TUNNELLING EFFECTS OF A GAUSSIAN WAVE PACKET IMPINGING ON A BARRIER

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Abstract: A general procedure based on momentum-like quantity provides the reflection and transmission amplitudes for a given barrier sandwiched by semiconductor reservoirs is presented. Furthermore, the evolution of the wave function stemming from an initial Gaussian wave packet located on the left hand side of the barrier with ignorable barrier overlap is obtained. The evolving wave function enables obtaining the associated probability and current densities space and time-wise. As application, the case of smooth double barrier is considered. The numerical results exhibit similar picture as obtained via propagator in the limited case of square barrier, *e.g.* repeated current density reversal at the barrier entrance, while being unidirectional at the exit. Presently, the treatment takes account of any barrier, inclusive of applied voltage. The basic quantity required is the value of the momentum-like quantity at the barrier entrance, which is obtained solving a Riccati equation governing the quantity, in question, whose value is known at the barrier exit in terms of the carrier energy and applied bias.

Keywords: quantum tunnelling, Gaussiam wave packet, potential barrier

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1. Introduction

In a previous paper [1] we dealt with the wave function resulting from an initial wave packet impinging on a square barrier. The procedure involved the relevant propagator. Consequently, through knowledge of the wave function we were able to obtain the associated probability and current densities, space and time-wise. However, the availability of the propagator, in general, for given barrier is limited and presently we shall deal with a procedure handling the situation involving any barrier, which can also take account of the influence of electric field. The work refers to a one dimensional case, as well as those appearing in the references, below. The case of applied transverse magnetic field requires further handling with regard to the dimensions of the impinging wave packet and will be dealt in subsequent work.

In the present work we consider a nanostructure made of a thin semi-insulating layer on either side of which a semiconducting, quite long, layer is attached. The semiconducting layers act as reservoirs, while a carrier along the width of the middle layer experiences the barrier potential.

In the literature one encounters papers dealing scattering of a particle initially in the form of wave packet impinging on a barrier. E.g. in [2] spatial probability density is reported at various times via numerical solution of the relevant Schrödinger equation in the cases of square well or square barrier. Paper [3] provides, in the case of double barrier, spatial distribution of the wave function absolute value at various times, as well as current densities at the barrier exit as function of time. The probability density in momentum representation in the case of square barrier is obtained analytically [4].

As, already, has been pointed out the propagator forms a useful tool for obtaining the wave function emanating from an initial wave packet impinging on a barrier. The case of square barriers and more general symmetric potentials of finite range the propagator is provided via employment of relevant green function [5]. A further way for obtaining propagators for tunnelling problems can be seen in [6].

As far as applications are concerned from the study of wave packet transmission through tunnelling barriers the reader can find in [7]. Essentially, they have to do with tunnelling times within the femptosecond region.

In section 2 a scheme leading to the wave function emanating from an initial wave packet impinging on any barrier, inclusive of applied electric field, is presented. From the wave function the associated probability and current density are obtained. Section 3 deals with numerical results concerning spatial distributions of probability and current densities at given times and furthermore their time evolution at the barrier entrance and exit. In addition, an example of the form of the real and imaginary part of the wave function is presented. Section 4 deals with conclusions.

2. Wave function emanating from an initial wave packet

As stated, earlier, we consider a nanostructure composed of a thin obstructive layer, whereby a barrier resides, together with a semiconductor reservoir attached on either side of the obstruction layer. A carrier along a straight line perpendicular to the obstructive layer experiences the barrier effect, within the portion of the line crossing the layer, while elsewhere the carrier is free in case of zero external applied field. For reasons of subsequent communication we introduce a 1D coordinate system with x-axis taken along a straight line as above, whose origin occupies the middle of the line portion through the layer. Furthermore, we denote the regions of the left hand side reservoir, the thin layer, and the right hand side reservoir by (1), (o), (2), correspondingly. Assuming the thickness of the obstructive layer to be $2a$ and the potential energy experienced by a carrier within the layer region along the x-axis expressed by $U_0(x)$,the total potential energy seen by a carrier upon application of bias, V, across the device takes the form

Potential energy		Region	
$U(x)=0$	$x\leq a$	(1)	(1)
$U(x)=U_0a-\frac{qV}{2a}(x+a)$	$-a\leq x\leq x$	(0)	(2)
$U(x)=qV$	$x\geq a$	(2)	(3)

q stands for the carrier charge (taken positive for reasons of simplicity). In what follows we consider the case whereby the carrier effective mass in the regions (1), (o), (2) is given correspondingly as, $m_j=\mu m_c, m_o=\mu_o m_c, m_2=\mu m_c$, where m_c s the carrier mass. For obtaining the reflection and transmission amplitudes we follow the procedure employed in [8]. As previously, we begin with relevant Hamiltonian

Region

$$H_j=-\frac{\hbar^2}{2\mu m_c}\frac{\partial^2}{\partial x^2} \qquad (1) \tag{4}$$

$$H_o=-\frac{\hbar^2}{2\mu_o m_c}\frac{\partial^2}{\partial x^2}+U(x) \qquad (0) \tag{5}$$

$$H_2=-\frac{\hbar^2}{2\mu m_c}\frac{\partial^2}{\partial x^2}-qV \qquad (2) \tag{6}$$

The Schrödinger equation in the regions (1), (o), (2) takes the form

$$\left[-\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial x^2}+U_i(x)\right]\Phi_i(x)=E\Phi_i(x) \qquad (i=1,o,2) \tag{7}$$

where $U_i(x)$ stands for the potential energy in the regions $i=(1,o,2)$ given in (1), (2), (3). Clearly, we have the same energy eigenvalue, E, in the three regions, given by

$$E=\frac{\hbar^2k^2}{2\mu m_c} \tag{8}$$

For the purpose of transmission the wave function is taken in the form

$$\Phi_i=e^{ikx}+Re^{-ikx} \tag{9}$$

$$\Phi_o=\Phi_o(x) \tag{10}$$

$$\Phi_2=Te^{ikx} \tag{11}$$

R and T stand correspondingly for the reflection and transmission amplitude, and k being the wave number of the incoming plane wave in region (1). The incoming kinetic energy is given by the energy eigenvalue (8), which is the incoming kinetic energy. Finally, from Schrödinger equation (7) in region (2) we obtain the wave number k associated with the transmitted wave in region (2) as

$$K=\frac{1}{\hbar}\sqrt{2\mu m_c+(E+qV)} \tag{12}$$

At this point we introduce the longitudinal momentum-like quantity (pseudo-momentum) in the region (o) as

$$P_o(x)=\frac{\hbar}{i}\frac{\Phi_o'(x)}{\Phi_o(x)} \tag{13}$$

$\Phi_o'(x)$ in (13) stands for the derivative of Φ_o with respect to x. Utilizing Schrödinger's equation (7), in region (o), in conjunction with (13) we are led to the equation governing $P_o(x)$ as

$$\frac{\hbar}{2m_o i}\frac{dP_o(x)}{dx}+\frac{P_o(x)^2}{2m_0}+U_o(x)-\frac{qV}{2a}(x+a)=E \tag{14}$$

We shall now proceed to obtain the reflection and transmission amplitudes, R and T, with the aid of the pseudo-momentum equation (8). We begin with the continuity conditions

$$\Phi_1(-a)=\Phi_o(-a), \qquad \frac{1}{\mu}\Phi_1'(-a)=\frac{1}{\mu_o}\Phi_o'(-a) \tag{15}$$

$$\Phi_o(a)=\Phi_2(a), \qquad \frac{1}{\mu_o}\Phi_o'(-a)=\frac{1}{\mu}\Phi_2'(a) \tag{16}$$

From (12) and (15) we obtain the pseudo-momentum value at the barrier exit as

$$P_o(a)=\frac{\mu}{\mu_o}\sqrt{2\mu m_c(E+qV)} \tag{17}$$

Solving, now, (14) under condition (17) we have $P_0(-a)$, the value of $P_0(x)$ at the barrier entrance, $x=-a$. Having obtained $P_o(-a)$ we can through combination of (13) in region (o) together with the aid of the continuity conditions (15) obtain the reflection amplitude as

$$R=\frac{\mu_o\hbar k-\mu p_0(-a)}{\mu_o\hbar k+\mu p_0(-a)}e^{-i2ka} \tag{18}$$

Utilizing (11) together with (16) the transmission amplitude can be expressed as

$$T=\Phi_o(a)e^{-iKa} \tag{19}$$

However, there remains to specify $\Phi_o(a)$ which can be obtained solving the differential equation $\Phi_o'(x)=\frac{i}{\hbar}P_o(x)\Phi_o(x)$ provided by (13). The solution, in question, is given by

$$\Phi_o(x)=\exp\left[\frac{i}{\hbar}\int_{-a}^{x}P_o(x')dx'\right]\Phi_o(-a) \tag{20}$$

Taking account of $\Phi_1(-a)=\Phi_o(-a)$ in (15) and furthermore (9), (18), (19) and (20) we arrive at the following expression for the transmission amplitude

$$T=\frac{2\mu_o\hbar k}{\mu_o\hbar k+\mu P_o(-a)}\exp\left[\frac{i}{\hbar}\int_{-a}^{a}P_o(x')dx'-i(k+K)a\right] \tag{21}$$

With the above we have at our disposal the wave function in the regions (1), (o), (2) relating to plane wave transmission as described in formulae(9), (10), (11). Our aim is to exploit knowledge of the above solution for obtaining the wave function, time and space-wise, emanating from an initial wave packet located within the left hand side region (1). Prior to proceeding to the problem, in question, it is necessary to note that the wave function solution is valid not only for $k, K \geq 0$ (incoming and transmitted wave), and in addition $k, K < 0$. This result provides a complete set of wave functions, necessary for attaining the purpose of the required wave function. In addition, since the wave function solution for (9), (10), (11) corresponds to a given k it would be useful denoting the solution, in question, as $\Phi_j(k,x)$, $(j = 1, o, 2)$.

As pointed out, earlier, our problem has to do with the time evolution of the wave function deriving from an initial wave packet lying effectively in region (1). The form of the initial wave packet is expressed as

$$\Phi(x) = \frac{1}{\left(2\pi s^2\right)^{1/4}} \exp\left[-\frac{1}{4s^2}\left(x - x_o\right)^2 + \frac{i}{\hbar} p_o \left(x - x_o\right)\right] \tag{22}$$

where x_0, p_o and s re respectively the wave packet center, mean momentum and mean spread. The parameters x_o and s are such the wave packet overlap with the barrier be negligible. On account of the fact that the wave packet (22) in the regions (o) and (2) is highly negligible we can proceed expanding (22) in plane waves via Fourier transform, although the procedure involves integration over x, which goes beyond region (1). We have

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi_g(k) e^{ikx} dk \tag{23}$$

where

$$\Phi_g(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi(x) e^{-ikx} dx = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{s} \, \exp\left[-s^2 \left(k - \frac{P_o}{\hbar}\right)^2 - ikx_o\right] \tag{24}$$

Owing to the linearity of Schrödinger's equation the expression

$$\Psi_j(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi_g(k) \Phi_j(k,x) \exp\left(-\frac{i}{\hbar} Et\right) dk, \quad E = \frac{\hbar^2 k^2}{2\mu m_c} \quad (j = 1, o, 2) \tag{25}$$

constitutes the required time dependent solution of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi_j = H_j \Psi_j \qquad (j = 1, o, 2) \tag{26}$$

H_j stands for the Hamiltonian in region $j, (j = 1, o, 2)$ given in (2).
At time $t = 0$ the wave function (25) in region (1) becomes

$$\Psi_j(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi_g(k) \left(e^{ikx} + Re^{-ikx}\right) dk \tag{27}$$

Under the condition whereby the initial wave function (22) has negligible overlap with the barrier region the reflection effect at time $t = 0$ is also negligible.

Therefore, the condition $\Psi_1(x,0)=\Phi(x)$ is essentially satisfied. Results concerning the wave function in all regions as time evolves, as well as with regard to probability and current density will be presented in the next section. Closing the present section we state the expressions for the probability and current densities, p_i and J_i, associated with the wave function $\Psi_i(x,t)$ in region .

$$p_i(x,t)=\left|\Psi_i(x,t)\right|^2, \quad J_i(x,t)=\frac{\hbar}{m_i}\mathrm{Im}\left[\Psi_i^*(x,t)\frac{\partial}{\partial t}\Psi_i(x,t)\right] \quad (i=1,o,2) \tag{28}$$

3. Numerical results

In this section we present results via which one can form a picture of the spatial distribution of the probability and current densities at given times, as well as their corresponding time evolution at the barrier entrance and exit. Example relating to the form of the wave function is also given. For the purpose of facilitating the numerical results, which follow, we introduce an appropriate dimensionless scheme utilizing as basic unit the unit of energy, $E_u = 0.1\mathrm{eV}\simeq 1.38062\times 10^{-13}$ erg. The choice of the above unit relies on the fact that the various barrier heights in the nanostructures are on the order of a few tenths of eV. On the basis of the unit, in question, together with the carrier particle mass, m_c, and Planck's constant, t, we form the units of time, length, and momentum correspondingly as

$$T_u=\frac{\hbar}{E_u}, \quad L_u=\frac{\hbar}{\sqrt{m_c E_u}}, \quad P_u=m_c\frac{L_u}{T_u}=\sqrt{m_c E_u} \tag{29}$$

Employing for m_c the electron mass $m_c = 9.109558\times 10^{-28}$ g, $\hbar = 1.054559\times 10^{-27}$ erg.s, the units in (29) take the values: $T_u = 6.58198\times 10^{-15}$ s, $L_u = 8.27901\times 10^{-15}$ cm, $P_u = 1.20811\times 10^{-20}$ g.cm/s.

Utilizing the above system of units we can deal with dimensionless quantities, just by setting in Schrödinger's equation (7) $\hbar=1$ and $m_c=1$. The various dimensional results are obtained from the acquired dimensionless quantities times their associated units, given in (29). Employing the procedure, in question, we can obtain via (25) the required wave function $\Psi_i(x,t)$ $(i=1,o,2)$ from which we can derive, via (28), the associated probability and current densities and, furthermore, the reflection and transmission amplitudes correspondingly through (18) and (21).

In what follows we shall deal with a potential energy barrier, $U_o(x)$, given by

$$U_o(x)=\frac{u_o}{4}\left\{\sin\left[\frac{2\pi}{\lambda}\left(x-\frac{\lambda}{4}\right)\right]+1\right\}^2 \tag{30}$$

extending over the range $-a\le x\le a$, u_0 being the barrier potential energy height. Taking $a=\lambda$ (30) represents a smooth double barrier.

In the ensuing results we make use of data in common with regard to the potential barrier being $u_o = 5E_u$, $\lambda = 4L_u$, while for the wave packet the width, the location, and mean momentum are taken correspondingly as $s=0.4L_u$,

$x_o = -25L_u$, $p_o = 1.5P_u$. Although in the previous section the scheme presented involved effective masses for the barrier region and the reservoirs, presently we are not making use of the parametric facility, in question. However, the general picture provided by the results is not essentially affected. The figures, below, refer to barrier potential energies, probability and current densities, as well as a case of wave function. In particular, Figure 1 depicts the barrier potential energy, without and with applied bias. Figure 2 in (a) depicts the initial probability density as well as its form after a short time, $t = 1T_u$, while in (b) the corresponding current densities. Figure 3 shows in (a) and (b) correspondingly probability and current densities at time, $t = 8T_u$. Figure 4 shows probability and current density evolutions at the barrier entrance free of bias and under $V = 2V_u$ bias. Figure 5 shows the corresponding probability and current density time evolutions of Figure 4 as appearing at the barrier exit. Finally, in Figure 6 are shown real and imaginary part of the form the wave function takes at time $t = 8T_u$ while the barrier is under bias $V = 2V_u$.

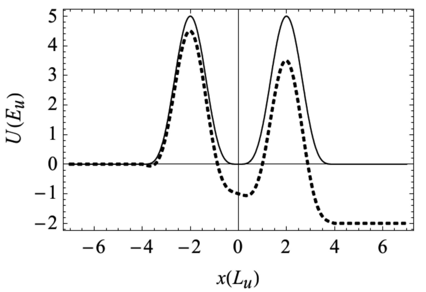

Figure 1. Continuous curve shows barrier potential energy for smooth double barrier, as obtained from formula (30) in region $(-a, a)$, $a = \lambda$, $\lambda = 4L_u$ and height $u_o = 5E_u$. Dashed curve shows barrier potential energy, above, under bias, $V = 2V_u$, in barrier region and part of the sandwiching reservoirs

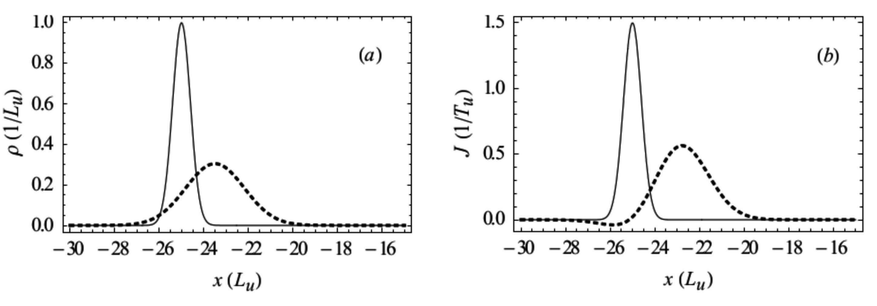

Figure 2. (a) Probability density spatial distributions emanating from an initial wave packet (data for s, x_o, p_o, as in common) at time $t = 0$ impinging on barrier (data for u_o, λ as in common) under bias, $V = 2V_u$ (solid curve) and at $t = 1T_u$ (dashed curve). (b) Corresponding spatial current density at time $t = 0$ (solid curve) and at $t = 1T_u$ (dashed curve)

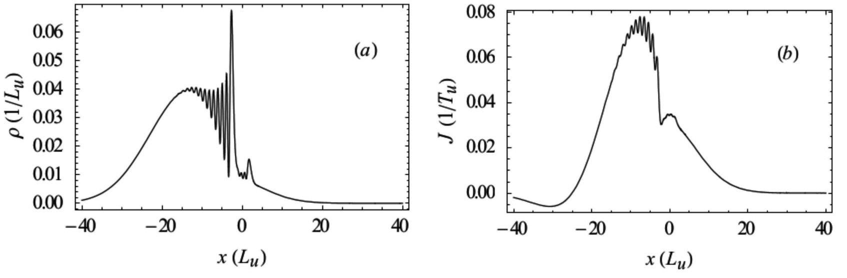

Figure 3. (a) Probability density spatial distribution at time $t = 8T_u$, emanating from an initial wave packet (data as in common) impinging on barrier under bias $V = 2V_u$ (rest of data as in common). (b) Corresponding current density spatial distribution

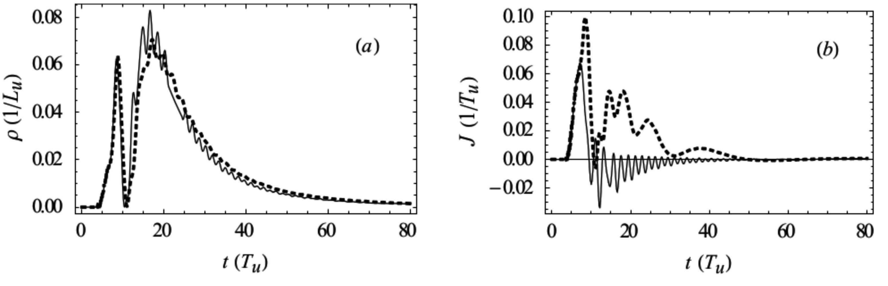

Figure 4. (a) Time evolution of probability density at the barrier entrance, $x = -4L_u$, emanating from an initial wave packet (data as in common) impinging on barrier (data as in common); Without bias, continuous curve, Dashed curve, bias $V = 2V_u$. (b) Corresponding current density time evolutions

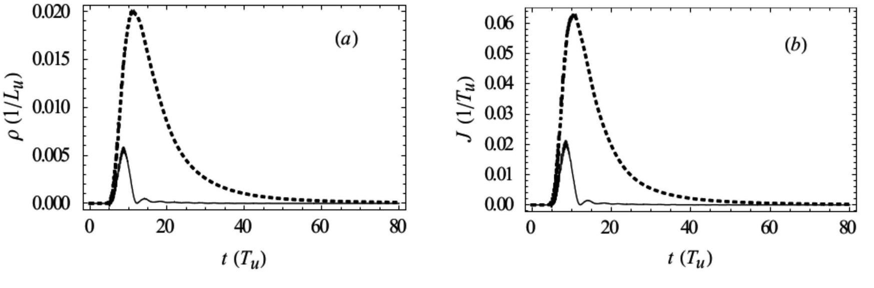

Figure 5. (a) Time evolution of probability density at the barrier exit, $x = 4L_u$, emanating from an initial wave packet (data as in common) impinging on barrier (data as in common); Without bias, continuous curve, Dashed curve, bias $V = 2V_u$. (b) Corresponding current density distributions

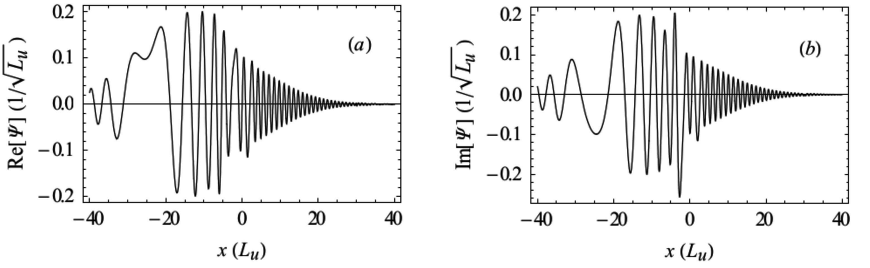

Figure 6. Shows large part of the wave function emanating from an initial wave packet (data as in common) impinging on barrier (data as in common) under bias, $V = 2V_u$, at time $t = 8T_u$. (a) refers to the real part of the wave function, while (b) to the imaginary part

4. Conclusion

Presently, we dealt with a limited number of parameters in conjunction with the tunneling effects of a Gaussian wave packet impinging on a barrier. However, the main characteristic lies in that the methodology, employed, applies for any barrier.

Another remark, worth mentioning, has to do with the oscillatory nature of the current density at the barrier entrance, in and out of the barrier, while it exits the barrier uni-directionally.

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