Significance and Novelty

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Significance and Novelty of the paper “Calculation of electron transport in branched semiconductor nanostructures using quantum network model”.

Significance

Electron transport in branched semiconductor nanostructures provides many possibilities for creating fundamentally new devices. The scientific significance of the paper is the formulation of an effective algorithm for calculating electron transport. The proposed algorithm has the following advantages.

1. *Programmability*. The algorithm is presented in the form of a program-friendly implementation. This is achieved due to the original system of agreements and notation (section 2.1).
2. *Completeness*. The algorithm contains all the elements necessary for calculating electron transport. First, in its framework, the scattering problem of an electron/hole in the junction is solved (section 2.3). The electron/hole scattering in the entire nanostructure is then calculated based on this (section 2.4). Finally, the electrical characteristics of the nanostructure are calculated taking into account electrons/holes statistics (section 3).
3. *Accuracy*. The algorithm is formulated in terms of an extended scattering matrix. This allows one to correctly perform calculations taking into account tunnel effects. Tunnel effects affect the scattering properties of nanostructure junctions.
4. *Universality*. The algorithm is designed for nanostructures with an arbitrary number of junctions. This is achieved due to the network combining formula (section 2.4.3).
5. *Flexibility*. The algorithm allows for different calculation methods for a particular nanostructure. This is achieved both by varying the methods of calculating scattering in the junction (sections 2.3.2 and 2.3.3) and by varying the order of combining network junctions according to the formula (92).
6. *Performance*. The algorithm provides high performance. This is achieved both by the possibility of partial calculation of scattering in analytical form (for example, section 4.1.3 and appendix B) and by the absence of the need for individual calculation of scattering in the same junctions (see example in section 4).
7. *Validity*. All parts of the algorithm have a rigorous mathematical proofs. The paper contains 16 propositions that are proven in detail, which makes it easier for the reader to check them.
8. *Realness*. The algorithm is designed to model not abstract mathematical constructions, but real nanostructures studied in modern experiments (see example in section 4).

The author programmed the proposed algorithm on C++ using an object-oriented paradigm. To test the algorithm, a QIY-network model was proposed (section 4.1). Using it, the author simulated several nanostructures relevant to modern nanoelectronics (switch, logic element XOR, etc.). The structure of four junctions is considered as a minimal non-trivial example (section 4.2). Analysis of its transport properties showed that they correspond to the expected ones. Thus, the algorithm proposed in the paper confirmed its effectiveness in modeling branched semiconductor nanostructures.

Novelty

The scientific significance of the proposed calculation algorithm is ensured by its novelty. It is achieved due to the following features.

1. *Agreements and notation*. To formulate the algorithm, it was necessary to develop an original system of agreements and notation (section 2.1). It combines both already known elements and new approaches. The proposed system also helps to increase the clearness of computations and reproducibility of results.
2. *Scattering boundary conditions*. To calculate the electron/hole scattering in the nanostructure junction, scattering boundary conditions in the integro-differential form are formulated (sections 2.3.1 and 2.3.2). They simplify the definition of the scattering problem and obtaining its solution in an analytical form, where possible. Also, these boundary conditions have a simple interpretation and allow one to easily formulate the resonant states problem (Appendix A).
3. *Adapted DN- and ND-map methods*. The DN- and ND-map methods known in the literature are written in terms of an extended scattering matrix as part of the original algorithm for calculating electron transport (section 2.3.3). The relevant expressions have been proven in detail (Appendix C).
4. *Network combining formula*. For the first time, the formula for combining a quantum network was obtained (section 2.4). It allows one to calculate the scattering of an electron/hole in an arbitrary branched nanostructure. For this, there is enough information about the scattering of an electron/hole in its typical junctions. This approach is particularly effective for large nanostructures with a small number of typical junctions. The network combining formula has been rigorously proven and tested on known special cases (Appendix D).
5. *Adaptation of the Landauer–Büttiker formalism*. The Landauer–Büttiker formalism known in the literature is adapted for the algorithm developed in the paper (section 3). For this purpose, the relevant propositions have been formulated and proved in detail (Appendix E). This made it possible to obtain a valid and complete algorithm for calculating electron transport.
6. *QIY-network*. As an example for testing the algorithm proposed in the paper, a quantum network of smooth Q-, I - and Y-junctions was presented (section 4). Such a network is the basis for modeling nanostructures based on two-dimensional electron gas. These structures are widely studied in modern experiments, which makes the QIY-network particularly relevant.

Thus, the new approaches proposed in the paper made it possible to obtain an improved algorithm for calculating the transport properties of branched nanostructures.