One Dimensional Quantum Scattering

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Introduction

In a mesoscopic level, particles behave in a way that can not be explained within the classical physics. They obey the laws of quantum mechanics. In the quantum realm, particles are treated like waves according to the de Broglie's principle.Therefore, the wave nature of electrons can be utilized in studying the interaction of electrons with one or more potential barriers. Usually, plane waves are used in representing the wave functions of quantum mechanical particles. In the following sections, the transmission of electrons through a single and double potential barriers is investigated. Despite the simplicity of these models, they can be extended to model important quantum devised, which are the heart of modern electronics. Thanks to the contemporary microelectronics manufacturing technologies, nano scaled one dimensional systems can be now realized. Important physical characteristics of these models such as transmissivity and reflectivity of electrons through the barriers are of interest because the transmission of electrons is directly connected to an electric conductivity. They will be calculated numerically and compared to the analytical solutions. The simplest system with a square potential barrier will be followed by the consideration of a more interesting-double barrier potential.

Theory

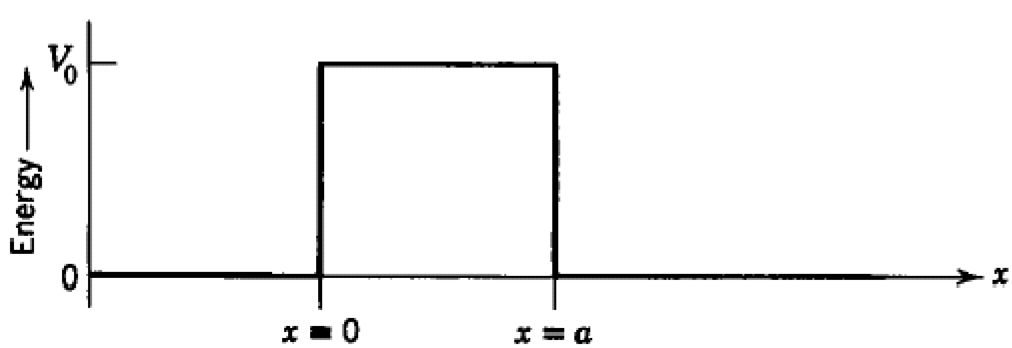

Figure 1. A single barrier potential

A single barrier potential in the figure1 has the potential height V_0 and the width a. It is subject to the incoming flux of electrons with the energy E from the left. Let us consider the following two cases with different energies. First, the energy of incoming particles is less than the potential barrier. In other words, $E < V_0$. Classically, the incoming particles would be reflected totally, so there would be zero transmission, and thus no particle penetrates the barrier. However, the quantum mechanics predicts the different picture of events. The equivalent of Newton's equation of motion in quantum mechanics is the Schrodinger equation, and for our system it is written as follows:

$$\left[-\frac{\hbar 2}{2m}\frac{d\,2}{dx2}+V\right]\Psi(x)=E\Psi(x) \qquad (1)$$

where m is the mass of an electron. The equation 1 yields the following expressions for the three region in the figure 1:

$$\Psi 1(x)=Aexp(ik1x)+Bexp(-ik1x) \qquad x\leq 0 \qquad (2)$$

$$\Psi 2(x)=Cexp(k2x)+Bexp(-k2x) \qquad a>x>0 \qquad (3)$$

$$\Psi 3(x)=Eexp(ik1(x-a)) \qquad x\geq a\,, \qquad (4)$$

where $k1=\sqrt{2mE}/\hbar$ and $k2=\sqrt{2m(V0-E)}/\hbar$. To find the reflection, the transmission and reflection coefficients we use are

$$R=\frac{|B\cdot|\,|B|}{|A|\cdot|A|}\ ,\ T=\frac{|E\cdot|\,|E|}{|A|\cdot|A|}\ . \qquad (5)$$

After a number of steps of derivations, the transmission coefficient is

$$T=\frac{1}{1+\frac{1}{4\varepsilon(1-\varepsilon)}sinh(\lambda\sqrt{1-\varepsilon})\cdot sinh(\lambda\sqrt{1-\varepsilon}\cdot}\ , \qquad (6)$$

where $\varepsilon = E/V0$ and $\lambda = a\sqrt{2mV0}/\hbar$. Because T is finite, a quantum mechanical particle can penetrate a barrier, and this is called the tunneling effect.
The same procedure is applied in finding the transmission coefficient for the case $E > V0$, and it is

$$T = \frac{1}{1+\frac{1}{4\varepsilon(1-\varepsilon)}sin(\lambda\sqrt{1-\varepsilon})\cdot sin(\lambda\sqrt{1-\varepsilon}\cdot} \qquad (7)$$

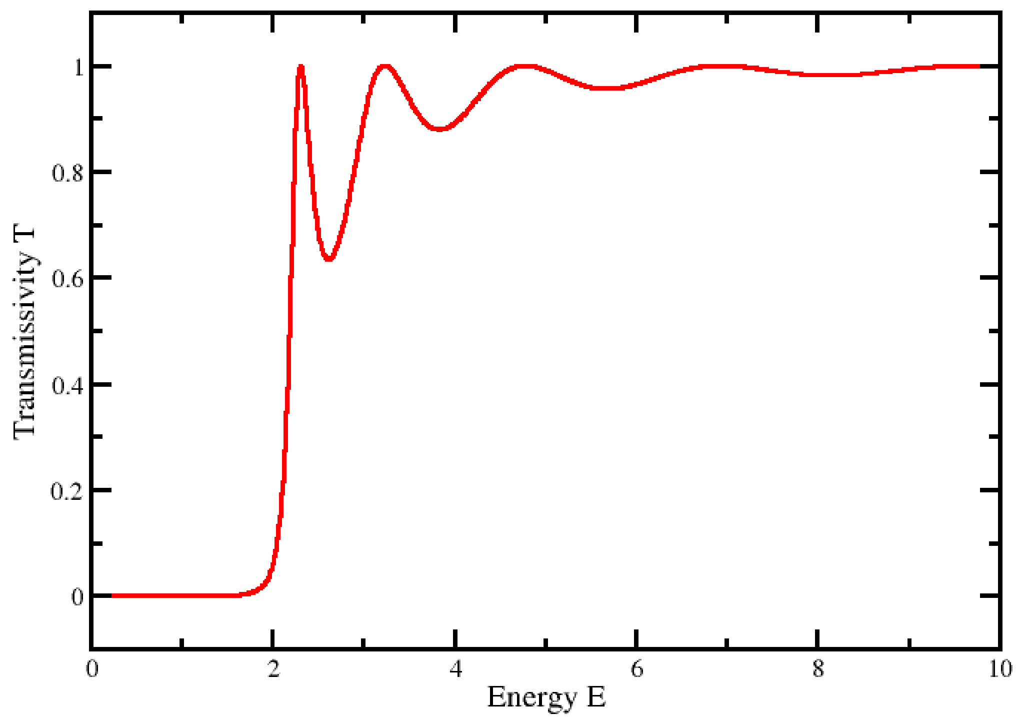

Figure 2. An exact transmissivity of a potential barrier.Here, $a = 2$, $\hbar = m = 1$, and $E = v0/2.$

The figure 2 shows the exact transmission coefficient for a single square barrier. It is seen from the figure that if $E \gg V0$, the transmission is equal to unity. Also, the maxima of the transmission coefficient, which is called resonances occur during the scattering. They are the result of a constructive interference between the incidence and the reflected waves. This phenomenon only occurs in the quantum regime because tiny particles manifest their wavelike nature.

Method

Although the Schrodinger equation 1 can be solved analytically for the second region, for the more complicated cases the procedure becomes complex or the analytic solution is unobtainable. First, we will solve the Schrodinger equation for $\Psi 2(x)$ in the case of a single barrier, and the method will be used also for the double barrier. We assume that $\Psi 1(x)$ and $\Psi 3(x)$ have been obtained analytically, but the coefficients A, B, and E will be determined during the process. The boundary conditions $x = 0$ and $x = a$ are

$$\Psi 1(0) = \Psi 2(0) \qquad (8)$$

$$\Psi 1(a) = \Psi 2(a) \qquad (9)$$

$$\Psi 1'(0) = \Psi 2'(0) \qquad (10)$$

$$\Psi 1'(a) = \Psi 2'(a) \qquad (11)$$

It is also worth to note that the wave functions and coefficients are complex variable.

To solve equation, the Runge-Kutta method of integration can be employed. The complete procedure of the Runge-Kutta method is described in the ref. [1].

The notation used, including the symbols, trace closely ref.[1]. If one choses $y1(x) = \Psi 2(x)$ and $y2(x) = \Psi 2'(x)$, the initial conditions at the point of initial integration point can be used. Because the potential is constant, the Schrodinger equation is a linear equation, and one can set $E = 1$. We start the integration from a to 0 using the Runge-Kutta algorithm. Our initial conditions are $y1(x) = \Psi 3(a) = 1$ and $y2(x) = \Psi 3'(a) = ik.$ The coefficients A and B are determined as the left edge of the barrier:

$$A + B = y1(0) \qquad (12)$$

$$ik(A - B) = y2(0). \qquad (13)$$

In calculation, the transmission coefficients we use is

$$T = |E| \cdot |E| / (|A| \cdot |A|) = 1/(|A| \cdot |A|). \qquad (14)$$

And the reflection coefficient by definition $R = 1 - T$.

The procedure is used also for the double barrier potential in the figure 6 since we find the wave functions in the intermediate regions numerically. Knowing only A and B will suffice to determine the transmission through the double barrier potential because $E = 1$.

Results

The results of the integration yield the following transmission versus energy graphs. In the figure 3, the calculated transmissivity and reflectivity of electrons through the single square barrier shown. Here, a=2, m=1, V0=2, and $\hbar$=1. From the figure 2 and 3 it is seen that the exact and computed values of the transmissivity are comparable. If the energy of the particles is lesser than the potential energy height, the transmissivity is low. An increase in energy results the higher transmissivity and the lower reflectivity. The resonant peaks in the graph indicate the existing interference between the incident and reflected waves.

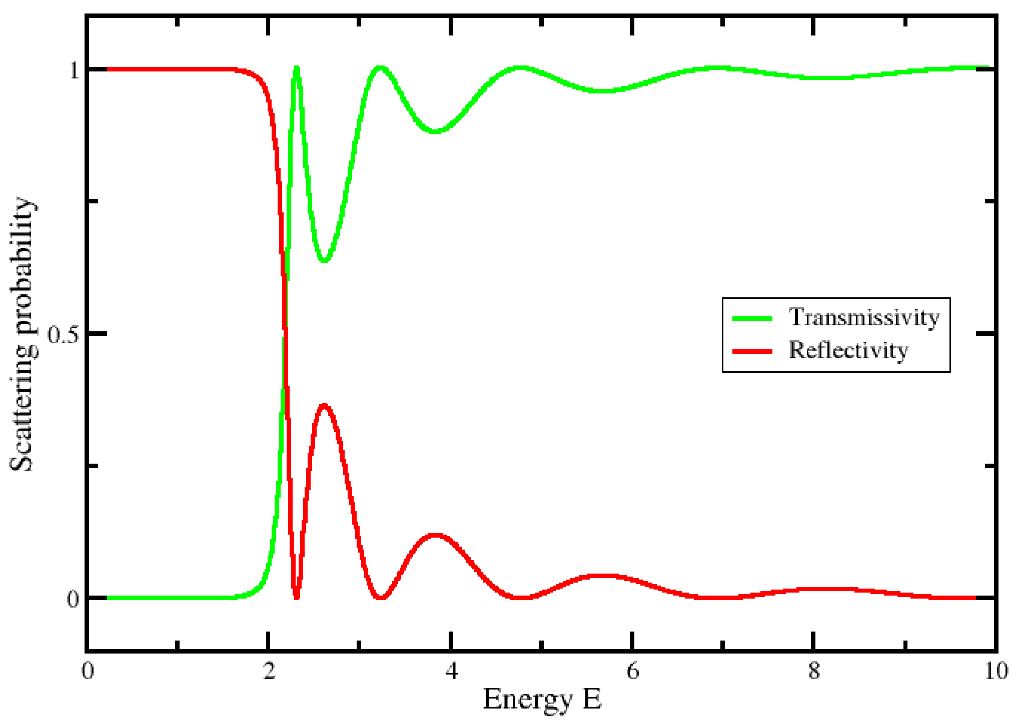

Figure 3. The transmissivity and the reflectivity of 1D barrier potential.

The figure shows the dependence of the occurrence of the resonance peaks on the barrier width. Although the thinner barriers transmit electrons with lower energies, they do not have noticeable resonance peaks.

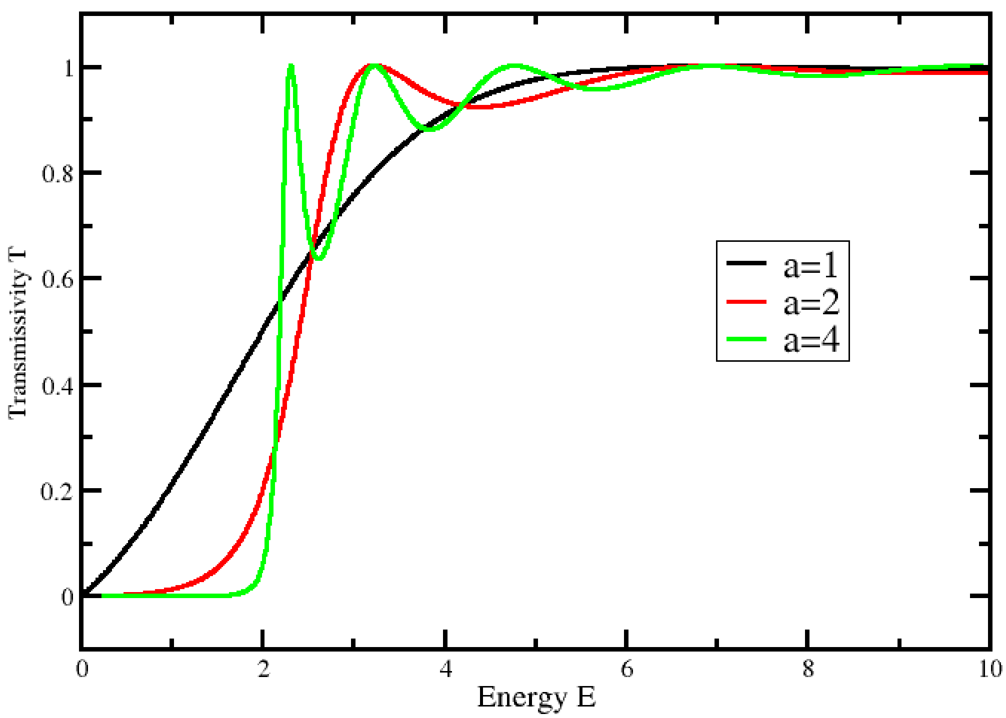

Figure 4. A transmissivity is as a function of an energy for various barrier widths.

The numerically obtained wave function in the second region is given in the figure 5. The eigenenergy, here, is half the barrier height. It is obvious that when the electrons are free, the real part of their wave functions are sine or cosine functions. When they are subject to a potential barrier, the wave function decays exponentially inside the barrier. Classically, it would be impossible for a particle to penetrate through the barrier, but a quantum particle has a finite probability of tunneling through the barrier. However, if the energy of the incident particle is large than the potential height, the wave function is oscillatory inside the barrier.

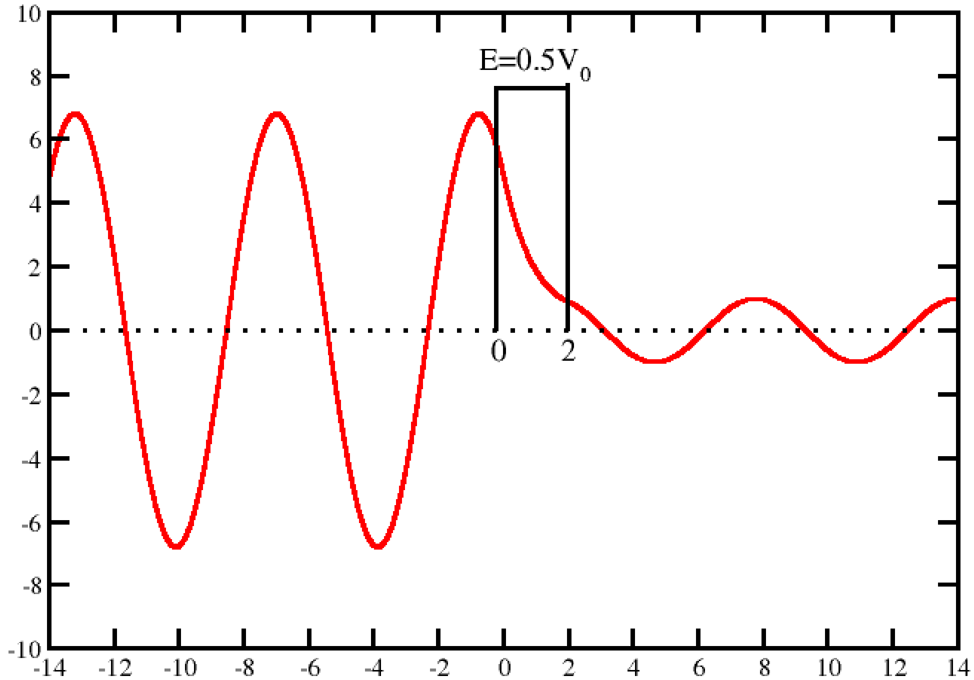

Figure 5. The electron wave function in the vicinity of a barrier potential

Let us now consider a double square potential given in the figure 6. The values of $x1$ *and* $x2$ may be changed. We would like to look at the symmetric and asymmetric double potentials. The incoming and the reflected waves are shown in the figure.

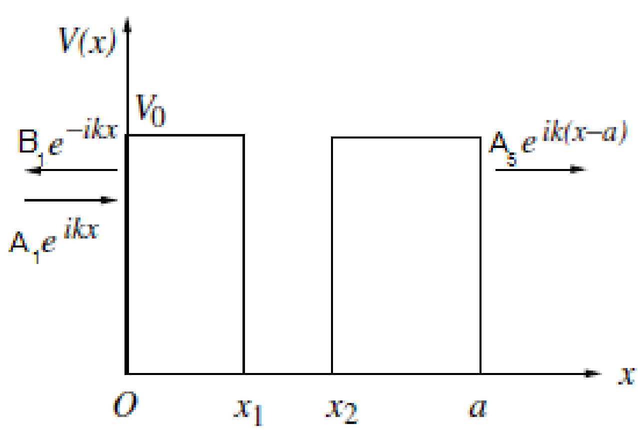

Figure 6. The double square quantum barrier potential.

As before, we can assume $A3 = 1$, and the transmission coefficient $T = 1/(|A1|\cdot|A1|)$. The integration is done from a to 0 point. This is very interesting problem because it has applications in quantum electronic devices. We have done calculations with electron's effective mass $m = 0.067me$ for the GaAs/Ga1-xAlxAs heterostructures. In the figure 7, the wave function is plotted for the symmetric potential with $V0 = 0.3\ eV,\ x1 = 5\ nm,\ x2 = 10\ nm,\ and\ a = 15\ nm.$ The wave functions in the absence of the barrier are oscillatory and decay exponentially inside the barrier. Here, the energy of electrons is smaller than the barrier height.

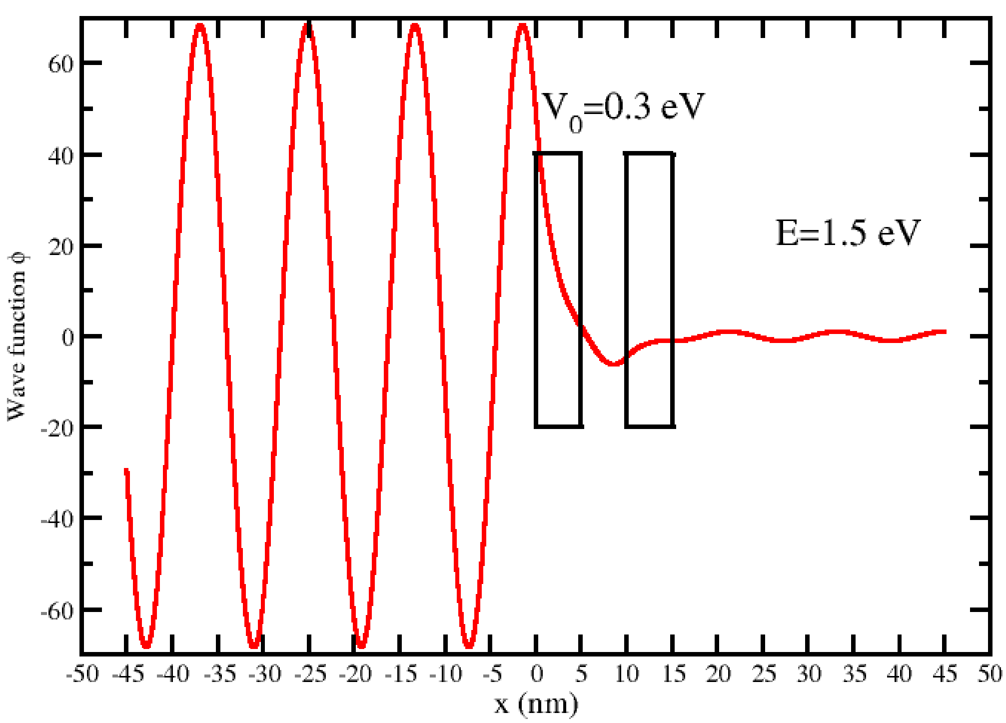

Figure 7. The electron wave function in the region of the double square barrier potential.

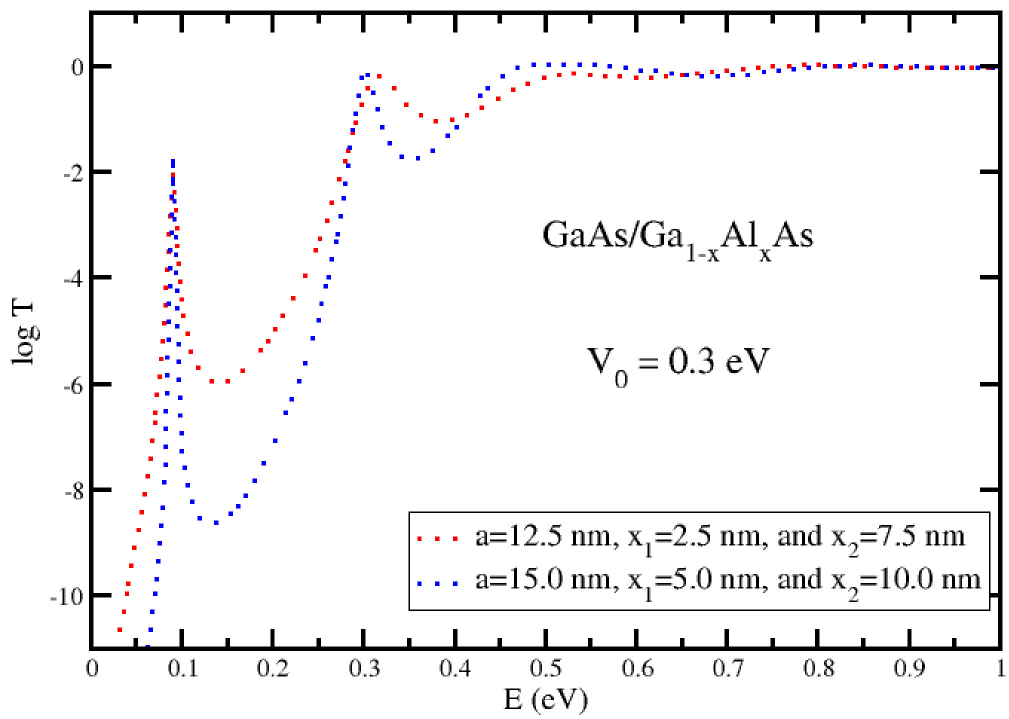

Figure 8. The energy dependence of the transmissivity for the double barrier potential with 0.3 eV height. Here, the barrier widths are 2.5 and 5.0 nm and the distance between the potentials is 5.0 nm.

The transmission coefficients for the asymmetric and symmetric double potentials are shown in the figure 8. There is a significant increase in transmissivity around a resonance energy $E \approx 0.09\ eV$ even though it is far less than the potential height.

It accounts for the interference pattern of oscillatory waves in the middle of barriers. The second height is slightly after the barrier height. The resonance peak for the symmetric double barrier is slightly larger than the asymmetric one. In tunneling through a single barrier is always less than one($E < V0$). Apparently, for the double barrier potential in certain energies it may be close to unity, so the double barrier may become transparent to the incoming particles. This is called a resonance tunneling. This phenomenon is used in resonant-tunneling diodes.

Conclusion

The Schrodinger equation is solved numerically for the single and double potential barriers using the Runge-Kutta algorithm. For the single barrier potential the transmissivity increases by increasing the energy, but it never reaches unity for the energies less than the potential height, whereas for the double barrier potential a resonant tunneling occurs for certain energies, and the barrier become transparent to the incident particles. This behavior of the double barrier potentials used in semiconductor heterostructures to make resonant-tunneling diodes.

References

1. T. Pang, An introduction to Computational Physics, 2006
2. N. Zetilli, Quantum Mechanics, 2001