

Scattering in abrupt heterostructures using a position dependent mass Hamiltonian

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Abstract. Transmission probabilities of the scattering problem with a position dependent mass are studied. After sketching the basis of the theory, within the context of the Schrödinger equation for spatially varying effective mass, the simplest problem, namely, transmission through a square well potential with a position dependent mass barrier is studied and its novel properties are obtained. The solutions presented here may be advantageous in the design of semiconductor devices.

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1 Introduction

One dimensional quantum wells (QW) and their analysis have played an increasingly significant role in various applications as well as the understanding of the properties of a variety of semiconductor devices [1–4]. The motivation for studying these problems is the recent developments in the nanofabrication of semiconductor devices, where one observes QW with very thin layers [5]. The effective mass of an electron (hole) in the thin layered QW varies with the composition rate. In such systems, the mass of the electron may change with the composition rate which depends on the position. Therefore, the corresponding Schrödinger equation should be formulated in a correct form.

Exact and quasi-exact solvability of the position dependent mass (PDM) Schrödinger equation has been the subject of recent interest [6–14]. It provides a useful model for the description of many physical systems [15–19]. Although it has been solved for a number of potentials and masses, the general solution has not yet been completed for square well potentials. Here we suggest a model that has been easily related to the QW structures with various PDM models. We will demonstrate a number of promising applications of the model.

Potential device applications, as well as purely scientific interest, provide the motivation for studies of the nature of the transport properties of the PDM electron through the barriers or wells. For realistic transport prop-

erties in semiconductors, the usual Schrödinger equation has to be replaced by the more general equation [24]:

$$\left(\frac{1}{4} (m^\alpha p m^\beta p m^\gamma + m^\gamma p m^\beta p m^\alpha) + V(z) - E \right) \psi(z) = 0 \quad (1)$$

with the constraint over the parameters: $\alpha + \beta + \gamma = -1$. In applications, the spatial variation of m is either neglected, or, alternatively various special cases of (1) have been suggested in the literature [25–27]. In this article we focus on abrupt heterostructures. It has been proven [18] that for sharp heterostructures $\alpha = \gamma$; otherwise the wavefunction is forced to vanish at the heterojunction boundary which is clearly an unphysical result.

In contrast to the solution of the PDM Schrödinger equation including Coulomb, Morse, harmonic oscillator, etc. type potentials [20–23], the study of the PDM Schrödinger equation including a constant potential has not attracted much attention in the literature. Such quantum systems have been found to be useful in the study of electronic properties of semiconductors. Generally, analysis of the scattering problem with PDM is based on the investigation of the simple problems, and it was pointed out that the transmission probability no longer tends to unity when incoming energy goes to infinity. The fundamental question remains open: whether the behavior of the transmission probability is generic or if it depends on the properties of the mass. To answer this question one has to obtain a general expression for the transmission probability by solving (1), for an arbitrary mass.

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The rest of the paper is organized as follows. In Section 2, we outline a specific formulation of the exactly solvable PDM Schrödinger equation to derive a general expression for the transmission amplitude of the wave through the square barrier. In Section 3, we apply our model to calculate the transmission coefficient of the wave through the barrier for various spatially varying effective masses. Finally, a summary of the work and conclusions are drawn in Section 4.

2 Theory

A typical QW structure is composed of a semiconductor thin film embedded between two semi-infinite semiconductor materials. For a compositional QW, the well material can be generated by alternate deposition of thin layers. For example, in a GaAs/Al_xGa_{1-x}As QW there exists a wide GaAs well, followed by an Al_xGa_{1-x}As barrier and a GaAs narrow well. The mole fraction x varies along the z -axis, therefore the mass of the electron may vary along the z -axis. The simplest model of the QW is that of a step potential and mass, both showing discontinuities at the same given point and constant inside and outside the well. Here we suggest a model by taking into account the spatial variation of the mass inside the barrier or well. Let us consider a potential barrier of width, d . The structure may be generated by continuously changing the alloy composition x of Al_xGa_{1-x}As from $x = 0$ to $x = 0.32$. The relation between alloy composition x and coordinate z is given by [28, 29]:

$$x = \frac{0.32z^2}{d^2}. \quad (2)$$

Now we turn our attention to the PDM Schrödinger equation (1). As we mentioned before, the continuity condition forces $\alpha = \gamma = 0$ and $\beta = -1$. With these choices the PDM Schrödinger equation (1), takes the form:

$$\left(p\frac{1}{2m}p + V_0 - E\right)\psi(z) = 0, \quad d > z > 0 \quad (3)$$

where V_0 is the constant potential associated with the barrier height, and E is the energy of the particle. In spite of its simple appearance the Schrödinger equation (3) cannot be solved analytically for arbitrary m . We note here that an exact solution of (1) including a constant potential can be obtained when $\alpha = \gamma = -1/4$ and $\beta = -1/2$, but in this case continuity conditions can not be satisfied. We look instead at the problem from a different point of view. Instead of the potential V_0 let us introduce the following potential [22],

$$V(z) = V_0 + \frac{\hbar^2}{8m^2} \left(m'' - \frac{7m'^2}{4m}\right), \quad d > z > 0 \quad (4)$$

where m is a function of z and m' and m'' denote first and second derivatives of m with respect to z . At this point it is worth mentioning that we will be interested in the potential which has a less pronounced cusp. Now, the

potential resembles a square barrier or well with smooth walls. The additional term is small compared with the original potential V_0 and does not change the shape of the potential. It is obvious that the conditions are satisfied for smoothly varying mass. With the potential (4) the Schrödinger equation can be exactly solved with a simple coordinate transformation and the wave function is given by

$$\psi(z) = \left(C_1 e^{-ikf(z)} + C_2 e^{ikf(z)}\right) m^{\frac{1}{4}} \quad (5)$$

where the function $f(z)$ is defined as $f(z) = \int \sqrt{m} dz$ and $k = \frac{\sqrt{2}}{\hbar}(E - V_0)$.

The results given above can easily be used to solve the Schrödinger equation including well and/or barrier potentials. Let us illustrate our procedure on a simple example. Consider the potential barrier

$$V(z) = \begin{cases} 0 & 0 > z, \quad z > d \\ V_0 + \frac{\hbar^2}{8m^2} \left(m'' - \frac{7m'^2}{4m}\right) & d > z > 0 \end{cases} \quad (6)$$

with mass barrier

$$m(z) = \begin{cases} m_0 & 0 > z, \quad z > d \\ m(z) & d > z > 0. \end{cases} \quad (7)$$

We assume that the mass of the particle m_0 is constant outside the barrier. Mass of the particle inside the barrier $m(z)$ is an arbitrary function of z . The general solution of the Schrödinger equation yields:

$$\psi(z) = \begin{cases} A_1 e^{ik'z} + A_2 e^{-ik'z} & z < 0 \\ (A_3 e^{-ikf(z)} + A_4 e^{ikf(z)}) m^{\frac{1}{4}} & d > z > 0 \\ A_5 e^{ik'z} & z > d \end{cases} \quad (8)$$

where $k' = \sqrt{2m_0 E}/\hbar$ and A_i are constants. For an abrupt heterostructure the continuity conditions are given by [18]

$$m^\alpha \psi(z) = \text{continuous}, \quad m^\beta \frac{d}{dz} m^\alpha \psi(z) = \text{continuous}. \quad (9)$$

The transmission coefficient, T , and reflection coefficient, R , are defined by

$$T = \frac{|A_5|^2}{|A_1|^2}, \quad R = \frac{|A_2|^2}{|A_1|^2}, \quad T + R = 1. \quad (10)$$

Using elementary quantum mechanical methods, algebraic computation applying boundary conditions, will lead to the following expression which is related with the transmission coefficient:

$$\frac{A_5}{A_1} = \frac{e^{ik'd} K_+(0) K_+^*(d) e^{ik(f(0)-f(d))}}{64kk'm_0m(0)^{7/4}m(d)^{5/4}f'(d)} - \frac{e^{ik'd} K_-(0) K_-^*(d) e^{-ik(f(0)-f(d))}}{64kk'm_0m(0)^{7/4}m(d)^{5/4}f'(d)} \quad (11)$$

and the coefficient related with the reflection of the wave:

$$\frac{A_2}{A_1} = \frac{K_-(0) K_-^*(d) e^{2ikf(d)} - K_+(0) K_+^*(d) e^{2ikf(0)}}{K_+^*(d) K_-^*(d) e^{2ikf(d)} - K_-^*(0) K_+^*(d) e^{2ikf(0)}} \quad (12)$$

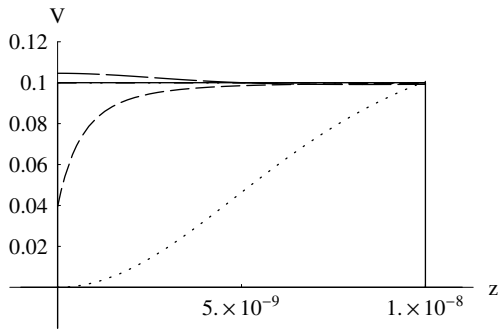


Fig. 1. Effect of the position dependent mass on the potential profile. The long dashed line, dashed line and dotted line show the effect of the m_a , m_c , and m_d , respectively, on the potential profile. The change in the potential profile due to $m_b(z)$ is plotted with long dashed lines and it is negligible.

where K_{\pm} are given by

$$K_{\pm}(a) = [4k'm(a)^2 \pm 4km_0m(a)f'(a) - im_0m'(a)] \quad (13)$$

$K_{\pm}^*(a)$ is conjugate of $K_{\pm}(a)$. The transmission and reflection coefficients can be computed using the relations (8) through (12). In the following section we will illustrate our model using some explicit examples.

3 Examples

In this section we discuss the dependence of the transmission probability on the position dependent mass by various choices of the mass $m(z)$. We give several examples for systems with different position dependent masses. Our criterion for the selection of masses is that the shape of the original potential does not change and the square root of $m(z)$ is analytically integrable. Moreover we made an attempt to include mass functions that are frequently used in the literature. In order to demonstrate our procedure, let us begin by considering the following spatially dependent effective masses found to be useful for studying transport properties in semiconductors:

$$\begin{aligned} m_a(z) &= m_0(\sigma + \delta z^2) \\ m_b(z) &= m_0\sigma e^{\sqrt{\delta}z} \\ m_c(z) &= m_0(\sigma + \tanh(\sqrt{\delta}z)) \\ m_d(z) &= m_0 \left(\frac{\sqrt{\sigma} + \delta z^2}{1 + \delta z^2} \right)^2 \end{aligned} \quad (14)$$

where δ is the length scale parameter and σ is a dimensionless parameter. Through out this section the parameters are chosen $\sigma = 0.0665$, $\delta = 0.0835$, and $V_0 = 100$ meV, height of the barrier and width of the barrier $d = 100$ Å.

It can be seen from Figure 1, the potential (4) closely resembles a square barrier with smooth walls for the masses $m_a(z)$, $m_b(z)$ and $m_c(z)$. We remark that when the mass rapidly changes with position z , the shape of the

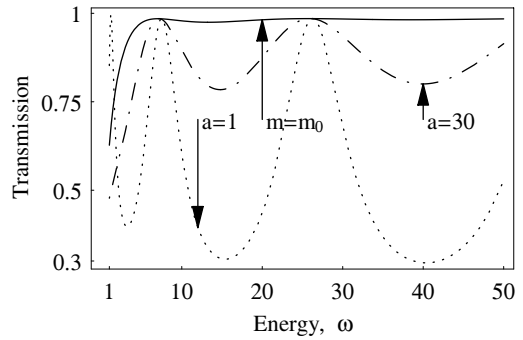


Fig. 2. The transmission coefficient T for a potential barrier with height V_0 and a mass discontinuities.

potential profile has a pronounced cusp. The potential (4) which includes the rapidly changing mass function $m_d(z)$ can be plotted as shown in Figure 1. We explicitly calculate transmission probability of the scattering problem employing various physically meaningful spatially varying effective masses in the following.

3.1 Mass barrier: $m(z) = \sigma m_1$

Consider now a simple mass barrier such that the mass changes at the potential discontinuities, but inside and outside the barrier it is a constant. In this case the potential V_0 remains the same. Since the tunneling effect is not qualitatively modified by the mass discontinuity, we have to leave aside the case where $E < V_0$. In the case $E > V_0$ the calculation for transmission coefficient can easily be done from the relation (11) and a plot of the transmission probability is illustrated in Figure 2 for various mass ratios. In the plot we defined the quantities:

$$\frac{m_1}{m_0} = a, \quad d = \frac{\pi\hbar}{\sqrt{m_0V_0}}, \quad \omega = \frac{E}{U_0}. \quad (15)$$

The graph shows clearly for $m_0 \geq m_1$ the transmission coefficient no longer tends to unity when E goes to infinity, but it becomes an oscillating function of E , as is discussed in [15,30]. In Figure 2, the curve denoted by $a = 1$, corresponds to the plot of transmission coefficient for $m = 0.0665m_0$. This is the conduction band edge effective mass of the electron in the GaAs structure. In the following we compute the transmission coefficients for the mass functions given in equation (14).

3.2 Mass barriers: $m_a(z)$, $m_b(z)$, $m_c(z)$ and $m_d(z)$

The mass functions given in equation (14) are used in various fields of physics. We mention here that mass function $m_a(z)$, may be useful to analyze the structures GaAs/ $Al_xGa_{1-x}As$. For example the effective band mass of the electron in the barrier can be written [28,31] as

$$m(x) = m_0(0.0665 + 0.0835x). \quad (16)$$

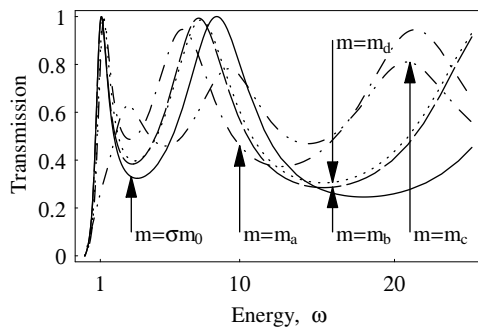


Fig. 3. The transmission coefficient T for a potential barrier with height V_0 and various position dependent mass discontinuities.

The relation between alloy composition x and the coordinate z is given in equation (2). For comparison we calculated transmission coefficients by using the relations (10) through (12) and they are illustrated in Figure 3.

4 Conclusion

In summary, we have discussed the exact solvability of the PDM Schrödinger equation including a constant potential. We have recovered a general expression for the transmission coefficient of the wave through the square potential barrier. We have presented calculations of transmission coefficients for various spatially varying effective masses.

Within the framework of the effective mass approximation, in some previous works [32] the electron was assumed to be confined in a square infinitely high potential well. In fact, a finite height potential well model is more realistic for describing the motion of the electron in the QW [33,34]. It is obvious that the model described in this article can easily be modified to study QW structures and superlattices [35].

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