Evaluation of channel transmission of nanoelectronic devices on low-dimensional structures with quantum confinement

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Abstract. A methodology has been developed for evaluation the channel transmission of nanoelectronic devices on low-dimensional 2D structures with quantum confinement and transverse current transfer. The advantage of the developed methodology is to ensure the numerical stability and increased speed of the computational model of channel transmission with a different number of heterostructure layers, which allows optimizing the calculation of the current-voltage characteristics of nanoelectronic devices and predicting their electrical parameters.

1. Introduction
The modern development of micro- and nanoelectronics has resulted in the creation of promising devices with superlattices (periodic structures of nanolayers of two or more semiconductor materials) that act as a low-dimensional channel. Such quantum structures are widely used to create generator [1-3], amplification [4-5], and converter [6] devices operating at terahertz frequencies. A large number of optoelectronic devices are also being implemented on the basis of superlattices, in particular, photodetectors (photodetectors [7-10] and solar cells [11-12]) and light-emitting devices (quantum cascade lasers [13-15] and LEDs [16-17]).

The most important parameter determining the electrical properties of devices on heterostructures is the transmission coefficient (the transmission of the heterostructure). The calculation of the current-voltage characteristics (CVC) of semiconductor devices is characterized by high time complexity, causes a problem with kinetics of CVC simulation because of repeated self-consistent calculation [18–20], which are optimized by applying a high-speed algorithm at the stage of calculating the heterostructure transmission. It is also important to use a numerically stable computational model to ensure satisfactory accuracy in calculating the CVC of the device. The superlattices, acting as a low-dimensional channel of semiconductor devices, have a complex potential relief, which cannot only increase the computation time of the algorithm, but also disrupt its numerical stability.

Thus, the actual task is to develop a method for evaluating the transmission of the channel of nanoelectronic devices on low-dimensional 2D structures with quantum confinement and transverse current transfer based on not only a high-speed, but also a numerically stable quantum-mechanical model for calculating the transmission coefficient of the semiconductor superlattices.

2. Methods
The basis of quantum-mechanical approaches to the description of electron transfer is the representation of semiconductor low-dimensional heterostructures in the form of an open quantum system. As approaches to calculating the transmission coefficient of superlattices, authors analyzed the transfer matrix method and the Green function method.

The transfer matrix method [21-23] is a method for calculating the transmission of a quantum structure, which consists in finding a matrix connecting the amplitudes of electron waves propagating in opposite directions at the boundary points of the structure. To implement this method, the quantum
region is divided into a finite number of small regions $N$ with a certain step, where the potential $U$ is constant. In such regions, the Schrödinger equation is analytically solved (using the Bastard boundary conditions), as a result of which the transfer matrix $M_{i,i+1}$, which reflects the transition of the wave function from the elementary region $i$ to region $i+1$, is derived. The resulting transport matrix $M_{1,N}$ in this case is calculated as the multiplication of all elementary matrices:

$$
M_{1,N} = \prod_{n=1}^{N-1} M_{i,i+1}.
$$

(1)

The transmission coefficient of the structure $T$ is defined as the ratio of the squared modulus of the amplitude of the transmitted wave to the squared modulus of the amplitude of the incident wave, which means that the resulting transfer matrix uniquely determines the transmission of the quantum structure:

$$
T = \frac{|k_N|^2}{|k_1|^2 \prod_{i=1}^{N} |M_{i,i+1}|^2}.
$$

(2)

Here $k_i = [2m_i(U_i - E)]^{1/2}/\hbar$ – the wave number of an electron with energy $E$ in the $i$-th region, $m_i$ – the effective electron mass in the $i$-th region, $\hbar$ – the Dirac constant.

The Green's function method [24-25] is a numerical method of calculating the transmission coefficient of the quantum structure. The Schrödinger equation in the implementation of this approach is given in matrix form (3) taking into account the discrete representation of the wave function and potential:

$$
[EI - H]\psi = 0.
$$

(3)

Here $E$ – the energy, $I$ – the identity matrix, $H$ – the Hamilton operator in matrix form, $\psi$ – the discretized wave function.

When considering the "contact-channel-contact" system, where the superlattice acts as a channel, the Schrödinger equation will change:

$$
[EI - H - \Sigma_L - \Sigma_R]\psi = \{S\}.
$$

(4)

In this equation $S$ – the vector describing the injection of electrons from the contact into the channel, $\Sigma_L, R$ – the matrix operator describing the outflow of electrons from the quantum region to the left (right) contact.

The nonequilibrium Green's function $G$ is the matrix by which the vector $\{S\}$ must be multiplied to obtain the vector of the wave function $\{\psi\}$:

$$
G = [EI - H - \Sigma_L - \Sigma_R]^{-1} = [H^*]^{-1}.
$$

(5)

By calculating the matrix $G$ according to the known parameters of the quantum system, we can calculate the transmission coefficient of the structure $T$:

$$
T = \sum_{n=1}^{N} [G^\dagger GF^R G^+]_{nn}.
$$

(6)
Here \( \Gamma^{L(R)} = j[\Sigma^{L(R)} - \Sigma^{L(R)}_\text{inc}] \) – the matrix characterizing the broadening of energy levels at the boundary of the left (right) contact with the channel, \( N \) – the finite number of regions under consideration, \( j \) – the imaginary unit.

The objects of modeling are low-dimensional channels of the resonant tunneling diode (RTD) [26–27] and the quantum cascade laser (QCL) [28] based on InGaAs / AlAs heterostructures with the number of quantum regions 5 and 61, respectively. The transmission coefficients are calculated for superlattices, the number of potential barriers of which varies from 2 (InGaAs / AlAs RTD) to 30 (InGaAs / AlAs QCL) with a step of 1. Comparison of computational algorithms that implement the calculation of the low-dimensional channel transmission of semiconductor devices by the transfer matrix method and the Green’s function method is carried out using the MATLAB system in two parameters: numerical stability and computation time.

The numerical stability of the method is understood as sensitivity of method to inaccuracies in the initial data [29]. Therefore, the method is stable if small errors in the initial values resulted in small errors in the solution. The matrix solution of the Schrödinger equation is a common step in the considered methods for calculating the transmission coefficient, which means that the numerical stability of the methods directly depends on the conditionality of the matrices that are used in calculating the transmission of the quantum structure. According to the perturbation theory, the condition number indicates how close the matrix is to degeneracy (with a high value of the matrix condition indicator, slight changes in the matrix significantly change the solution of the system of equations). In the MATLAB system, the matrix condition number is calculated using the built-in function \text{cond}, the use of which makes it possible to evaluate the condition of the matrices \( M \) of the equation (1) and \( H^* \) of the equation (5), and hence the numerical stability of the transfer matrix method and the Green’s function method.

Using the \text{tic} and \text{toc} functions built into MATLAB, the computation time of the methods for 100 energy values from 0 to 1.2 eV is calculated. An analysis of the numerical stability of the calculation of channel transmission with a concomitant assessment of the ratio between the computation times of the two methods for heterostructures with the corresponding number of quantum regions using the profiler \text{profile} yielded the following results.

3. Results

Having visualized the dependence of the transmission coefficient calculated by the considered methods on energy (Figure 1), one can note a violation of the numerical stability of the transfer matrix method with an increase in the number of layers in the superlattice, namely, when considering the 7-barrier structure at low energy values, unexpected “bursts” and gaps of transmission (the inability to calculate the transmission coefficient at certain energy values) are observed, which indicates a slight instability of the calculation method at low energy values. In the structure consisting of 30 barriers, one can observe an excess of the transmission of the unit — its limiting value — over the entire energy range under consideration (with the exception of the energy corresponding to resonance peaks). At the same time, the Green’s function method demonstrates good stability regardless of the number of layers in the heterostructure, as evidenced by the calculated values presented in Figure 1.

The observed result can be confirmed by calculating the condition number of the matrices \( M \) and \( H^* \). Indeed, the condition number of the matrix \( H^* \) does not exceed \( 10^5 \) in the regions of resonance energy and \( 10^3 \) in all other regions of the energy, regardless of the number of layers in the superlattice (Figure 2). The resulting matrix \( M \), starting from the calculation of the transmission of the 7-barrier structure, shows an extremely high (~ \( 10^{16} \)) condition number at low energy values, and with an increase in the number of layers in the superlattice, high values of condition number of the matrix are observed in the remaining energy sections, except for resonance ones. With an increase in the number of quantum regions in the structure, the energy range with the limiting values of the condition number (~ \( 10^{16} \)) increases, i.e. it is possible to predict how many layers in the superlattice the calculation of the transmission coefficient at a certain energy value will lose stability.
Figure 1. The transmission coefficient of the superlattices with the number of quantum regions 15 (a) and 61 (b).

Figure 2. Dependences of the condition number of the matrices M (a) and H* (b), corresponding to the transfer matrix method and the Green's function method, on the energy and number of quantum regions.

So, when calculating transmission by the transfer matrix method at an energy close to zero, the resulting matrix M shows the limiting values of condition number in a structure with 7 potential barriers (Figure 2), when the numerical stability of the method for calculating transmission at an energy of 1.2 eV is violated in a structure with 23 potential barriers. The H* matrix at the same energy values shows a low values of condition number that varies in a narrow range of values (for the matrix corresponding to E = 1.2 eV, the condition number remains in the range from 40 to 85) with an increase in the number of layers in the superlattice (Figure 2).
The computation time of the methods increases according to the linear (transfer matrix method) and quadratic law (Green’s function method) with an increase in the number of layers in the superlattice (Figure 3). The transfer matrix method, despite the expected instability, demonstrates the computation time by an order of magnitude less than the Green's function method.

![Figure 3: Dependence of the computation time of the transfer matrix method (a) and the Green's function method (b) on the number of quantum regions of superlattices; evaluation of the computation time of methods for heterostructures with 15 (c) and 61 (d) quantum regions using the profiler profile.](image)

4. Discussion

The calculated condition numbers of the matrices made it possible to confirm the results observed in the transmission modeling by the considered methods. So, if you calculate a structure with a large number of layers included in it (from 15 or more in the structure under consideration), the transfer matrix method loses numerical stability due to an ill-conditioned resulting matrix, however, it remains possible to calculate transmission at higher energy values, which does not require is used when calculating the CVC of a semiconductor device in connection with the influence of the electron supply function. This means that the transfer matrix method is preferable for calculating heterostructures with a small number of quantum regions. By calculating the dependence of the condition number of the resulting matrix M on the number of layers in the structure, it is possible to predict the numerical stability of the solution at a certain energy value, and therefore determine the energy range in which it is possible to stably calculate the transmission of the superlattice of the configuration of interest.

The Green's function method has proved to be a more universal method for modeling semiconductor superlattices, since the algorithm for calculating the transmission of the heterostructures under consideration (the number of quantum regions of the structure varied from 5 to 61 in steps of 2) remains stable, which confirms the good values of condition number (no more than $10^6$) of the matrix $H^*$ (Figure 2). Evaluation of the implementation time showed that the
computational time of this method is an order of magnitude longer than that of the transfer matrix
method.

Based on the results obtained, a methodology has been developed for assessing the transmission of
a low-dimensional channel of arbitrary complexity, which ensures the stability and high speed of the
algorithm for calculating the transmission coefficient of both double-barrier structures (InGaAs / AlAs
RTD) and multilayer superlattices (InGaAs / AlAs QCL), which allows to optimize the kinetics of
CVC simulation of a wide class of semiconductor devices.

5. Conclusions

Thus, the developed methodology for evaluation the channel transmission of nanoelectronic devices
on low-dimensional 2D structures with quantum confinement and transverse current transfer is based
on the application of such an approach to calculating the transmission of heterostructures, which, on
the one hand, is due to the complexity of the potential channel relief and, on the other hand, is adapted
to change the channel profile in the kinetics of the CVC during operation of the nanoelectronic device.
The developed methodology provides stability and high speed of the computational model of a
heterostructure channel transmission of arbitrary complexity.

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