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Numerical method to calculate the quantum transmission, resonance and eigenvalue energies: application to a biased multibarrier systems

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ABSTRACT

A novel method to calculate the quantum transmission, resonance and eigenvalue energies forming the sub-bands structure of non-symmetrical, non-periodical semiconducting heterostructure potential has been proposed in this paper. The method can be applied on a multilayer system with varying thickness of the layer and effective mass of electrons and holes. Assuming an approximated effective mass and using Bastard's boundary conditions, Schrödinger equation at each media is solved and then using a confirmed recurrence method, the transmission and reflection coefficients and the energy quantification condition are expressed. They are simple combination of coupled equations. Schrödinger's equation solutions are Airy functions or plane waves, depending on the electrical potential energy slope. To illustrate the feasibility of the proposed method, the N barriers – $(N-1)$ wells structure for $N=3$, 5, 8, 9, 17 and 35 are studied. All results show very good agreements with previously published results obtained from applying different methods on similar systems.

1. Introduction

The interest in artificial multilayered semiconducting structures stimulate the speedy development of new and fast functional devices. This provides an increasing impulsion on the comprehension of the quantum-tunneling problems [1,2]. Both theoretical and experimental studies and applications of the resonant tunneling phenomenon are very interesting subjects. In the case of double-barrier structures, this phenomenon has been studied by many researchers during the last twenty years [3–5]. For the transmission coefficient across arbitrary potential barriers, a one-dimensional matrix method based on a multistep potential approximation and a multistep electron mass are developed [6]. Multiple-barriers resonant tunneling has been encouraged since the original work of Tsu and Esaki [1] and Chang et al. [7]. Their studies are motivated by their wide applications in high speed electronic devices (lasers, modulators, photodetectors, and signal processing devices). Bloch theorem allows the study of ordered systems which are distinguished by their periodicity [8]. The case of disordered superlattices is very hard since the translation symmetry of the system is broken [9–13]. Ko and Inkson developed a scattering-matrix formalism to study electron transmission coefficient for nonperiodic semiconductor heterostructures [14]. The transfer matrix method was used by Jatindranath [15] to solve the time independent Schrödinger equation, using the same method Simion et al. [16] studied the resonant tunneling in multilayered heterostructures, and in the same way Fedirko et al. [17] developed an efficient approach for computer simulation of stationary scattering and tunneling transfer across one-dimensional potential barrier. Resonant tunneling in electrically biased multibarrier systems has been intensively studied [18–27] by a computational model using the exact Airy function formalism and the transfer-matrix technique. These multiple applications of the transfer matrix method proved its very large magnitudes, however, such method involves some difficulties in the mathematical derivation and programming especially for beginners. The argument of the Airy function contains parameter field in the denominator, then the low voltage area is generally not included in the calculations based on Airy functions and some results are lost. If necessary, we use the asymptotic form of the Airy functions and their derivatives [18]. Asenova et al. [28] studied the tunneling and current density in short period strained AlN/GaN superlattices.

Maiz et al. [29–31] proposed a simple method to calculate the band structure of nonperiodic multilayer unbiased semiconducting heterostructures and used an airy function approach to study quantum anharmonic oscillator. Maiz [32,33] applied his method to calculate the energy levels for electrons, holes and deduced the transition energy.

This paper is organized as follows: in Section 2 we introduce our new method for the calculations of the quantum transmission

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and reflection coefficients across electrically biased multibarrier systems and the energy eigenvalues. In Section 3 this novel method is applied to N barriers – $(N-1)$ Wells structure (N=3, 5, 8, 9, 17 and 35). Results are presented and discussed in Section 4.

2. Theoretical approach

2.1. Analytical forms of the quantum transmission and reflection coefficients

As shown in Fig. 1a, we have considered a general case of a quantum heterostructure constituted by $(n+2)$ semiconductor layers. Table 1 shows the characteristics of the different layers. For the ith semiconductor layer SCi, the thickness and the electron effective mass are designed respectively by h_i and m_i^*, where m_0 is the free electron mass. The Schrödinger equation for different layers is given by

$$\frac{\partial^2\Psi_0}{\partial x^2} = K_0^2\Psi_0, \quad \text{for } x \le 0$$
$$\frac{\partial^2\Psi_i}{\partial x^2} = K_i^2\Psi_i \quad \text{for } x_{i-1} \le x \le x_i$$
$$\frac{\partial^2\Psi_{n+1}}{\partial x^2} = K_{n+1}^2\Psi_{n+1} \quad \text{for } x \ge x_n \tag{1}$$

where $K_0^2 = 2m_0^*(V_0 - E)/\hbar^2$, $K_i^2 = 2m_i^*(V_i(x) - E)/\hbar^2$, and $K_{n+1}^2 = 2m_{n+1}^*(V_{n+1} - E)/\hbar^2$.

For $x_{i-1} \le x \le x_i$, the linear potential energy is given by: $V_i(x) = V(x_{i-1}) + eS_i\,x = V_{i-1} + eS_i x$, where x denotes the distance from the interface x_{i-1}. Here S_i is the slop of the electrical potential, e the electron charge and E the incident electron energy. The thickness of the SCi layer is $h_i = (x_i - x_{i-1})$. The electron motion in the plans of layers is not taken account in this study. The general solution of the one-dimensional Schrödinger's equation $\Psi_i(x)$ for an electron with incident energy E in the SCi layer can be expressed as a linear combination of two functions ϕ_i and φ_i as

$$\Psi_i(x) = \alpha_i\phi_i(X) + \beta_i\varphi_i(X) \tag{2}$$

where α_i and β_i are constant and:

- for linear potential $(S_i \neq 0)$: $\varphi_i(X) = Ai(X)$ and $\phi_i(X) = Bi(X)$ where Ai and Bi are the Airy functions, and $X = \left(2m_i^*/\hbar^2\right)^{1/3}(V_i + eS_ix - E)/(-S_i)^{2/3}$.
- for constant potential $(S_i = 0)$: $\phi_i(X) = \exp(-X)$ and $\varphi_i(X) = \exp(X)$ where $X = K_ix$, and $K_i^2 = 2m_i^*(V_i - E)/\hbar^2$ is the modulus of the wave vector.

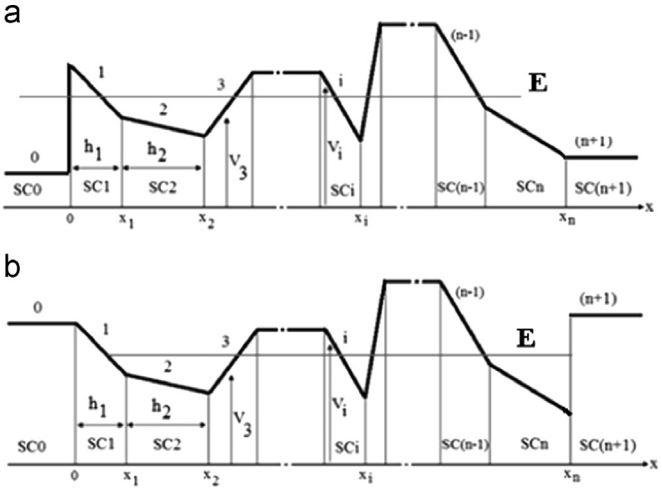

Fig. 1. (a) Potential energy profile of multilayer system to study the transmission phenomena. (b) Potential energy profile of multilayer system to study the energy bound states.

Table 1
Characteristics of a $(n+1)$ layers semiconducting system.

Layer index	Effective mass (m_0)	Thickness (nm)	Potential slope (V/nm)	Barrier height difference
0	m_0^*	h_0	$S_0 = 0$	$V(0)$
1	m_1^*	h_1	S_1	$V_1 = V(0) + eS_1x$
i	m_i^*	h_i	S_i	$V_i(x) = V(x_{i-1}) + eS_i(x - x_{i-1})$
$n+1$	m_{n+1}^*	h_{n+1}	$S_{n+1} = 0$	$V(x_n)$

For $x \le 0$, the solution of the Schrödinger equation is $\Psi_0(X) = \alpha_0\phi_0(X) + \beta_0\varphi_0(X)$, with $\phi_0(X) = e^{-K0x}$, $\varphi_0(X) = e^{K0x}$ and $\alpha_0 \neq 0$. However, for $x \ge 0$, the solution of the Schrödinger equation is $\Psi_{n+1}(X) = \alpha_{n+1}\phi_{n+1}(X)$ with $\phi_{(n+1)}(X) = e^{-K(n+1)x}$, since there is no incoming wave.

According to Bastard's boundary conditions [34], the wave function and its first derivative divided by the effective mass must be continuous at each interfacex_i:

$$\Psi_i(x_{i+1}) = \Psi_{i+1}(x_{i+1}) \text{ and } \Psi_i'(x_{i+1})/m_i^* = \Psi_{i+1}'(x_{i+1})/m_{i+1}^* \tag{3}$$

where the prime denotes the first derivative with respect to x. Using this notation $\tilde{\Psi}_i(x_i) = \Psi_i'(x_i)/m_i^*$, one can write Bastard's boundary condition at each interface as

$$\Psi_i(x_{i+1}) = \Psi_{i+1}(x_{i+1}) \text{ and } \tilde{\Psi}_i(x_{i+1}) = \tilde{\Psi}_{i+1}(x_{i+1}) \tag{4}$$

Writing this previous condition at each interface leads to the following system of coupled equations:

$$\begin{cases}
\alpha_0\phi_0(0) + \beta_0\varphi_0(0) = \alpha_1\phi_1(0) + \beta_1\varphi_1(0)\\
\alpha_0\tilde{\phi}_0(0) + \beta_0\tilde{\varphi}_0(0) = \alpha_1\tilde{\phi}_1(0) + \beta_1\tilde{\varphi}_1(0)\\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
\alpha_i\phi_i(h_i) + \beta_i\varphi_i(h_i) = \alpha_{i+1}\phi_{i+1}(0) + \beta_{i+1}\varphi_{i+1}(0)\\
\alpha_i\tilde{\phi}_i(h_i) + \beta_i\tilde{\varphi}_i(h_i) = \alpha_{i+1}\tilde{\phi}_{i+1}(0) + \beta_{i+1}\tilde{\varphi}_{i+1}(0)\\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
\alpha_n\phi_n(h_n) + \beta_n\varphi_n(h_n) = \alpha_{n+1}\phi_{n+1}(0)\\
\alpha_n\tilde{\phi}_n(h_n) + \beta_n\tilde{\varphi}_n(h_n) = \alpha_{n+1}\tilde{\phi}_{n+1}(0)
\end{cases} \tag{5}$$

The expressions of $\alpha_i$and β_i as a function of $\alpha_{i-1}$and β_{i-1} are given by the following equations system:

$$\begin{cases}
\alpha_1\Omega_{\phi\varphi}(1,0,1,0)\\
\quad = \alpha_0\Omega_{\phi\varphi}(0,0,1,0) + \beta_0\Omega_{\varphi\varphi}(0,0,1,0)\\
\beta_1\Omega_{\varphi\phi}(1,0,1,0)\\
\quad = \alpha_0\Omega_{\phi\phi}(0,0,1,0) + \beta_0\Omega_{\varphi\phi}(0,0,1,0)\\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
\alpha_i\Omega_{\phi\varphi}(i,0,i,0) = \alpha_{i-1}\Omega_{\phi\varphi}(i-1,h_{i-1},i,0)\\
\qquad\qquad + \beta_{i-1}\Omega_{\varphi\varphi}(i-1,h_{i-1},i,0)\\
\beta_i\Omega_{\varphi\phi}(i,0,i,0) = \alpha_{i-1}\Omega_{\phi\phi}(i-1,h_{i-1},i,0)\\
\qquad\qquad + \beta_{i-1}\Omega_{\varphi\phi}(i-1,h_{i-1},i,0)\\
\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
\alpha_{n+1}\Omega_{\phi\varphi}(n+1,0,n,h_n) = \alpha_n\Omega_{\phi\varphi}(n,h_n,n,h_n)\\
\alpha_{n+1}\Omega_{\phi\phi}(n+1,0,n,h_n) = \beta_n\Omega_{\varphi\phi}(n,h_n,n,h_n)
\end{cases} \tag{6}$$

where $\Omega_{XY}(a,b,c,d) = X_a(b) \times \tilde{Y}_c(d) - \tilde{X}_a(b) \times Y_c(d)$.