Triangular quantum profiles: transmission probability and energy spectrum

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Abstract: Analytical expressions for the transition probability and the energy spectrum of the 1D Schrdinger equation with position-dependent mass are presented for the triangular quantum barrier and quantum well. The transmission coefficient is obtained by using the wave functions written in terms of Airy's functions and of the solutions of Kummer's differential equation. In order to show the validity of our analysis, an example by taking some numerical values for a GaAs heterostructure is presented.

Key words: Heterostructure, quantum well, quantum barrier, tunneling, semiconductor

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1. Introduction

Quantum well [1,2], quantum dot [3,4], and quantum wire [5,6] heterostructures, which are classified as low-dimensional semiconductor quantum systems, have become an important part of semiconductor studies. Theoretical and practical investigation gives some possibilities for producing high quality quantum heterostructures. Materials consisting of GaAs/AlAs have been widely used in the investigation of the above heterostructures. However, new types of materials have also been taken into account, such as, for example, silicon carbide (SiC) [7].

To study semiconductor heterostructures within theoretical and practical frameworks could give some clues that may be helpful to advance the semiconductor technology, such as the development of some optoelectronic and communication devices based on quantum mechanical tunneling, some visible lasers based on the electronic spectrum of double quantum wells [8], and quantum cascade lasers based on the electronic transition between levels of the conduction band [9]. Among the other quantum heterostructures, triangular quantum wells are also important systems since the absorption coefficient value is reduced in the experimental measurement of the electroabsorption when triangular quantum wells are used [10]. Moreover, the current absorption spectra of the triangular quantum profile could operate with lower driving voltages [11].

Quantum mechanical tunneling is a fundamental subject within the study of semiconductor quantum systems. This is because the study of tunneling helps to understand the physical properties of the related system and gives some hints about the lasing in quantum well lasers and electron transport in some devices [12]. According to the above points, it could be interesting to find the transmission coefficient for the triangular quantum barrier including a numerical presentation and to study the bound states of the triangular quantum well for the 1D Schrdinger equation. We find that the transmission probability oscillates within the range of

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energy but this behavior is very slight. The numerical computation is presented for the triangular quantum barrier made of GaAs heterostructure where the thickness is $a = 7$ nm while its maximum value is $V_0 = 450$ meV. It is observed that our numerical results are in agreement with the ones obtained for the constant mass case [13]. We point out that the energy levels of the triangular quantum well are finite and the potential parameter α controls the bound state numbers. In computation, we take the values of the mass parameters as $0.067m_0$ for GaAs, where m_0 is the free electron mass.

In the present work, we study the transmission probability of the 1D Schrdinger equation for the triangular potential barrier by writing the related wave functions in terms of Airy's functions and in terms of the solutions of Kummer's differential equation, namely the confluent hypergeometric functions of the first kind. Among the approaches and methods used to study quantum heterostructures [12], our formalism is based on solving the Schrdinger equation coming from the Hamiltonian written for the case of position-dependent mass [14]. In this case, the generalization of the standard Hamiltonian is not trivial because the linear momentum and mass operator no longer commute. We propose a mass function depending on a spatial coordinate to solve the 1D effective Schrdinger equation. Our formalism also includes an approach where we ignore the terms including the derivatives of mass in the 1D effective Schrdinger equation by assuming that one of the mass parameters goes to zero.

2. Analytical expressions

The generalized Hamiltonian for the case where the mass depends on the spatial coordinate is given as [14]

$$\mathcal{H} = \frac{1}{2} \left[p \frac{1}{m} p \right] + V \,, \tag{1}$$

where p is the linear momentum operator and V is the operator that defines the potential function. The 1D Schrdinger equation for the position-dependent mass obtained from the above Hamiltonian is written as [14]

$$\left\{ \frac{d^2}{dx^2} - \frac{dm(x)/dx}{m(x)} \frac{d}{dx} + Hm(x)[E - V(x)] \right\} \phi(x) = 0 \,, \tag{2}$$

where $H = 2/\hbar^2$.

We tend to parameterize the mass as

$$m(x) = M_0 - M_1 x \,, \tag{3}$$

where M_0 and M_1 are arbitrary parameters. For the rest of the computation, we assume that the terms including the derivatives of the mass can be ignored when the mass parameter $M_1 \to 0$.

2.1. Transmission probability

The triangular quantum barrier is defined as (Figure 1) [13]

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ V_0 - \alpha x & \text{for} \quad 0 < x < a \\ 0 & \text{for} \quad x > a, \end{cases} \tag{4}$$

where V_0 represents the maximum value of the potential profile and α controls the thickness of the quantum barrier.
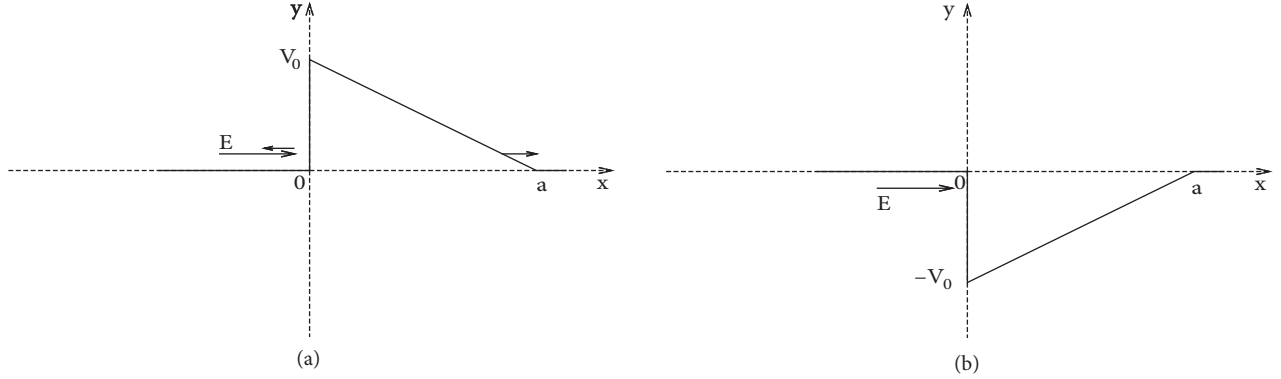
Figure 1. Graphical representation of the triangular quantum barrier (a) and triangular quantum well (b).

Inserting Eqs. (3) and (4) into Eq. (2), taking into account the above assumption, and using a new variable $y = (HEM_1)^{1/3} x$, we obtain the following equation:

$$\left[\frac{d^2}{dy^2} - y\right] \phi_I(y) = 0,\tag{5}$$

where solutions are expressed in terms of Airy's functions. We write the solution for the region I $(x < 0)$ as [15]

$$\phi_I(y) = b_1 Ai(y) + b_2 Bi(y).\tag{6}$$

Similarly, we obtain the following equation for the region II $(0 < x < a)$:

$$\left\{\frac{d^2}{dx^2} - [a_1 x^2 + a_2 x + a_3]\right\} \phi_{II}(x) = 0,\tag{7}$$

which can be written by using a new variable, $y = x + \frac{a_2}{2a_1}$, as

$$\left\{\frac{d^2}{dy^2} - [a_1 y^2 + A_I]\right\} \phi_{II}(y) = 0,\tag{8}$$

where

$$a_1 = HM_1\alpha,\tag{9a}$$

$$a_2 = -H[M_0\alpha + M_1(V_0 - E)],\tag{9b}$$

$$a_3 = HM_0(E - V_0),\tag{9c}$$

and $A_I = \frac{4a_1 a_3 - a_2^2}{4a_1}$.

In order to get a more suitable form of Eq. (8), we use a new variable $z = \sqrt{a_1}\, y^2$ and a trial wave function in terms of z as $\phi_{II}(y) = e^{-z/2} f(z)$, which gives

$$\left\{z\frac{d^2}{dz^2} - \left(z - \frac{1}{2}\right)\frac{d}{dz} - \frac{1}{4}\left[1 + \frac{A_I}{4a_1}\right]\right\} f(z) = 0,\tag{10}$$

which is a kind of Kummer's differential equation having the form [15]

$$x\frac{d^2y(x)}{dx^2} + (c-x)\frac{dy(x)}{dx} - by(x) = 0.\tag{11}$$

Two linear independent solutions of the above equation are written as [15]

$$y(x) \sim {}_1F_1(b;c;x) + U(b;c;x),\tag{12}$$

where ${}_1F_1(b;c;x)$ is the confluent hypergeometric function of the first kind and the second part is given as

$$U(b;c;x) = \pi\csc(\pi c)\left[\frac{{}_1\bar{F}_1(b;c;x)}{\Gamma(b-c+1)} - x^{1-c}\frac{1}{\Gamma(b)}{}_1\bar{F}_1(b-c+1;2-c;x)\right],\tag{13}$$

where ${}_1\bar{F}_1(b;c;x)$ is the regularized confluent hypergeometric function of the first kind [15].

With the help of Eq. (12) we write the solution for region II as

$$f(z) = b_3\,{}_1F_1(\frac{1}{4}[1+\frac{A_I}{4a_1}];\frac{1}{2};z) + b_4U(\frac{1}{4}[1+\frac{A_I}{4a_1}];\frac{1}{2};z).\tag{14}$$

Following the same steps for region I, we obtain the following equation:

$$\left[\frac{d^2}{dy^2} - y\right]\phi_{III}(y) = 0,\tag{15}$$

where we define a new variable as $y = (HEM_1)^{1/3}x - \frac{HEM_0}{(HEM_1)^{2/3}}$. We write the physical solution for region III as

$$\phi_{III}(y) = b_5Ai(y),\tag{16}$$

where we use the properties given as $\lim_{x\to+\infty}Bi(x)\to\infty$, $\lim_{x\to-\infty}Bi(x)\to 0$, and $Bi(0) = \frac{1}{\sqrt[6]{3}\,\Gamma(\frac{2}{3})}$ [15].

Using the continuity conditions for $\phi(x)$ and $d\phi(x)/dx$ at $x=0$ and at $x=a$ and after straightforward calculations, we obtain the following expressions:

$$b_1Ai(y_1) + b_2Bi(y_1) = b_3f_1' + b_4f_7,\tag{17a}$$

$$(HEM_1)^{1/3}[b_1Ai'(y_1) + b_2Bi'(y_1)] = b_3f_8 + b_4f_9,\tag{17b}$$

$$b_5Ai(y_3) = b_3g_1' + b_4g_7,\tag{17c}$$

$$(HEM_1)^{1/3}b_5Ai'(y_3) = b_3g_8 + b_4g_9,\tag{17d}$$

where prime in $Ai(y)$ and $Bi(y)$ denote derivatives in the above expressions and the following abbreviations are used:

$$f_1 = \sqrt{a_1}\, y_2 e^{-y_2^2 \sqrt{a_1}/2} \, _1F_1\Big(\frac{1}{4}\Big[1 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{1}{2}; \sqrt{a_1}\, y_2^2\Big), \tag{18a}$$

$$f_2 = \sqrt{a_1}\, y_2 e^{-y_2^2 \sqrt{a_1}/2} \, _1F_1\Big(\frac{1}{4}\Big[5 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{3}{2}; \sqrt{a_1}\, y_2^2\Big), \tag{18b}$$

$$f_3 = \pi \csc\frac{\pi}{2} \sqrt{a_1}\, y_2 \frac{e^{-y_2^2 \sqrt{a_1}/2}}{\Gamma(\frac{3}{4} + \frac{A_I}{4\sqrt{a_1}})} \, _1\bar{F}_1\Big(\frac{1}{4}\Big[1 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{1}{2}; \sqrt{a_1}\, y_2^2\Big), \tag{18c}$$

$$f_4 = \pi \csc\frac{\pi}{2} \sqrt{a_1}\, y_2 \frac{e^{-y_2^2 \sqrt{a_1}/2}}{2\Gamma(\frac{3}{4} + \frac{A_I}{4\sqrt{a_1}})} \Big(1 + \frac{A_I}{\sqrt{a_1}}\Big) \, _1\bar{F}_1\Big(\frac{1}{4}\Big[5 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{3}{2}; \sqrt{a_1}\, y_2^2\Big). \tag{18d}$$

$$f_5 = \pi \csc\frac{\pi}{2} \sqrt{a_1}\, y_2 \frac{e^{-y_2^2 \sqrt{a_1}/2}}{\Gamma(\frac{1}{4} + \frac{A_I}{4\sqrt{a_1}})} \, _1\bar{F}_1\Big(\frac{1}{4}\Big[3 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{3}{2}; \sqrt{a_1}\, y_2^2\Big), \tag{19a}$$

$$f_6 = \pi \csc\frac{\pi}{2} \sqrt{a_1}\, y_2 \frac{e^{-y_2^2 \sqrt{a_1}/2}}{2\Gamma(\frac{1}{4} + \frac{A_I}{\sqrt{a_1}})} \Big(3 + \frac{A_I}{\sqrt{a_1}}\Big) \, _1\bar{F}_1\Big(\frac{1}{4}\Big[7 + \frac{A_I}{\sqrt{a_1}}\Big]; \frac{5}{2}; \sqrt{a_1}\, y_2^2\Big), \tag{19b}$$

$$f_1' = \frac{f_1}{\sqrt{a_1}\, y_2}, \tag{19c}$$

$$f_3' = \frac{f_3}{\sqrt{a_1}\, y_2}, \tag{19d}$$

$$f_5' = \frac{f_5}{a_1^{1/4} y_2}, \tag{19e}$$

$$f_7 = f_3' - f_5', \tag{19f}$$

$$f_8 = f_2 - f_1, \tag{19g}$$

$$f_9 = f_4 + f_5 - f_3 - f_6. \tag{19h}$$

$$g_1 = f_1(y_2 \to y_4); g_2 = f_2(y_2 \to y_4); g_3 = f_3(y_2 \to y_4); g_4 = f_4(y_2 \to y_4),$$

$$g_5 = f_5(y_2 \to y_4); g_6 = f_6(y_2 \to y_4); g_1' = f_1'(y_2 \to y_4); g_3' = f_3'(y_2 \to y_4),$$

$$g_5' = f_5'(y_2 \to y_4); g_7 = g_3' - g_5'; g_8 = g_2 - g_1; g_9 = g_4 + g_5 - g_3 - g_6. \tag{20}$$

We use $\frac{d}{dz}\, _1F_1(b; c; z) = \frac{b}{c}\, _1F_1(b + 1; c + 1; z)$ and $\frac{d}{dz}\, _1\bar{F}_1(b; c; z) = b\, _1\bar{F}_1(b + 1; c + 1; z)$ to obtain the above expressions [15]. The arguments of the above functions coming from the continuity conditions at $x = 0$ and

$x = a$ are given as

$$y_1 = -\frac{HEM_0}{(HEM_1)^{2/3}} \, , \tag{21a}$$

$$y_2 = \frac{a_2}{2a_1} \, , \tag{21b}$$

$$y_3 = (HEM_1)^{1/3} \, a - \frac{HEM_0}{(HEM_1)^{2/3}} \, , \tag{21c}$$

$$y_4 = a + \frac{a_2}{2a_1} \, . \tag{21d}$$

With the help of Eqs. (18)–(20), Eqs. (17a)–(17d) gives us the transmission probability as

$$T = \left| \frac{t_1}{t_2} \right|^2 \, , \tag{22}$$

where

$$t_1 = \frac{1}{\pi} (HEM_1)^{1/3} \left[g_1' g_9 - g_8 g_7 \right] \, , \tag{23a}$$

$$t_2 = \left[g_9 Ai(y_3) - (HEM_1)^{1/3} g_7 Ai'(y_3) \right] \left[(HEM_1)^{1/3} f_1' Bi'(y_1) - f_8 Bi(y_1) \right]$$

$$\times \left[(HEM_1)^{1/3} g_1' Ai'(y_3) - g_8 Ai(y_3) \right] \left[(HEM_1)^{1/3} f_7 Bi'(y_1) - f_9 Bi(y_1) \right] \, , \tag{23b}$$

where the following property of Airy's functions $Ai(y)Bi'(y) - Ai'(y)Bi(y) = \frac{1}{\pi}$ [15] is used.

To check the validity of our formalism, we compute the transmission coefficient in Eq. (22) numerically. For this aim, the following parameters are used: $V_0 = 450$ meV, $a = 7$ nm [16], the mass made of GaAs $M_0 = 0.067 m_0$ where m_0 is the free electron mass of 9.1×10^{-31} kg [12], $\hbar = 1.05 \times 10^{-34}$ Js, and $M_1 = M_0$. Figure 2 shows the dependence of the transmission probability on the energy of the incident particle. It is seen that the transmission probability is very slight within the energy range and goes to one while the energy increases. We plot the dependence of the transmission coefficient on the height and width of the quantum barrier in Figures 3 and 4, respectively. The parameter values of mass are the same as the ones used in Figure 2, but Figures 3 and 4 are plotted for $E = 0.1$ eV. In both figures, the transmission probability is exactly one for initial values of V_0 and a, respectively. Its value decreases while the values of height and width of the quantum barrier increase. The fluctuations of the transmission coefficient are very small, as observed in Figure 2. Figure 5 shows the varying of the tunneling coefficient according to the energy of the incident particle. It is observed that the tunneling coefficient is also very slight within the energy range, as in Figure 2.

2.2. Bound states
In order to study the bound states of the triangular quantum well, we parameterize the potential profile as (Figure 1)

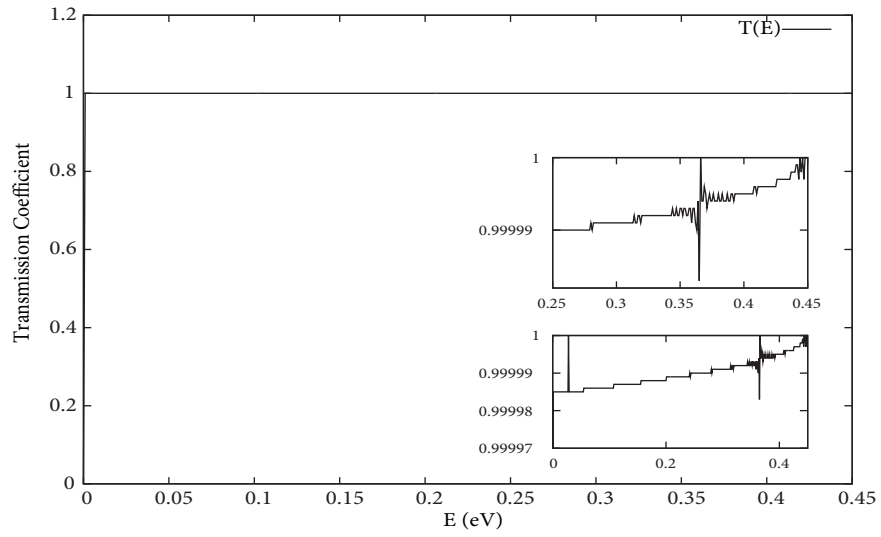$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ -V_0 - \alpha x & \text{for} \quad 0 < x < a \\ 0 & \text{for} \quad x > a. \end{cases} \tag{24}$$

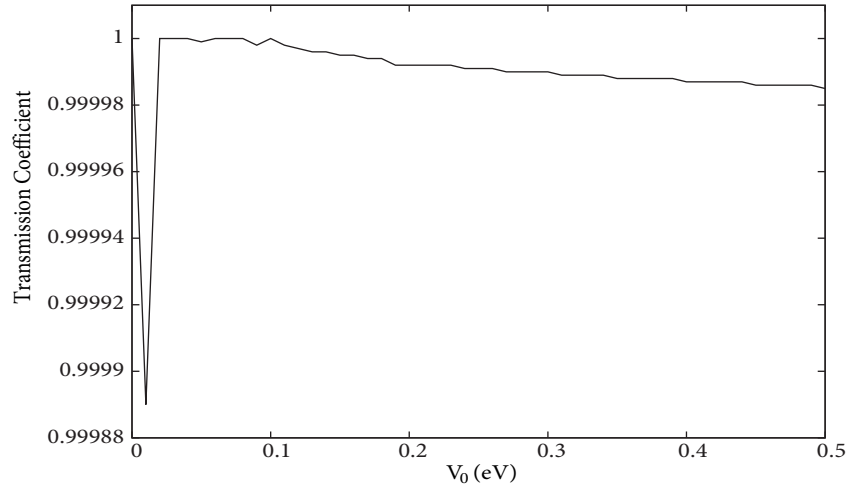**Figure 2.** The transmission probability for the triangular quantum barrier versus E.

Figure 3. The variation of transmission probability versus height of barrier V_0.
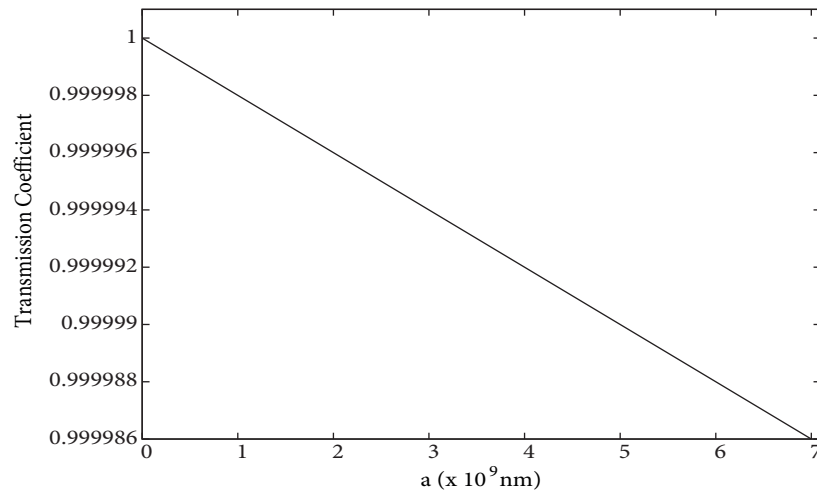

Figure 4. The transmission probability versus the width of barrier a.
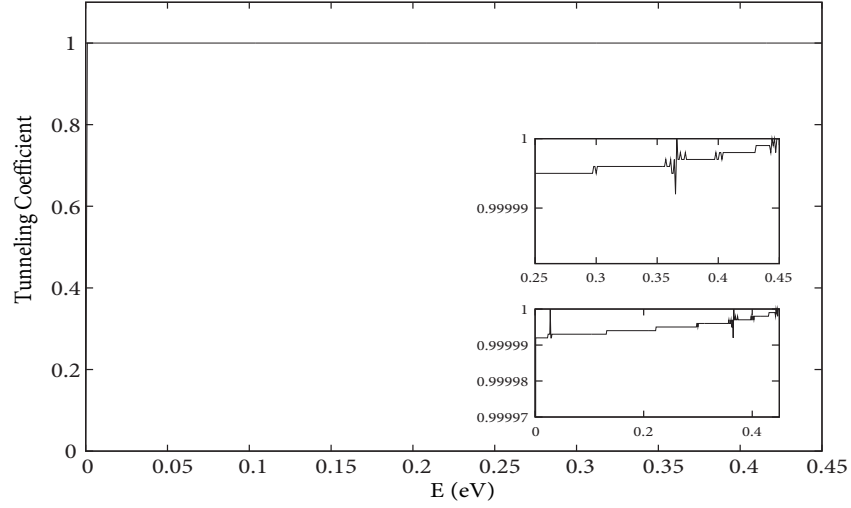
Figure 5. The tunneling coefficient for the triangular quantum barrier versus E.

In this case, we obtain a differential equation similar to the one given in Eq. (10) with the following abbreviations:

$$a_1' = HM_1\alpha = a_1\,, \tag{25a}$$

$$a_2' = -H[M_0\alpha - M_1(V_0 + E)]\,, \tag{25b}$$

$$a_3' = HM_0(E + V_0)\,, \tag{25c}$$

and $B_I = \frac{4a_1'a_3' - a_2'^2}{4a_1'}$, which gives a physically acceptable solution as

$$f(z) \sim {}_1F_1\big(\frac{1}{4}\,[1 + \frac{B_I}{4a_1'}]; \frac{1}{2}; z\big)\,. \tag{26}$$

In order to get a finite solution, it must be

$$\frac{1}{4}\big(1 + \frac{B_I}{4a_1'}\big) = -n\ (n \in \mathbb{N})\,, \tag{27}$$

which is a quantization condition for the bound states. We write the energy spectra of the triangular quantum well as

$$E_n = -V_0 - \frac{M_0\alpha}{M_1} + 2\big(\frac{\alpha^3}{M_1}\big)^{1/4}\sqrt{1 + 4n}\,. \tag{28}$$

It is worth noting that the parameter α in the potential profile depends on the diffusion length (or the Debye length) L_D inversely, which controls the number of the bound states [16]. In order to get some numerical values for the bound states we choose the parameter set as $M_1 = M_0 = 0.067m_0$ and $\alpha = 0.01V_0$ and we present our results in the Table. It shows that the results are in agreement with the ones stated in the literature [16].

Table. Some energy eigenvalues for the triangular quantum profile (eV).

	Ref. [16]	Our results
E_1	-0.20986	-0.29407
E_2	-0.00630	-0.00871

As a final remark, we briefly discuss the effect of an external electric field on the quantum system considered here. For this case, the potential is written as an 'effective' potential as follows:

$$V_{eff} = V(x) + V_E(x), \tag{29}$$

where $V_E(x)$ denotes the potential part arising from the external electric field. The second term in Eq. (29) depends on the electric field strength linearly [17], so we expect that the obtained expressions for transmission coefficient and also the energy levels have additional terms including the electric field strength.

3. Conclusions

In the present work, we have analyzed the transmission probability for the 1D Schrdinger equation with position-dependent mass for the triangular quantum barrier by applying the continuity conditions on the wave functions, which are written in terms of Airy's functions and the solutions of Kummer's equation. For this aim, we have solved the Schrdinger equation obtained from a nonstandard Hamiltonian written for the case where the mass and linear momentum operator does not commute. We have ignored the terms including the derivatives of mass in the Schrdinger equation for $M_1 \to 0$ to obtain the analytical solutions. We have given the dependence of the transmission probability not only on the energy but also on the height and width of the barrier, respectively. We have observed that the transmission coefficient decreases while the values of parameters E, V_0, and a increase, as expected, and the fluctuations of the transmission probability are very small. We have also studied the bound states of the triangular quantum well and observed that the number of the bound states is finite depending on the mass parameter M_1 and on the diffusion length.

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