Quantum transport properties of one dimensional barriers: a simple approach to calculate transfer matrices

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We present a simple method for calculating the transfer matrix of a one dimensional system consisting of a number of rectangular barriers of arbitrary shape. We also make use of the Cayley-Hamilton theorem and the spectral theory of finite complex matrices to calculate high powers of matrices in a simple way, obtaining analytic expressions that are easily evaluated. We give an example of the transmission coefficient and conduction bands for a complex-basis superlattice. The method provides an intuitive approach to the construction for the transfer matrix.

Keywords: Transfer matrix; superlattices; electronic transport.

Presentamos un método simple para el calculo de la matriz de transferencia de un sistema unidimensional que consiste de un numero de barreras rectangulares de forma arbitraria. También hacemos uso del teorema de Cayley-Hamilton y la teoría espectral de matrices complejas finitas para calcular, de una manera sencilla, potencias grandes de las matrices; obteniendo expresiones analíticas que son fácilmente evaluables. Damos un ejemplo del coeficiente de transmisión y bandas de conducción para una superred de base compleja. El método provee una manera intuitiva para la construcción de la matriz de transferencia.

Descriptores: Matriz de transferencia; superredes; transporte electrónico.

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Binary-type superlattices (SL) in recent years have found a great number of applications [1] including semiconductor-diode lasers, electro-optical modulators and infrared detectors among others. Thanks to the great advances in crystal growing techniques, specially molecular beam epitaxy, it is now possible to grow with high precision semiconductor SL's of more than two materials, the so called complex-basis superlattices. These structures often exhibit superior electronics, optical and transport characteristics compared to binary SL's. Furthermore, this kind of structures are becoming more important from the technological point of view because of the potential applications in nanotechnology.

One way to investigate the transport properties of SL's is by calculating the transfer matrix of the structure, although many techniques have been given in the literature [2–4], such as Green function methods, envelope functions, etc.

In this paper, we report a technique based on the transfer matrix method to calculate the transmission coefficient and other transport properties of complex-basis superlattices. We also show two alternative ways to calculate high powers of transfer matrices that arise when dealing with large SL's.

We are interested in structures composed of a sequence of arbitrary potential barriers, as the one shown in Fig. (1) [2]. We now calculate the transfer matrix corresponding to an arbitrary barrier in the structure.

Let

$$\phi_L(z_1) = \begin{pmatrix} Ae^{ik_1 z_1} \\ Be^{-ik_1 z_1} \end{pmatrix}, \tag{1}$$

and

$$\phi_R(z_1) = \begin{pmatrix} Ce^{ik_2 z_1} \\ De^{-ik_2 z_1} \end{pmatrix}, \tag{2}$$

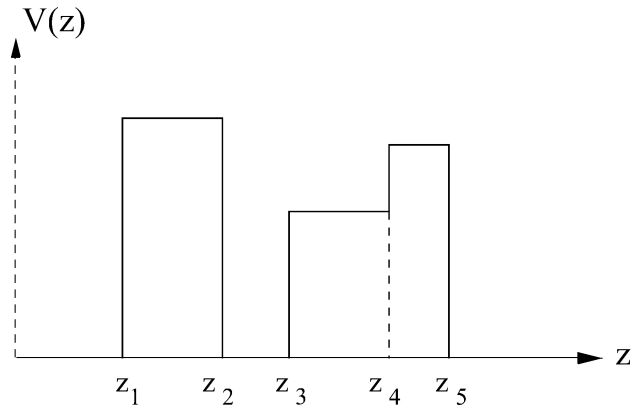

FIGURE 1. A general potential profile used to calculate the transfer matrix from z_1 to z_5. Two different kind of matrices are used in order to calculate the transmission.

be the state vectors [5] to the left and right of z_1, respectively, where z_1 is a point in the graph where the potential has a discontinuity. The continuity conditions of the state vectors at the interface lead us to the following relation

$$\phi_L(z_1) = M(z_1)\phi_R(z_1), \tag{3}$$

where

$$M(z_1) = \frac{1}{2}\begin{pmatrix} 1+r & 1-r \\ 1-r & 1+r \end{pmatrix}, \tag{4}$$

is a transition matrix between regions with different values for the potential and $r = k_2 m_1/k_1 m_2$ [6]. Similar matrices are defined for every point where the potential changes like

in z_2, z_3 etc. It is important to notice that this matrix is independent of the position of the barrier, a property that will be used later.

In the above equations the wave vectors are given by

$$k_i = \sqrt{\frac{2m_i}{\hbar^2}(E - V_i)}, \tag{5}$$

and m_i is the effective mass.

There is a transporting matrix [7] that connects the points z_1 and z_2 inside the barrier, that is

$$\phi_L(z_1) = M(z_2, z_1)\phi_R(z_2), \tag{6}$$

given by

$$M(z_2, z_1) = \begin{pmatrix} e^{-ik_2 l} & 0 \\ 0 & e^{ik_2 l} \end{pmatrix}, \tag{7}$$

where $l = z_2 - z_1$. A similar transporting matrix can be defined for any pair of points as long as the potential remains constant. If the electron's energy is less than V for this part of the graph then we will have that $k \to ik$. The total transfer matrix for this first barrier will be

$$M(z_1, z_2) = M(z_1)M(z_2, z_1)M(z_2). \tag{8}$$

The calculation for the multiple barrier graph can be obtained using a few simple rules. 1. Every point in the graph with a discontinuity in the potential will have a transition matrix, like the one in Eq. (4). 2. Every section in the graph with constant potential will have a transporting matrix like the one in Eq. (7). Notice that k may be real or complex depending on the value of the potential in that section of the graph. The total transfer matrix from one point to another in the graph will be given by a simple product of 2×2 matrices starting from the left.

These rules are easily generalized in the following way. Let's call z_i to every point in the z axis in which there is a change in the potential, and k_i is given in Eq. (5), the wave vector corresponding to the potential V_i between z_{i-1} and z_i.

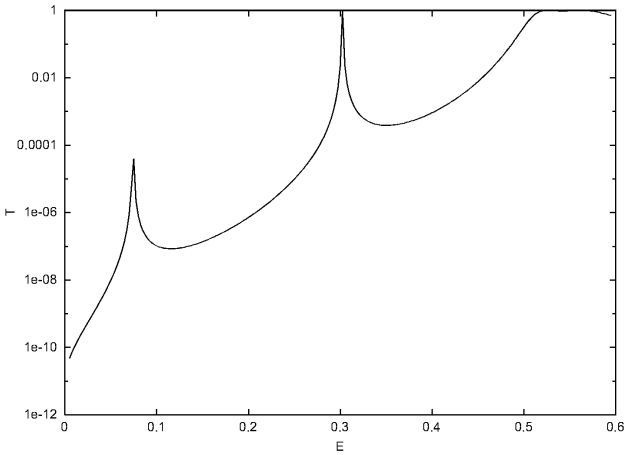

FIGURE 2. Plot of the transmission coefficient for a $Al_{0.45}Ga_{0.55}As$/GaAs DBRT structure with 5 nm barriers and a 5.5 nm GaAs well. The energy is given in eV.

The transition matrix $M(z_i)$ corresponding to the point z_i will be defined by

$$\begin{pmatrix} A_i e^{ik_i z_i} \\ B_i e^{-ik_i z_i} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+r_i & 1-r_i \\ 1-r_i & 1+r_i \end{pmatrix} \times \begin{pmatrix} A_{i+1} e^{ik_{i+1} z_i} \\ B_{i+1} e^{-ik_{i+1} z_i} \end{pmatrix}, \tag{9}$$

where $r_i = k_{i+1}m_i/k_i m_{i+1}$. We notice that this transition matrix changes the state vector into another one with a different wave vector at the same point. In contrast, the transporting matrix $M(z_{i+1}, z_i)$ from one point to another takes the state vector with the same momentum but to a different point along the axis. This is so because we are transporting the wave vector in a region where the potential is constant. Therefore we have

$$\begin{pmatrix} A_{i+1} e^{ik_{i+1} z_i} \\ B_{i+1} e^{-ik_{i+1} z_i} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} e^{-ik_{i+1} l_i} & 0 \\ 0 & e^{ik_{i+1} l_i} \end{pmatrix} \times \times \begin{pmatrix} A_{i+1} e^{ik_{i+1} z_{i+1}} \\ B_{i+1} e^{-ik_{i+1} z_{i+1}} \end{pmatrix}, \tag{10}$$

where $l_i = z_{i+1} - z_i$. For instance, in order to calculate the transmission for an arbitrary number of barriers, we have

$$\begin{pmatrix} A_1 e^{ik_1 z_1} \\ B_1 e^{-ik_1 z_1} \end{pmatrix} = \left[\prod_{i=1}^{N-1} [M(z_i)M(z_{i+1}, z_i)\right] M(z_N) \times \begin{pmatrix} A_{N+1} e^{ik_{N+1} z_N} \\ B_{N+1} e^{-ik_{N+1} z_N} \end{pmatrix}, \tag{11}$$

where N is the number of discontinuities in the graph. The transmission coefficient can be calculated from the equation $A_1 e^{ik_1 z_1} = M_{11} A_{N+1} e^{ik_{N+1} z_N}$ to get

$$T = \left|\frac{A_{N+1}}{A_1}\right|^2 = \frac{1}{|M_{11}|^2}, \tag{12}$$

where M is the total transfer matrix from z_1 to z_N, and M_{11} is the element (1,1).

As an example [11], we consider a $Al_{0.45}Ga_{0.55}As$/GaAs double-barrier resonant tunneling (DBRT) structure. In Fig. 2 we plot the transmission coefficient as function of energy calculated with the method just described.

If we consider now a periodic repetition of the potential profile of Fig. 1, we obtain what is known in the literature as a complex-basis superlattice. Using the formalism previously described the transfer matrix M for the basis can be calculated. The total transfer matrix of the entire superlattice will be the product of N single basis transfer matrices M, or M^N.

In this case, the product of N identical transfer matrices that arises can be easily obtained by using the Cayley-Hamilton theorem [8], which allows one to express powers of a unimodular matrix M, as in our case, in the following form [9]

$$M^N = U_{N-1}M - U_{N-2}, \tag{13}$$

where $U_n(t)$ is the nth Chebyshev polynomial of the second kind, and $2t$ is the trace of M. There is another way to calculate high powers of a matrix and this is given by the spectral theory of finite complex matrices [10]. In this technique, the Nth power of the matrix M is expressed as

$$M^N = \lambda_1^N E_1 + \lambda_2^N E_2, \tag{14}$$

where λ_i are the eigenvalues of M and E_i are two idempotent matrices associated with M. The matrices E_i have the following properties: $E_1 + E_2 = 1$ and $E_i E_j = E_i \delta_{ij}$. This second approach to the calculation of powers of a matrix may be more computationally convenient when N is very large, because there is no need to evaluate the Chebyshev polynomials.

It is important to stress that equations 13 and 14, when inserted in 12, will give a compact analytic expression for the transmission coefficient of a system composed of identical barriers or bases. This is an important point, because it is well known that the use of transfer matrices will give rise to numerical instabilities that arise because the coefficients in a given layer are evaluated from those in previous layers, and the numerical errors increase with the growing exponentials [12, 13]. However, this problem appears when explicit multiplication of transfer matrices is done, getting worse for larger systems. In our case, no multiplication is performed and hence numerical instabilities are absent. This feature makes our method specially well suited for very long systems.

Once the total transfer matrix M for a certain graph has been calculated, the transmission coefficient will be given by $T{=}|M_{11}|^{-2}$. As an example we calculate the transmission coefficient for a superlattice composed of 5 structures as the one shown in Fig. 1. The composition is, starting from the first barrier, $Al_{0.5}Ga_{0.5}As/GaAs/Al_{0.3}Ga_{0.7}As/Al_{0.4}Ga_{0.6}As/GaAs$, with widths 8, 5, 9 and 4 nm respectively, with a distance within bases of 4 nm. The calculated transmission coefficient is shown in Fig. 3.

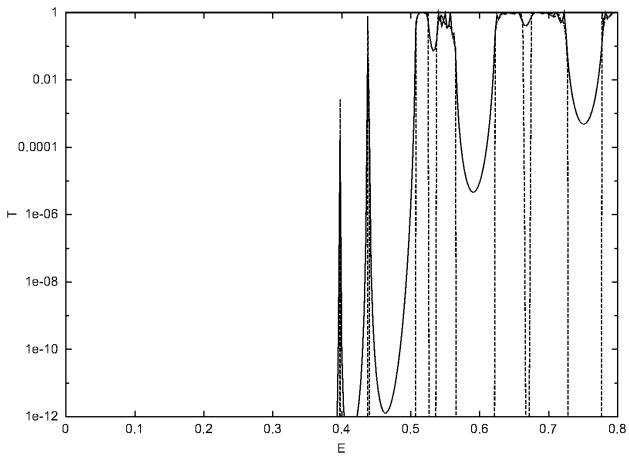

FIGURE 3. Plot of the transmission coefficient for a superlattice with $N = 5$ (solid line) and another with $N = 100$, as described in the text. The energy is given in eV.

Consider now a superlattice with the same basis as before but with $N = 100$. In this case we use Eq. (14) to calculate the $100th$ power of the single basis transfer matrix. Comparison with the $N = 5$ case shows that the transmission peaks become narrower leaving large regions of energy when the transmission sharply goes to zero, a property useful for filter design.

We would like to stress the simplicity of our approach compared to other calculations [14,15]. This simplicity arises from two main reasons. First, the use of state vectors instead of wave function coefficients eliminates the position dependence in the transition matrices. Second, because of this we can make use of matrix theorems to simplify the calculation of powers of matrices and obtain the total transfer matrix in a simple expression. We have shown how to obtain the transmission coefficient with this approach. Other physical properties can be easily calculated as well. In Fig. 4 we show the electronic band structure for the above superlattice as function of the concentration x of the first barrier in Fig. 1. Notice that drawing a vertical line at $x = 0.5$, the intersections with the bands give the same values for energy that those in Fig. 3 for the $N = 100$ system.

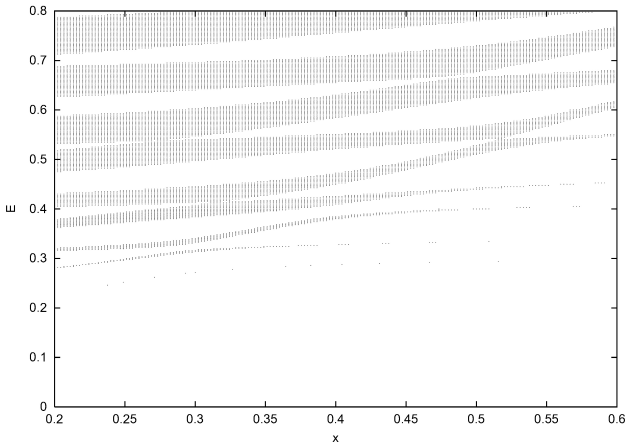

FIGURE 4. Electronic band structure as function of the Al concentration x, of the first barrier in Fig. 1. The energy is in eV.

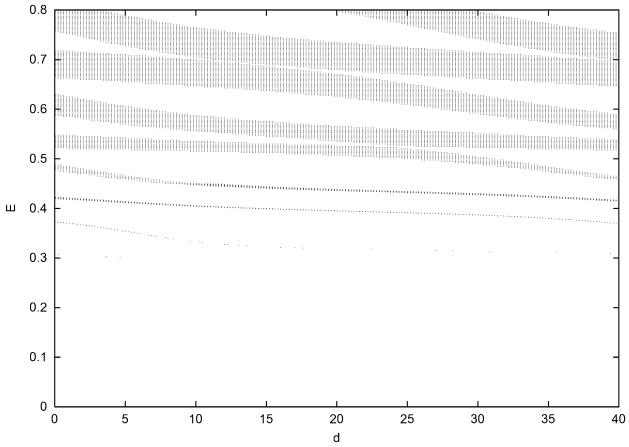

FIGURE 5. Electronic band structure as function of the well distance d (in Angstroms) for the same system as in Fig 4.

Figure 5 shows also the band diagram but as a function of the width in the well located between the first and second barriers in Fig. 1. These are obtained using the relation $\cos(kd) = TrM_T/2$, where d is the SL period, k the crystal momentum and M_T is the total transfer matrix for one basis in the infinite superlattice.

In conclusion, we report in this paper a simple and straightforward way to calculate the transfer matrix of a system composed of a number of rectangular barriers of arbitrary shape. Also, we give a way to simplify the calculation of the transfer matrix for a system composed of a large number of identical structures, or bases. This arises from the use of second type transfer matrices that do not depend on the position of the barrier, making them identical and therefore we can make use of either the Cayley-Hamilton theorem or the spectral theory for the calculation of powers of a matrix.

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