m_2 & |x| \leq x_0 \end{cases} \tag{26}$$

In this case, from (3), $M(x) = (g'(x))^2$, such that

$$g(x) = \begin{cases} \sqrt{\frac{m_1}{m_0}}\, x + \alpha, & x < -x_0 \\ \sqrt{\frac{m_2}{m_0}}\, x, & |x| \leq x_0 \\ \sqrt{\frac{m_1}{m_0}}\, x - \alpha, & x > x_0 \end{cases} \tag{27}$$

with $\alpha = \left(\sqrt{\frac{m_1}{m_0}} - \sqrt{\frac{m_2}{m_0}}\right) x_0$. Another example would be

$$m(x) = \begin{cases} m_1, & x < x_0 \\ m_2, & x \geq x_0 \end{cases} \tag{28}$$

Hence, the transformation $g(x)$ is

$$g(x) = \begin{cases} \sqrt{\frac{m_1}{m_0}}\, x, & x \leq x_0 \\ \sqrt{\frac{m_2}{m_0}}\, x + \alpha, & x_0 \leq x \end{cases} \tag{29}$$

with $\alpha = \left(\sqrt{\frac{m_1}{m_0}} - \sqrt{\frac{m_2}{m_0}}\right) x_0$. Next, the Schrödinger equation (10) with a free particle confined in an infinite square well potential is considered. In such a case, the solution of (10) with $U(u) = 0$ will be

$$\varphi_n(u) = A\, Sin(k_0 u) \tag{30}$$

where A is a constant and $k_0 = \sqrt{\frac{2m_0 E}{\hbar^2}}$. The boundary conditions $\varphi_n(0) = \varphi_n(L) = 0$ lead to $k_0 = \frac{n\pi}{L}$, thus the corresponding wave function for the case of staggered mass distribution will be

$$\psi_n(x) = A\, Sin(k_0 g(x)) = \sqrt{\frac{m_1 m_2}{{m_0}^2}} \begin{cases} Sin\left(k_0 \sqrt{\frac{m_1}{m_0}}\, x\right), & 0 \leq x < x_0 \\ Sin\left(k_0 \sqrt{\frac{m_2}{m_0}}\, x + k_0 \alpha\right), & x_0 \leq x \leq \ell \end{cases} \tag{31}$$

where $A = \sqrt{\frac{m_1 m_2}{{m_0}^2}}$ is required for the continuity of the wave function. Dealing with a free particle in an infinite well potential in a constant mass frame, the corresponding boundary conditions for the wave functions in the context of variable mass are $\psi_n(0) = \psi_n(\ell) = 0$, where according with the transformation (29), $\ell = \sqrt{\frac{m_0}{m_2}}\,(L - \alpha)$. Fig. 2 shows some details of these solutions. As in the previous example, the wave functions have no longer symmetrical. This is because the transformation $g(x)$ deforms the *x*-space where the mass is varying with the position. In fact, it is possible to notice that the wave functions are skewed toward the major mass.

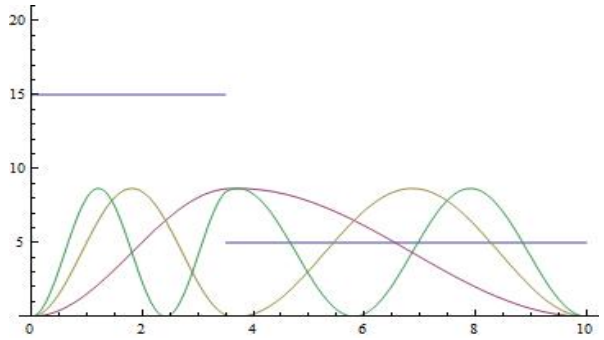

Fig. 2 Free particle confined in an infinite square well potential. The probability density $|\psi_n(x)|^2$, $n = 1, 2, 3$ in (31) and the mass distribution $m(x)$ given in (28). $m_1 = 15$, $m_2 = 5$, $x_0 = 3.5$ and $\hbar = m_0 = 1$

As in the example given in Section II, a harmonic oscillator potential $U(u) = \beta^2 u^2$ is used to link the Schrödinger equation with constant mass with its corresponding varying mass problem. Hence, the solution given in (17) and the energy spectra $E_n = \beta(2n + 1)$ will be considered. Then, the corresponding problem with varying mass is solved for a mass distribution given in (28). In such a case, according with (25), the potential will be $V(x) = \beta^2 (g(x))^2$ which, by using the transformation (29), can be written as

$$V(x)=\begin{cases}\beta^2\left(\sqrt{\frac{m_1}{m_0}}\,x\right)^2 & x<x_0\\ \beta^2\left(\sqrt{\frac{m_2}{m_0}}\,x+\alpha\right)^2 & x\geq x_0.\end{cases} \quad (32)$$

Likewise, from (14) and (17), the corresponding wave functions are

$$\psi(x)=\begin{cases}N\,exp\left[-\frac{\beta\sqrt{\frac{m_1}{m_0}}x}{2}\right]H_n\left(\sqrt{\beta\frac{m_1}{m_0}}x\right) & x<x_0\\ N\,exp\left[-\frac{\beta\left(\sqrt{\beta\frac{m_2}{m_0}}x+a\right)}{2}\right]H_n\left(\sqrt{\beta\frac{m_2}{m_0}}x+a\right) & x\geq x_0\end{cases} \quad (33)$$

where in this case $N=\sqrt{\frac{\sqrt{\beta}}{2^n n!\sqrt{\pi}}}\left(\frac{m_1 m_2}{m_0^2}\right)^{1/4}$. The factor involved with the masses m_1, m_2, and m_0 is necessary to guarantee the continuity of the wave-functions. Fig. 3 shows a harmonic oscillator which is deformed by the transformation $g(x)$ generated by the staggered mass distribution (28).

Different approaches for studying the Schrödinger equation with position-dependent mass for the case of staggered mass distribution have been applied. In this context, by taking a staggered potential, reflection and transmission coefficients have been calculated [17]. Also, by using a model of step-type mass, interface connection rules for abrupt heterojunctions between two different semiconductors are obtained [18]. The envelop-function approximation method has been applied for studying super-lattices [19]. The analytical solution of a smooth potential with mass step has been solved [20]. In [21], transmission coefficients and mooring energies for electrons moving in a double potential barrier are calculated. To do that, the multi-step potential approximation method is used with the mass varying as shown above.

The proposed method may be applied to make calculations on transmission coefficients when staggered masses are considered. Besides that, other interesting amounts such as transition probabilities or matrix elements can be calculated.

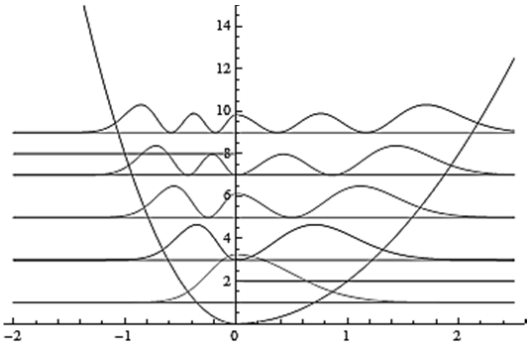

Fig. 3 Potential (32), the probability density $|\psi_n(x)|^2$ given in (33), the energy spectra $E_n=\beta(2n+1),\ n=0,1,2,3,4$ and the mass distribution $m(x)$ given in (28). $m_1=8, m_2=2,\ x_0=0,\ \beta=1$ and $\hbar=m_0=1$

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