International Journal of Theoretical Physics, Vol. 43, No. 2, February 2004 (© 2004)

Differential Equation for the Transfer Matrix

I. A. Shelykh[1,2,3] and V. K. Ivanov[1]

An electron propagating through a crystal toward an interface can either reflect or transmit. The determination of its transmission and reflection probabilities represents an actual task in such fields as nanoelectronics, magnetoelectronics, or spin electronics. Within the framework of the effective mass approximation the problem can be reduced to the tunneling of the quantum particle through one-dimensional potential barrier. The tunneling process can be described by means of the transfer matrix, which contains all the information about the energetic dependence of the transmission and reflection coefficients. In the present work the differential equation for the transfer matrix of the arbitrary potential barrier is derived. The method proposed represents an alternative way of the calculation of the transfer matrix.

KEY WORDS: tunneling; quantum interference; transfer matrix.

1. INTRODUCTION

Since the appearance of the pioneering work of Esaki and Tsu (Tsu and Esaki, 1973), the carrier tunneling in semiconductor superlattices has been the focus of a number of theoretical and experimental works in the field of mesoscopic physics. As was shown (Esaki and Chang, 1976; Tsu and Esaki, 1973; Vessel *et al.*, 1984), the quantum interference of the ballistic carriers in such structures leads to the resonant current–voltage characteristics (CVC) and to the formation of regions with negative differential conductivity. This is due to the oscillating dependence of the transmission coefficient of the multibarrier structures on the carrier energy. The standard method of calculation for the energy dependence of the transmission coefficient is based on the transfer matrix method proposed in (Tsu and Esaki, 1973). This method was used while considering the optical properties of quantum microcavities and photonic crystals (Ańdreani, 1994; Ivchenko and Pikus, 1997; Kosobukin, 1993; Savona *et al.*, 1999), the ballistic transport in modulated quantum wires (Bagraev *et al.*, 2000; Kim *et al.*, 1999; Kim and Satanin,

[1] St. Petersburg State Polytechnical University, Politechnicheskaya, St-Petersburg, Russia.
[2] LASMEA, UMR 6602 CNRS, Université Blaise Pascal, av des Landais, Aubière, France.
[3] To whom correspondence should be addressed at St. Petersburg State Polytechnical University, 29, Politechnicheskaya, 195251, St-Petersburg, Russia; e-mail: ivshel@mail.ru.

0020-7748/04/0200-0477/0 © 2004 Plenum Publishing Corporation

1999) and wires in inhomogeneous magnetic field (Kousuke Yakubo, 2001), and for determining of the miniband structure and interface states of infinite or semi infinite superlattices (Trzeciakowski, 1988; Vladimirova and Kavokin, 1995). The transfer matrix method allows the determination of the positions of the transmission resonances through multibarrier structures for arbitrary values of the system's characteristic parameters.

The present work is devoted to the derivation of the integral and differential equations that describe the transfer matrix of an arbitrary potential barrier.

2. DEFINITION OF THE TRANSFER MATRIX

Let us consider a potential barrier, localized in the region $[x_{\min}; x_{\max}]$ and having some arbitrary shape. Outside this region let us put the potential constant.

$$U = \begin{cases} U_0, & x < x_{\min} \\ U(x), & x_{\min} < x < x_{\min} \\ U_1, & x > x_{\max} \end{cases}$$

If the energy of a particle ε exceeds the potentials U_0 and U_1, its wave function can be represented in the regions outside the barrier as a linear combination of two plane waves. Within the barrier region it can be determined from the Schrodinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x)\right]\Psi(x) = \varepsilon\Psi(x) \tag{1}$$

where m is the effective mass of the particle assumed to be independent on the coordinate. Let us suppose that $\Psi_1(x)$ and $\Psi_2(x)$ are two linear independent solutions of this equation. The wave function in the overall space can thus be represented as

$$\Psi = \begin{cases} A_0 e^{ik_o x} + B_0 e^{-ik_o x}, & x < x_{\min} \\ C\Psi_1(x) + D\Psi_2(x), & x_{\min} < x < x_{\max} \\ A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}, & x > x_{\max} \end{cases}$$

where $\hbar k_0 = \sqrt{2m(E - U_0)}$, $\hbar k_1 = \sqrt{2m(E - U_1)}$. The coefficients A_0, B_0, A_1, B_1 describe the amplitudes of the plane waves in the right and left regions. They are connected by the transfer matrix $\mathbf{T}$ (Tsu and Esaki, 1973), so that

$$\mathbf{X}_1 = \mathbf{T}\mathbf{X}_0 \tag{2}$$

$$\mathbf{X}_1 = \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \quad \mathbf{X}_0 = \begin{pmatrix} A_0 \\ B_0 \end{pmatrix}, \quad \mathbf{T} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \tag{2a}$$

which can be determined as (Liu and Stamp, 1993):

$$\mathbf{T} = \begin{pmatrix} \tau_1^* e^{i(k_0-k_1)L} & \tau_2^* e^{-i(k_0+k_1)L} \\ \tau_2 e^{i(k_0+k_1)L} & \tau_1 e^{i(k_1-k_0)L} \end{pmatrix}$$

$$\tau_1 = e^{ik_1L}(\Psi_1' - ik_1\Psi_1) + ik_0 e^{-ik_1L}(\Psi_2' - ik_1\Psi_2),$$

$$\tau_2 = e^{ik_1L}(\Psi_1' - ik_1\Psi_1) - ik_0 e^{-ik_1L}(\Psi_2' - ik_1\Psi_2)$$

where $L = x_{\max} - x_{\min}$, $\Psi_1(x)$ and $\Psi_2(x)$ represent two solutions of the Cauchy problem for the Eq. (1) with the following initial conditions

$$\Psi_1(x_{\min}) = 1; \quad \Psi_1'(x_{\min}) = 0$$

$$\Psi_2(x_{\min}) = 0; \quad \Psi_2'(x_{\min}) = 1$$

The amplitudes of the transmission A and reflection B can be determined from the following set of the algebraic equations

$$\begin{pmatrix} A \\ 0 \end{pmatrix} = \mathbf{T} \begin{pmatrix} B \\ 1 \end{pmatrix}$$

Thus, the transmission and reflection coefficients are

$$R = |B|^2 = \left| \frac{\tau_2}{\tau_1} \right|^2 \tag{3}$$

$$T = \frac{k_1}{K_0}|A|^2 = \frac{k_1}{k_0|\tau_1|^2} \tag{3a}$$

and all the characteristics of the transport are determined by the elements of the transfer matrix.

3. DERIVATION OF THE DIFFERENTIAL EQUATION FOR THE TRANSFER MATRIX

Now, let us obtain the differential equation for the transfer matrix of the arbitrary smooth potential barrier. For this purpose, let us consider the scattering potential $U(x)$, where $U(x)$ is a finite smooth function in $[-\infty, +\infty]$. We can approximate the real shape of the barrier by a sequence of the rectangular layers. By increasing the number of layers, one increases the precision of the approximation. Let us assume that the particle energy always exceeds the barrier height. Then, in the jth layer the particle's wavefunction can be represented as

$$\psi_j = A_j e^{ik_j x} + B_j e^{-ik_j x}$$

where $k_j = \frac{1}{\hbar}\sqrt{2m[E - U(x_j)]}$. Using the boundary conditions, it is easy to establish the connection between A_{j+1}, B_{j+1} and A_j, B_j. One has

$$A_j e^{ik_j x_j} + B_j e^{-ik_j x_j} = A_{j+1} e^{ik_{j+1} x_j} + B_{j+1} e^{-ik_{j+1} x_j}$$
$$k_j \left(A_j e^{ik_j x_j} - B_j e^{-ik_j x_j}\right) = k_{j+1}\left(A_{j+1} e^{ik_{j+1} x_j} - B_{j+1} e^{-ik_{j+1} x_j}\right)$$

Introducing the vectors $\mathbf{X}_j = \binom{A_j}{B_j}$, $\mathbf{X}_{j+1} = \binom{A_{j+1}}{B_{j+1}}$, it is easy to show that

$$\mathbf{X}_{j+1} = \mathbf{D}_j \mathbf{X}_j$$

where

$$D_j = \mathbf{C}(k_{j+1}, x_j)\mathbf{D}(k_j, k_{j+1})\mathbf{C}^{-1}(k_j, x_j)$$
$$\mathbf{C}(k_1, x_m) = \begin{pmatrix} e^{ik_i x_m} & 0 \\ 0 & e^{-ik_i x_m} \end{pmatrix}$$
$$\mathbf{D}(k_j, k_{j+1}) = \begin{pmatrix} \dfrac{k_{j+1} + k_j}{2k_{j+1}} & \dfrac{k_{j+1} - k_j}{2k_{j+1}} \\ \dfrac{k_{j+1} - k_j}{2k_{j+1}} & \dfrac{k_{j+1} + k_j}{2k_{j+1}} \end{pmatrix}$$

The transfer matrix through the whole barrier is a product of the transfer matrices of the n layers

$$\mathbf{T} = \prod_{j=0}^{n} \mathbf{D}_j = \mathbf{C}(k_t, x_{\max}) \left\{ \prod_{j=0}^{n} \mathbf{D}(k_j, k_{j+1})\mathbf{C}^{-1}(k_j, x_j - x_{j-1}) \right\} \mathbf{C}^{-1}(k_f, x_{\min}) \tag{4}$$

where k_f is a wave number of the incident particle, k_t- of the transmitted particle. The factors $\mathbf{C}(x_t, x_{\max})$ and $\mathbf{C}^{-1}(k_f, x_{\min})$ change only the phase of the matrix elements of $\mathbf{T}$, and according to (3) do not change the transmission and reflection coefficients. Thus, in the following discussion we will use the matrix

$$\mathbf{T}' = \prod_{j=1}^{n} \mathbf{D}(k_j, k_{j+1})\mathbf{C}^{-1}(k_j, x_j - x_{j-1})$$

which is equivalent to the matrix $\mathbf{T}$.

Now let us increase the number of the layers to put the thickness of the each layer dx infinitely small, $dx \to 0$. The matrices $\mathbf{D}$ and $\mathbf{C}$ can now be considered to depend on the continuous coordinate x. Using the Taylor expansion for the elements of the matrices $\mathbf{D}$ and $\mathbf{C}$ and leaving only the term linear in dx, it is easy to show

$$\mathbf{D}(x)\mathbf{C}^{-1}(x) = \mathbf{I} + \mathbf{V}(x)\,dx \tag{5}$$

where **I** is a unity matrix,

$$\mathbf{V}(x) = \begin{pmatrix} -\dfrac{1}{2k(x)}\dfrac{\partial k}{\partial x} - ik(x) & \dfrac{1}{2k(x)}\dfrac{\partial k}{\partial x} \\ \dfrac{1}{2k(x)}\dfrac{\partial k}{\partial x} & -\dfrac{1}{2k(x)}\dfrac{\partial k}{\partial x} + ik(x) \end{pmatrix}$$

$$k(x) = \frac{\sqrt{2m[E - U(x)]}}{\hbar} \tag{6}$$

Let us consider the total transfer matrix, which can be calculated as a product of all the matrices (15) from $x = x_{\min}$ to $x = x_{\max}$.

$$\begin{aligned}\mathbf{T}' &= \prod_j (\mathbf{I} + \mathbf{V}(x_j)) = \mathbf{I} + \sum_j \mathbf{V}(x_j) + \sum_{j<l} \mathbf{V}(x_j)\mathbf{V}(x_l) + \cdots \\ &+ \sum_{j<l<\ldots s} \mathbf{V}(x_j)\mathbf{V}(x_l)\cdots\mathbf{V}(x_s) + \cdots = \mathbf{I} + \int_{x_{\min}}^{x_{\max}} dx_1 \mathbf{V}(x_1) \\ &+ \int_{x_{\min}}^{x_{\max}} dx_1 \int_{x_{\min}}^{x_1} dx_2 \mathbf{V}(x_1)\mathbf{V}(x_2) + \cdots + \int_{x_{\min}}^{x_{\max}} dx_1 \int_{x_{\min}}^{x_1} dx_2 \cdots \\ &\times \int_{x_{\min}}^{x_{n-1}} dx_n \mathbf{V}(x_1)\mathbf{V}(x_2)\cdots\mathbf{V}(x_n) + \cdots = \mathbf{I} + \sum_{n=1}^{\infty} \mathbf{T}^{(n)}\end{aligned} \tag{7}$$

where

$$\mathbf{T}^{(n)} = \int_{x_{\min}}^{x_{\max}} dx_1 \int_{x_{\min}}^{x_1} dx_2 \cdots \int_{x_{\min}}^{x_{n-1}} dx_n \mathbf{V}(x_1)\mathbf{V}(x_2)\cdots\mathbf{V}(x_n)$$

The formula (7) gives a representation of the transfer matrix in the form of a series of integrals. Let us introduce a coordinate-dependent matrix

$$\mathbf{T}(x) = \prod_{x_j < x} \mathbf{D}(x_j)$$

Using $\mathbf{T}(x)$ the transfer matrix $\mathbf{T}'$ can be determined as $\mathbf{T} = \mathbf{T}(x_{\max})$. It is easy to show, that $\mathbf{T}(x)$ obeys the following differential equation

$$\mathbf{T}(x_{\min}) = \mathbf{I} \tag{8}$$

$$\frac{\partial \mathbf{T}}{\partial x} = \mathbf{V}(x)\mathbf{T} \tag{8a}$$

In fact, transforming this equation into the integral one

$$\mathbf{T}(x) = \mathbf{I} + \int_{x_{\min}}^{x} \mathbf{V}(x')\mathbf{T}(x')\,dx' \tag{9}$$

and iterating (9), one easily obtains the series (7).

In conclusion, we have demonstrated that the transfer matrix satisfies the differential equation equivalent to the integral equation. It can be found directly without solving the Schrodinger equation for any smooth potential barrier. The method proposed represents an alternative way of the calculation of the transfer matrix.

REFERENCES

Ańdreani, L. C. (1994). *Phys. Lett. A* **102**, 99.

Bagraev, N. T., Gehlhoff, W., Ivanov, V. K., Klyachkin, L. E., Malyarenko, A. M., and Shelykh, I. A. (2000). *Semiconductors* **34**, 462.

Esaki, L. and Chang, L. L. (1974). *Phys. Rev. Lett.* **33**, 495.

Ivchenko, E. L. and Pikus, G. E. (1997). *Superlattices and Other Heterostructures: Symmetry and Optical Phenomena*, Springer, Berlin.

Kim, C. S. and Satanin, A. M. (1999). *JETP*, **115**, 211.

Kim, C. S., Satanin, A. M., Joe, Y. S., and Cosby, R. M. (1999). *Phys. Rev. B* **60**, 10962.

Kosobukin, V. A. (1993). *Fiz. Tv. Tela* **35**, 884.

Kousuke Yakubo (2001). *JPSJ* **70**, 3331.

Liu, X. W. and Stamp, A. P. (1993). *Phys. Rev. B* **47**, 6605.

Savona, V., Andreani, L. C., Schwendimann, P., Quattropani, A. (1999). *Sol. St. Comm.* **93**, 733.

Trzeciakowski, W. (1988). *Phys. Rev. B* **38**, 4322.

Tsu, R. and Esaki, L. (1973). *Appl. Phys. Lett.* **22**, 562.

Vessel, M. O., Lee, J., Lockwood, H. F. (1983). *J. Appl. Phys.* **54**, 5206.

Vladimirova, M. R. and Kavokin, A. V. (1995). *Fiz. Tv. Tela* **37**, 2163.