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A general formula for the transmission coefficient through a barrier and application to $I-V$ characteristic*

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A general formula providing the transmission coefficient through a given barrier, sandwiched by semiconductor reservoirs under bias is presented in terms of the incoming carrier energy and the logarithmic wave function derivative at the start of the barrier. Furthermore, the formula involves the carrier effective masses in the barrier and reservoir regions. The procedure employed is based on solving an appropriate Riccati equation governing the logarithmic derivative along the barrier width at the end of which it is known in terms of the carrier energy and applied bias. On account of the facility provided for obtaining the transmission coefficient we obtained the $I-V$ characteristic of a quantum dot carved barrier, which exhibits a region of quite a large negative differential resistance together with a high peak to valley ratio. Under the circumstances, the possibility of developing a nanostructure switch utilizing a small variation in the applied bias exists.

Keywords: *transmission coefficient, momentum related quantity, $I-V$ characteristic*

1. Introduction

In a previous paper [1] the $I-V$ characteristic for a truncated parabolic barrier was obtained. The methodology employed, relied on finding the scattering wave function pertaining to the problem, from which the transmission coefficient in terms of the applied voltage was obtained. Once the transmission coefficient becomes available, the $I-V$ characteristic can be acquired via the Tsu-Esaki formalism [2, 3]. Another way of reaching the transmission coefficient is based on the analytical transfer matrix (ATM) method [4, 5]. With the ATM procedure one can tackle the transmission coefficient for any form of barrier, which in general requires numerical handling.

In the present work we consider a nanostructure made of a thin semi-insulating layer with a semiconducting layer attached on either side. The semiconducting layers act as reservoirs, while a carrier along the width of the middle layer experiences the barrier potential energy. The aim of the present work is to provide a scheme for obtaining the transmission coefficient associated with the barrier potential energy inclusive of its modification by the application of an electric field across the nanostructure. With the facility of handling the transmission coefficient, in general, the $I-V$ characteristic of the nanostructure readily follows.

In Section 2 we proceed to obtain a formula for the transmission coefficient under bias on the basis of a momentum related quantity, $p(x)$, proportional to the logarithmic wave function derivative. The coefficient of proportionality is $\hbar/i$, and x stands for the carrier spatial coordinate along the barrier width. The reason for the above modification lies in showing the emergence of coincidence of the quantum mechanical equation governing $p(x)$ with the classical equation of energy conservation in the limit $\hbar \to 0$. Details concerning the above follow in the subsequent section.

In Section 3 the formalism developed for obtaining the transmission coefficient as a function of the applied voltage is employed numerically in the case of a barrier carved in the form of a parabolic dot under bias. The result is subsequently employed in conjunction with the

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Tsu-Esaki formalism for the $I-V$ characteristic. The study shows the possibility of having a region in the applied voltage whereby the $I-V$ characteristic exhibits an increased negative differential resistance (strong drop in current over a short interval of V) with appreciable peak to valley ratio.

2. Transmission coefficient

As pointed out earlier, our nanostructure consists of a thin obstructive layer with a semiconducting reservoir attached on either side. For the purpose of facilitating subsequent discussions we introduce a tri-orthogonal reference frame, $Oxyz$, relative to the nanostructure, as follows. The x-axis is taken perpendicular to the thin layer, and the origin occupies the middle of the perpendicular line through the layer in question. The y and z-axes are taken so that, together with the x-axis, they form a tri-orthogonal system. The carrier motion in the x-direction is governed by combination of the barrier and applied field force together with the prevailing thermal state of affairs. The motion in the yz- plane is essentially of thermal origin. For reasons of subsequent communication, we shall denote the regions in the left reservoir, the thin semi-insulating layer, and the right reservoir by (1), (0) and (2) correspondingly. Assuming the thickness of the thin obstructive layer to be $2a$ and the potential energy experienced by a carrier within the layer region in the x-direction expressed by $U_o(x)$, the potential energy seen by a carrier upon application of a bias, V, across the device can take the form:

$$U(x) = 0, x \leq -a \qquad (region(1)) \tag{1a}$$

$$U(x) = U_o(x) - q\varepsilon(x+a),\ -a < x < a\ (region(0)) \tag{1b}$$

$$U(x) = -2q\varepsilon a,\ x \geq a \qquad (region(2)) \tag{1c}$$

q stands for the carrier's charge and $\varepsilon = V/2a$ for the electric field experienced by the charge in the obstructive layer region. It should be noted that a certain displacement in the electric field is required for taking account of the layer dielectric properties.

We consider the case whereby the carrier effective mass in the three potential energy regions, (1), (0), (2), to be given correspondingly by $m_1 = \mu_1 m_c, m_o = \mu_o m_c,\ m_2 = \mu_2 m_c$, where m_c stands for the carrier mass. The usual way for obtaining the transmission coefficient, in this case, requires the scattering solution of the relevant Schrödinger equation

$$[-\frac{\hbar^2}{2m_i}\frac{\partial^2}{\partial x^2} + U_i(x)]\Psi_i(x) = E\Psi_i(x)(i = 1,0,2) \tag{2}$$

where $U_i(x)$ is given by (1a,1b,1c). The scattering wave function in the three regions attains, as usual, the form

$$\Psi_1 = e^{ik_1x} + Re^{-ik_1x}, \quad x \leq -a \tag{3a}$$

$$\Psi_o = \Psi_o(x), \quad -a \leq x \leq a \tag{3b}$$

$$\Psi_2 = Te^{ik_2x} \quad x \geq a \tag{3c}$$

Ψ_1 is made out of an incoming and a reflected wave, while Ψ_2 stands for an outgoing wave, and Ψ_o is the prevailing wave function within the barrier region. For obtaining the tunneling solution of (2) in terms of the wave function (3a, 3b, 3c), apart form considering energy conservation throughout the three regions, the probability and current densities at the barrier boundaries must be continuous. These conditions are guaranteed by:

$$\Psi_1(-a) = \Psi_o(-a), \Psi_o(a) = \Psi_2(a) \tag{4a}$$

$$\frac{1}{m_1}\Psi_1'(-a) = \frac{1}{m_o}\Psi_o'(-a), \frac{1}{m_o}\Psi_o'(a) = \frac{1}{m_2}\Psi_2'(a) \tag{4b}$$

where in (4b) prime indicates spatial derivative.

It should be noted that the wave function (3), as it stands, is not normalized, but as it is well known this does not affect the outcome for the transmission coefficient utilizing such a solution to the Schrödinger equation (2) as long as the conditions (4a, 4b) are satisfied.

Once the tunneling solution becomes available the transmission coefficient, T_r, can be obtained utilizing the expressions for incoming and outgoing current densities

$$J_{inc} = \frac{\hbar k_1}{m_1} \tag{5a}$$

$$J_{out} = \frac{\hbar k_2}{m_2} |T|^2 \tag{5b}$$

where k_1 and k_2 are related to the energy eigenvalue, E, via

$$\hbar k_1 = \sqrt{2m_1 E}, \quad \hbar k_2 = \sqrt{2m_2(E+qV)} \tag{6}$$

The transmission coefficient takes the form

$$T_r(E,V) = \frac{J_{out}}{J_{inc}} = \sqrt{\frac{\mu_1(E+qV)}{\mu_2 E}}\,|T|^2 \tag{7}$$

In order to find the coefficient T one has to solve Schrödinger's equation (2) under the continuity conditions (4a, 4b). Cases suitable for analytical treatment are limited, and in general one has to proceed numerically.

In what follows we shall present another way for handling the tunneling problem, based on some sort of momentum related quantity, $p(x)$, constructed via the momentum operator, $-i\hbar\partial/\partial x$, as

$$p(x) = \frac{\hbar}{i}\frac{\Psi'(x)}{\Psi(x)} \tag{8}$$

The quantity $p(x)$ is in general complex. Prior to proceeding with $p(x)$ for our tunneling purposes, certain remarks concerning $p(x)$ would seem in order. Taking into account that $\Psi(x)$ satisfies Schrödinger's equation, one is led to the following equation for $p(x)$

$$E = \frac{p^2}{2m} + U(x) + \frac{\hbar}{2mi}\frac{\partial p}{\partial x} \tag{9}$$

Clearly, in the limit of $\hbar \to 0$ (classical regime) (9) goes to the classical expression for energy conservation, and provides the classical local momentum value. The last term in (9) takes care of the quantum situation for a given energy, E, and potential energy, $U(x)$. It is precisely the last term in (9) that makes the difference between the classical and quantum mechanical considerations and enables transmission across a barrier even if the impinging particle's kinetic energy is smaller than the barrier's height.

Let us, now proceed to handle tunneling via equation (9) for p, taking account of the continuity conditions (4a, 4b). The forms of the required solutions for p in the regions (1) and (2), denoted by p_1 and p_2, are easily accessible from the corresponding forms of the wave functions Ψ_1 and Ψ_2 We have, via (8)

$$p_1 = \hbar k_1 \frac{e^{ik_1x} - Re^{-ik_1x}}{e^{ik_1x} + Re^{-ik_1x}}, p_2 = \hbar k_2 \tag{10}$$

where $\hbar k_1$ and $\hbar k_2$ are given in terms of the energy eigenvalue, E, through (6). Clearly, p_2 is fully specified, while for p_1 the reflection amplitude, R, has to be determined. The solution for p_o in the barrier region has to be obtained from the associated Riccati equation (9) with $U(x) = U_o(x) - qV(x+a)/2a$ and $m = \mu_o m_c$. Under the continuity condition at $x = a$, $p_o(a)$ can be expressed as

$$p_o(a) = \frac{\mu_o}{\mu_2}\sqrt{2\mu_2 m_c(E+qV)} \tag{11}$$

For obtaining the above condition we have made use of the relations $p_o(a) = \hbar\Psi_o'(a)/i\Psi_o(a) = \hbar m_o\Psi_2'(a)/im_2\Psi_o(a)$, which incorporate the continuity conditions (4b) at $x = a$.

Let us now assume that the solution to (9) in the barrier region satisfying the condition (11) is available. Taking account of the probability and current continuity conditions (4a, 4b) at $x = -a$ expressed as

$$\hbar\Psi_o'(-a)/i\Psi_o(-a) = \hbar m_o\Psi_1'(-a)/im_1\Psi_1(-a) =$$

$$m_o p_1(-a)/m_1,$$

we obtain, utilizing (10)

$$p_o(-a)=\frac{\mu_o}{\mu_1}\sqrt{2\mu_1 m_c E}\frac{e^{-ik_1a}-Re^{ik_1a}}{e^{-ik_1a}+Re^{ik_1a}} \quad (12)$$

Form (12) we can determine the reflection coefficient $|R|^2$ from which we can form the expression for the transmission coefficient, via

$$T_r=1-|R|^2 \quad (13)$$

which takes the form

$$T_r(E,V)=\frac{Q1}{Q2+Q3} \quad (14)$$

where

$$\begin{aligned} Q1 &= 4\mu_o\mu_1\sqrt{2\mu_1 m_c E}Re[p_o(-a)] \\ Q2 &= 2\mu_o^2\mu_1 m_c E+\mu_1^2|p_o(-a)|^2 \\ Q3 &= 2\mu_o\mu_1\sqrt{2\mu_1 m_c E}Re[p_o(-a)] \end{aligned} \quad (15)$$

Formula (14) supplies the transmission coefficient for any barrier, provided one can solve the Riccati equation (9), associated with the barrier region under condition (11). The equation, in question, can be solved analytically in certain cases, but in general numerically. It should be noted here, that the method, laid above, bears similarities to the ATM method [4, 5], but the present procedure appears simpler, as far as the process for obtaining the transmission coefficient is concerned. It essentially involves solving a Riccati equation in the barrier region.

3. $I-V$ characteristic and numerical results

For the $I-V$ characteristic relating to a barrier nanostructure consisting of a barrier with a reservoir attached on either side we employ the Tsu-Esaki formula [2, 3]. In our case it is modified to account for the case of different effective masses in the barrier and reservoir regions [1]. For the current density in terms of the applied voltage, V, and temperature, T, we have:

$$\begin{aligned} J(V)=\frac{em_c\kappa T}{2\pi^2\hbar^3}\int_0^\infty & T_r(E,V) \\ \times\{\mu_1\, ln\left[1+\exp\left(\tfrac{E_{fl}-E}{kT}\right)\right] & \\ -\mu_2 ln\left[1+\exp\left(\tfrac{E_{fr}-qV-E}{kT}\right)\right]\Big\}\, dE & \end{aligned} \quad (16)$$

where κ stands for the Boltzmann constant and E_{fl}, E_{fr} are correspondingly the chemical potentials for the left and right hand side reservoirs at temperature T and zero field. When $\mu_1=\mu_2$, $E_{fl}=E_{fr}$. In case $\mu_1\neq\mu_2$, for given E_{fl} one can obtain E_{fr} solving $J(V=0)=0$ with respect to E_{fr}.

In what follows, we shall proceed with numerical evaluations utilizing as a basic unit the energy unit, $E_u=0.1$ eV$=1.602191710^{-13}$ erg from which, via $\hbar^2/m_cL_u^2=E_u$, the unit of length is derived as $L_u=\hbar/\sqrt{m_cE_u}$. The momentum unit becomes $p_u=\hbar/L_u=\sqrt{m_cE_u}$. The voltage unit is given as $V_u=E_u/e$, where e stands for the absolute value of the electron charge. Finally, the current density unit, J_u, will be the product of the pre-factor of the integral in (16) times E_u, i.e. $J_u=em_c\kappa TE_u/2\pi^2\hbar^3$or $J_u=e\kappa T/2\pi^2\hbar L_u^2$. Furthermore, for reasons of simplicity, we shall be dealing with the absolute value of the electron charge, e, which will be taken as the charge for our carriers.

Let us now consider a nanostructure with barrier potential energy $U_o(x)=u_ox^2/a^2$ in the region $-a<x<a$. The potential energy seen by a carrier under applied voltage, V, in the whole range of the nanostructure, which includes the reservoirs, is described by (1a, 1b, 1c) and takes the form

$$\begin{aligned} U(x)=\Theta(x+a)0+[\Theta(x+a)-\Theta(x-a)] & \\ \times[u_o\frac{x^2}{a^2}-e\frac{V}{2a}(x+a)]+\Theta(x-a)eV & \end{aligned} \quad (17)$$

where Θ stands, as usual, for the step unit function. An instance of the carrier potential energy (17) is depicted in Fig. 1, whereby the combined potential energy experienced by a carrier due to a parabolic quantum dot carved square barrier and an applied electric field extending in the attached reservoirs, each on either side of the barrier.

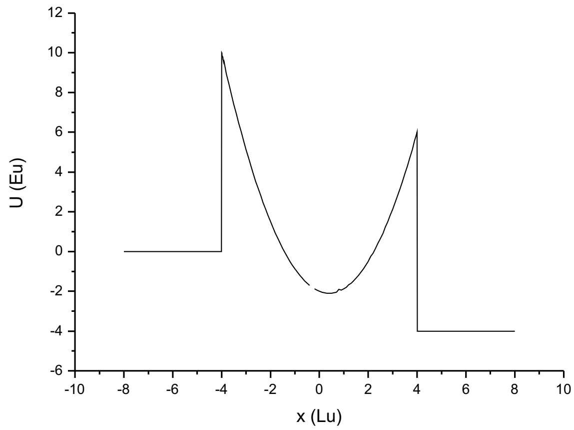

Fig. 1. The combined potential energy experienced by a carrier (formula 17). Data: Barrier height $u_o = 1$ eV, applied voltage $V = 0.4$ Volt, and barrier width $2a = 8L_u$. Horizontal axis in units $L_u = 0.872928$ nm, and vertical in $E_u = 0.1$ eV.

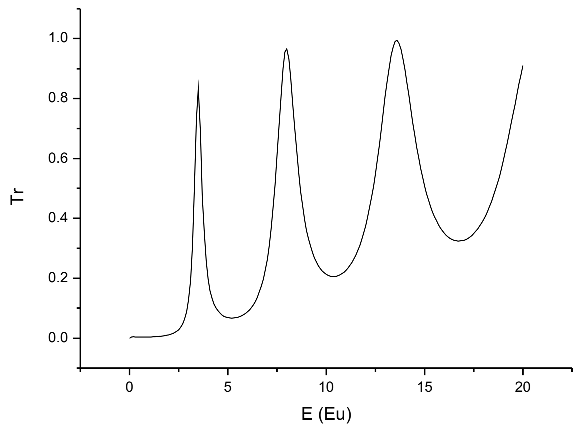

Fig. 2. Transmission coefficient oscillations as a function of the carrier energy. Data: Barrier height, u_o, applied voltage, V, and barrier width, $2a$, as in Fig. 1. Furthermore, the effective masses in the three regions of the nanostructure are characterized by the parameters $\mu_1 = \mu_2 = 0.02$, and $\mu_o = 0.1$. Horizontal axis in units E_u.

Employing the momentum-like Riccati equation (9) in the barrier region under condition (11), we can obtain the quantity $p_o(-a)$ which via (14) leads to the corresponding transmission coefficient. The procedure involves numerical solution which for a given V supplies $T_r(E,V)$ for a dense sequence of values of E ranging from 0 to quite a large value of E. Subsequently using interpolation we can obtain a continuous function of the transmission coefficient in terms of E for the given applied voltage, V. An example of the function, in question, is given in Fig. 2.

Once we are able to obtain the transmission coefficient for a given V and a sufficiently large range of E we proceed via (16) to obtain the current density for the applied voltage, V. It should be noted that the value of the logarithmic expression in the curly brackets in the integrand in (16) beyond a certain value of E becomes essentially zero. Repeating the procedure for a dense sequence of V starting from zero we are led to a graph for the current density in terms of the applied voltage, V, for a given temperature, T. Fig. 3 provides such an example.

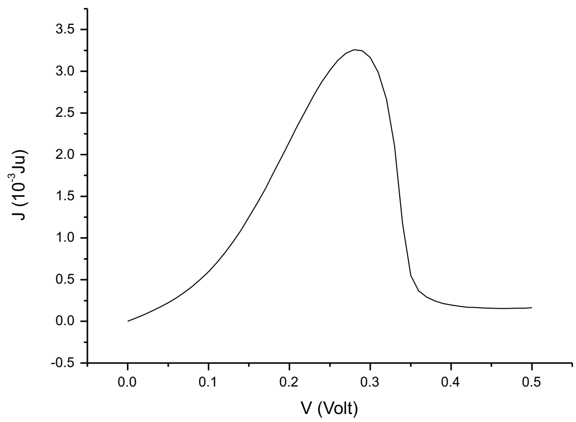

Fig. 3. Strong drop in current density as a function of applied voltage. Data: As in Fig. 2, apart from V, which now is a variable, and furthermore the left hand side reservoir chemical potential $E_{fl} = 0.1eV$ and the device temperature $T = 300$ K, for which $Ju = 1.255$ Cb/nm^2·s.

4. Conclusion

The work provides a facility for obtaining the transmission coefficient for a given barrier, under bias, which can be used for reaching the associated $I - V$ characteristic. In this way one can infer useful properties of nanostructures.

Presently, the nanostructure considered provides an $I-V$ characteristic with extremely high negative differential resistance. As can be seen from Fig. 3 the drop in current from peak to valley occurs over an extremely small change in V (approximately 0.06 V) with a very high peak to valley ratio, a fact pointing to the possibility of accessing some sort of nanoswitch.

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