Transmission Coefficient Calculation Methods for Semiconductor Nanostructures Modeling

Fedyay A., Marienkov V.
National Technical University of Ukraine "KPI", Kyiv, Ukraine, e-mail: artem.fedyay@gmail.com

***Abstract* – Existent method of transmission coefficient calculation is analyzed and compared by adequacy and application area. New analytical method for parabolic well was developed, based upon functions of parabolic cylinder. Recommendations on application are done based on fulfilled analysis for each model.**

Keywords – nanostructures modeling; quantum transport; transmission coefficient

I. INTRODUCTION

Calculation of electric current through semiconductor nanostructures with transverse electron transport (superlattices, resonant tunneling diodes (RTD), components of single-electronics, low-dimensional ballistic structures, etc.) mainly reduces to "scattering problem", in which transmission coefficient acts the main role. A family of analytical methods, based on transfer matrices; numerical methods, perturbation theory and other methods are using for defining coefficient calculation by now. However, publications about the limits of applicability and critical features of each method are absent. Choice of one or another method is defined by personal preferences of the author, rather than deep knowledge of methods' specifics. Wrong choice can make modeling process either more complex or less adequate, or misled into doubtful conclusion. Motivation of the current work is eliminating the gaps in knowledge about critical features of each method and methods' relation to each other.

II. THE TRANSFER-MATRIX METHODS

The transfer-matrix method is used to find a transmission coefficient through the quantum system, in which potential energy of electron is or can be approximated by a piecewise-constant function (Fig. 1, a), a piecewise-linear (Fig. 1, b) or a piecewise-parabolic function (Fig. 1, c).

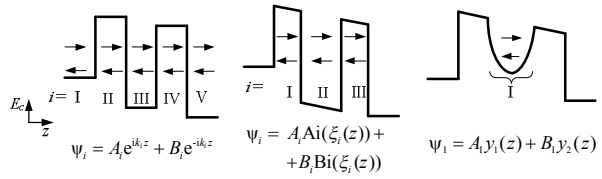

Figure. 1. Types and approximation of potential relief for nanostructure with double barrier: *a*) flat-bands, *b*) linear voltage drop, *c*) linear voltage drop in case of parabolic well.

Solutions of the effective mass Schrödinger equation in the form of plane waves, the Airy functions and parabolic cylinder functions correspond to these cases, respectively.

General goal of the transfer matrix method is to find a matrix $\mathbf{M} = [m_{11}, m_{12}; m_{21}, m_{22}]$, connecting amplitudes of incident and reflected waves in the left (A_L and B_L) and right (A_R and B_R) bulk regions of the structure (so-called "reservoirs"): $[A_R\ B_R]^T = \mathbf{M}[A_L\ B_L]^T$.

Once the form of Schrödinger equation is known, **M** matrix is can be found by imposing boundary conditions on the wave function and its derivative at the heteroboundaries. Having **M**, transmission coefficient can be calculated by the formula $T = |t|^2(|k_R|m_L)/(|k_L|m_R)$, where $k_{L(R)}$ and $m_{L(R)}$ are z-components of wave vector and electron effective mass in the left (right) reservoir; $t = m_{11} + m_{12}m_{21}/m_{22}$.

A. Plane Waves

Qualitative knowledge about the processes in nanostructures at small bias can be obtained by assuming that bands are shifting, nevertheless remaining flat within each layer, as shown in Fig. 1, *a* [1]. This allowing seeking for solutions of the Schrödinger equation in the each layer in the form of plane waves:

$$\psi_i(\xi_i(z)) = A_i \exp(\mathrm{i}k_i z) + B_i \exp(-\mathrm{i}k_i z).$$

B. The Airy functions

If neglecting space charge, the best approach is linear voltage drop along the nanostructure (Fig. 1, *b*). The solutions of the Schrödinger equation at the i-th area (i = 1, 2, 3) in such conditions are superposition of the Airy function Ai and complementary Airy function Bi [2]:

$$\psi_i(\xi_i(z)) = A_i \mathrm{Ai}((\xi_i(z)) + B_i \mathrm{Bi}((\xi_i(z)),$$

where $\xi_i(z)$ is a function, obtained by replacing the variable during obtaining the Airy equation from the Schrödinger equation.

C. Functions of parabolical cylinder

This method has been developed by the authors of this article and can be used for any piecewise-quadratic potential relief, or the one that can be approximated by them.

By the proper variation of stoichiometric composition in the well, a parabolic quantum well formation can be reached (region I in Fig 1, *c*). The solution of the Schrödinger equation for region I (Fig. 3, *c*) is a sum of parabolic cylinder functions:

$$\psi_1(z) = A_1 y_1\{\xi(x(z))\} + B_1 y_2\{\xi(x(z))\},$$

where

$$y_1 = \mathrm{e}^{-\frac{\xi^2}{4}} M\left(\frac{1}{2}\lambda + \frac{1}{4}; \frac{1}{2}; \frac{1}{2}\xi^2\right),$$

$$y_2 = \xi \mathrm{e}^{-\frac{\xi^2}{4}} M\left(\frac{1}{2}\lambda + \frac{3}{4}; \frac{3}{2}; \frac{1}{2}\xi^2\right),$$

$\xi(z)$ – function, obtained by the replacing a variable during obtaining equation of a parabolic cylinder from Schrödinger equation $M(a;b;z)$ is a degenerate hypergeometric series.

One of the applications of these RTDs is multi-valued logic, as RTD's current-voltage characteristics in principle can have the same number of peaks as metastable levels in the quantum well, and RTD with a parabolic well has equidistance peaks at its the VAC.

III. THEORY OF PERTURBATIONS

Using a perturbation theory, for some nanostructures, such as RTD, analytical functions can be obtained, which can fairly approximate shape of $T(E_z)$. For RTD such function is a sum of Lorentz-type functions:

$$T(E_z) = \sum_{i=1}^{N} \frac{\Gamma_i^2}{\Gamma_{\Sigma,i}^2 + 4(E_z - E_i)^2}. \qquad (1)$$

where Γ_i is a «natural» broadening; E_i are positions of the i-th metastable energy level in the quantum well, $\Gamma_{\Sigma,i} = \Gamma_i + \Gamma_p$ are total broadening of the i-th level; Γ_p is a relaxation broadening, N is a total number of energy levels in the quantum well.

IV. NUMERICAL METHODS

To solve the Schrödinger equation numerically, three-point conservative finite-difference scheme of second order accuracy on a uniform grid is usually built [3]. To obtain this scheme, integro-interpolation method is used for interior points, and quantum transmitting boundary method is used for boundary points [4].

As no assumptions about the form of potential are required in the numerical methods, they are applicable for potential relief of arbitrary form.

V. COMPARATIVE ANALYSIS

Implementation of the transmission matrices method is quite simple, although numerical realization is required in practice due to complexity of the form of transmission coefficient. We have shown that numerical instability of the final matrix calculation increase drastically, when the number of matrices excides 5-9 (for typical layers' sizes). Until the method is stable, it is exact (within underlying assumptions) contrary to numerical methods, and can be used to check numerical methods correctness or for setting initial guess during self-consistent calculations.

Application of the Lorentsian functions is restricted by double-barrier RTD only. Superposition of the Lorentsian functions at zero bias is a good approximation of the transmission function, calculated by transmission matrices method at low energies (which are typically relevant); as energy approaches barrier height, derivation between the two functions becomes significant (Fig. 2). Under relatively small bias, given method preserve the trends of the Airy functions method, slightly differing from it (Fig. 3).

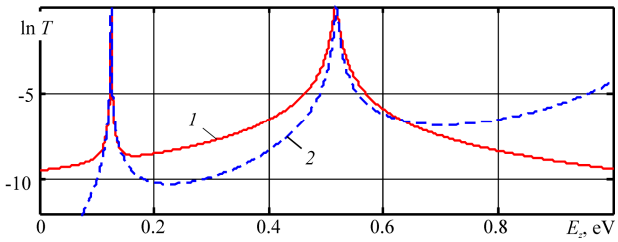

Figure 2. RTD transmission coefficient, calculated by the method of plane waves, numerically (both – *1*) and method of Lorentzian functions (*2*).

Lorentsian functions offer analytical approximation of transmission coefficient, and, consequently, allow fast and stable qualitative analysis. They are formulating through the energy levels and their broadening, which are intuitively understandable; other methods lack such kind of quantities.

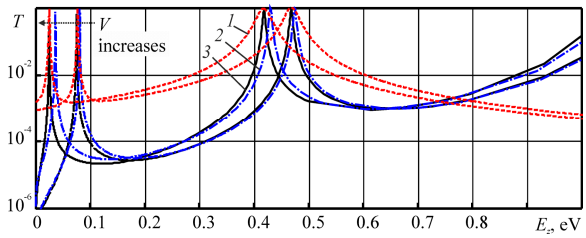

Figure 3. Transmission coefficient of RTD under 0.1 V and 0.2 V, calsulated by Lorentsian functions method (*1*), plane-waves method (*2*), the Airy functions method (*3*).

Quantitative modeling of devices with transverse electron transport is possible only by using numerical methods, which allows taking into account space charge and many-body effects [5]. If realized properly within linear voltage drop approximation, it should coincide with transmission matrices method, as shown in Fig. 2.

REFERENCES

[1] R. Tsu , L. Esaki, "Tunneling in a finite superlattice", Appl. Phys. Letters, vol. 22, pp. 562–564, 1973.

[2] C.S. Lent, D.J. Kirkner, "The quantum transmitting boundary method", J. Appl. Phys., vol. 67, pp. 6353–6359, 1990.

[3] K.F. Brennan, C.J. Summers, "Theory of resonant tunneling in a variably spaced multiquantum well structure: An Airy function approach" J. Appl. Phys., vol. 61, pp. 614–623, 1987.

[4] V. Moskalyuk, A. Fediai; "Simplified analytical model of resonant-tunneling diode", 32nd International Spring Seminar on Electronics Technology, pp.1-5, 13–17 May 2009.

[5] V.A. Moskaliuk, V.I. Timofeev, A.V. Fedyay, "Simulation of transverse electron transport in resonant tunneling diode", 32nd International Spring Seminar on Electronics Technology, pp. 365–369, 12–16 May 2010.