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In memoriam Vladimir A. Geyler (1943–2007)

Numerical Simulation of Electron Scattering by Nanotube Junctions

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Abstract. We demonstrate the possibility of computing the intensity of electronic transport through various junctions of three-dimensional metallic nanotubes. In particular, we observe that the magnetic field can be used to control the switch of electron in Y-type junctions. Keeping in mind the asymptotic modeling of reliable nanostructures by quantum graphs, we conjecture that the scattering matrix of the graph should be the same as the scattering matrix of its nanosize-prototype. The numerical computation of the latter gives a method for determining the "gluing" conditions at a graph. Exploring this conjecture, we show that the Kirchhoff conditions (which are commonly used on graphs) cannot be applied to model reliable junctions. This work is a natural extension of the paper [1], but it is written in a self-consistent manner.

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1. INTRODUCTION

Studies of the electron transport through Y-branch junctions of waveguides have attracted considerable attention in the last decades (see, e.g., [2, 3]). The interest to the topic increased recently in view of the progress in artificial formation of carbon nanotube-junctions [4]. In the paper, we discuss the procedure of numerical computation of the junction's scattering properties and demonstrate its efficiency by various examples. In particular, we observe that the magnetic field can be used to control the electron transport through Y-type junctions. Hopefully, this observation can be applied for the practical construction of electron switches.

There is another motivation for this work as well. As is known, the electron motion through nanotubes is essentially one-dimensional. In particular, an asymptotically one-dimensional description comes in a natural way by virtue of the adiabatic analysis of band nanotubes with variable cross-section [5–7]. However, the one-dimensional analysis fails at junctions. Normally, the modeling by graphs is used as a convenient tool to study scattering properties of branched quantum wires or nanotubes. However, such a model contains an uncertainty in the boundary (gluing) conditions at vertex point(s).

The paper is aimed, in particular, at suggesting a way to determine the gluing condition. We discuss the motivations to identify the scattering matrix of the graph with the scattering matrix of its nanosize-prototype; the latter can be computed numerically. Then, in view of the simplicity of the graph model, the gluing condition is restored explicitly by the scattering matrix of the graph. We examine graph models equipped with some "standard" gluing conditions and demonstrate that they are not adequate for reliable junctions.

2. SCATTERING MATRIX AND COMPUTATIONAL APPROACH

We model the nanotube junction by a domain Ω which coincides with a finite family of semi-infinite cylinders (channels) outside a ball of sufficiently large radius. Let the motion of electrons in Ω be governed by the Schrödinger equation

$$\mathcal{H}\Psi = E\Psi \tag{1}$$

† Deceased on February 17, 2008.

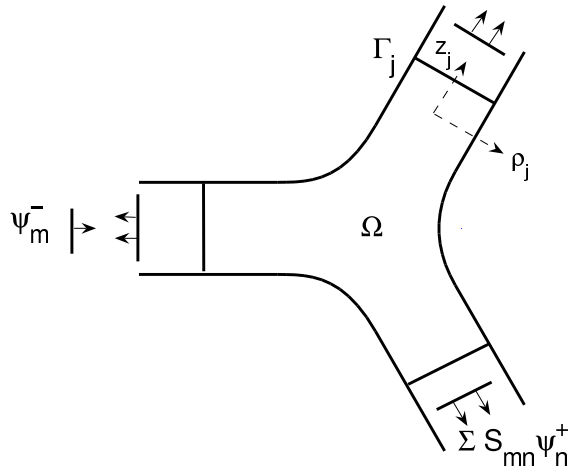

Fig. 1. On the definition and computation of the S-matrix.

with some boundary condition at $\partial\Omega$. We assume that at each channel the operator $\mathcal{H}$ admits the separation of variables, and thus Eq. (1) has solutions of the form

$$\psi^{\pm}_{m_j} = \frac{\mathrm{e}^{\pm \mathrm{i}\nu_{m_j} z_j}}{\sqrt{\nu_{m_j}}} \Phi_{m_j}(\rho_j)\,, \tag{2}$$

where $j = 1, \ldots, N$ is the index of a channel, (z_j, ρ_j) are the longitudinal and transverse coordinates at each channel (see Fig. 1), and $\Phi_{m_j}(\rho_j)$ is the normalized eigenfunction of the transverse eigenvalue problem

$$\mathcal{H}_\perp \Phi = \lambda \Phi \tag{3}$$

with appropriate boundary conditions on $\partial\Omega\big|_{z_j=\mathrm{const}}$. We assume the completeness of $\Phi_{m_j}(\rho_j)$ for each j.

Solutions (2) with $\nu_{m_j} = \sqrt{E - \lambda_{m_j}}$ are called *modes*. Let, for each j, finitely many eigenvalues λ_{m_j} $(m_j = 1, \ldots, M_j)$ of the problem (3) satisfy the inequality

$$\lambda_{m_j} < E\,. \tag{4}$$

The values of E at which M_j jumps are said to be *energy thresholds*. The modes satisfying condition (4) are said to be *propagating* (incoming for the minus and outgoing for the plus sign).[1] Provided that this leads to no ambiguity, we assume that the propagating modes are enumerated in some way throughout all channels and omit the subscript j, $\psi^{\pm}_{m_j} \rightsquigarrow \psi^{\pm}_m$. Denote the total number of propagating modes (incoming and outgoing) by $2M$.

The electronic transport through a junction is completely characterized by the *scattering matrix*. We introduce this matrix in the following way.

Consider an E such that $M > 0$. In this case (see [8]), there is a set of solutions to the problem (1) with the following asymptotics as $z \to +\infty$:

$$\widetilde{\psi}^{-}_m + \sum_{n=1}^{M} S_{mn} \widetilde{\psi}^{+}_n + O\left(\mathrm{e}^{-\delta z}\right)\,, \qquad m = 1, \ldots, M\,, \tag{5}$$

where $z = \min\{z_1, \ldots, z_N\}$, $\delta > 0$, $\widetilde{\psi}^{\pm}_{m_j} = \psi^{\pm}_{m_j} \eta_j(z_j)$, and $\eta_j(z)$ is a smooth cut-off function vanishing everywhere on Ω except for the jth channel, where it is equal to one. The coefficients S_{mn} in (5) form a unique $M \times M$ unitary scattering matrix $S = \|S_{mn}\|$. Taking into account the above agreement on the enumeration of modes, one can clearly interpret a solution with the asymptotics (5) as the scattering of the incoming mode ψ^{-}_m by a junction (see Fig. 1).

Difficulties related to the numerical computation of the scattering matrix arose from its definition on an infinite domain. To reduce the problem to a bounded domain, consider the truncation of Ω by planes crossing the channels. By Γ_j, $j = 1, \ldots, N$, we denote the parts of these planes inside Ω (see Fig. 1).

[1] In another terminology, the channel j is said to be *open for the mode* m_j if (4) holds.

To introduce the artificial boundary conditions on Γ_j, consider the operators which are called the *Dirichlet-to-Neumann maps*:[2]

$$\Psi\Big|_{\Gamma_j} \mapsto \mathcal{T}_j(E)\Psi\Big|_{\Gamma_j} = \sum_{m_j=1}^{\infty} \mathrm{i}\nu_{m_j} a_{m_j} \Phi_{m_j}(\rho_j)\,, \tag{6}$$

$$a_{m_j} = \int_{\Gamma_j} \Psi\Big|_{\Gamma_j} \Phi_{m_j}\,\mathrm{d}\sigma\,, \qquad \nu_{m_j} = \begin{cases} \sqrt{E-\lambda_{m_j}} > 0\,, & \lambda_{m_j} < E, \\ \mathrm{i}\sqrt{\left|E-\lambda_{m_j}\right|}\,, & \lambda_{m_j} > E\,. \end{cases}$$

Clearly $\mathcal{T}_j\psi^{\pm}_{m_j}|_{\Gamma_j} = \pm\nu_{m_j}\psi^{\pm}_{m_j}|_{\Gamma_j}$, and thus the operator $(\partial/\partial z_j - \mathcal{T}_j)$ is "transparent" for outgoing modes but not transparent for incoming modes,

$$\big(\partial/\partial z_j - \mathcal{T}_j\big)\psi^{+}_{m_j}\big|_{\Gamma_j} = 0 \quad \text{and} \quad \big(\partial/\partial z_j - \mathcal{T}_j\big)\psi^{-}_{m_j}\big|_{\Gamma_j} = -2\mathrm{i}\nu_{m_j}\psi^{-}_{m_j}\big|_{\Gamma_j}\,.$$

Let $\mathbf{P}_m$ be the boundary-value problem for Eq. (1) on the truncated domain with boundary condition preserved on the truncated part of $\partial\Omega$. We close the problem by an additional boundary condition on $\Gamma = \sum_j \Gamma_j$ of the form

$$\Big(\frac{\partial}{\partial z_j} - \mathcal{T}_j\Big)\Psi\Big|_{\Gamma} = -2\mathrm{i}\nu_m\widetilde{\psi}^{-}_{m}\Big|_{\Gamma} \tag{7}$$

(here we again apply the enumeration of modes). It has been proved [11, 12] that the solution Ψ_m to the problem $\mathbf{P}_m$ can be extended to the unbounded domain Ω with the asymptotics (5). Thus, by obtaining all solutions Ψ_m, $m = 1, \ldots, M$, numerically, one can compute the scattering matrix as

$$S_{mn} = \big[\operatorname{diag}\|\sqrt{\nu_m}\|\big]\,\big\langle \Psi_m, \psi^{+}_{n}\big\rangle\,\Big|_{\Gamma}\big[\operatorname{diag}\|\sqrt{\nu_m}\|\big]^{-1}\,. \tag{8}$$

Remark. In general, the operators $\mathcal{T}_j$ cannot be found explicitly, since their definition (6) requires summation of both propagating modes and infinitely many evanescent modes. The natural approach is to replace these operators by their projections to open channels (propagating modes) only. The error which is introduced by this approximation is expected to be exponentially small provided that the truncating boundaries Γ_j are put sufficiently far from the junction.

Another approach to the computation of the scattering matrix (also related to the approximation of the operators $\mathcal{T}_j$) was discussed in [9, 10] (see the references therein).

3. NUMERICAL RESULTS: SCATTERING BY Y-JUNCTION

3.1. *Specification of the Examined Problem*

For the sake of brevity, we consider only $\mathcal{H} = -(\nabla + \mathrm{i}A)^2$ with the Dirichlet boundary conditions. This choice corresponds (in dimensionless units) to the one-electron effective-mass approximation of electronic transport in a metallic nanotube under the presence of a magnetic field.

We discuss the numerical results for the *"Y-type"* junction ($N = 3$). To reduce the number of parameters of the problem to a reasonable minimum, we focus on the consideration of a junction with identical circular cross-sections (assuming the unit radius of cross-section throughout the paper) of channels. Let the generatrices of half-cylinders be specified by directional vectors {1,0,0} (1st channel), $\{\cos(\pi-\varphi), -\sin\varphi, 0\}$ (2nd channel), and $\{\cos(\pi-\varphi), \sin\varphi, 0\}$ (3rd channel), see Fig. 3. The angle φ is said to be the *opening angle* of a junction.

For simplicity, assume that

$$A = \begin{cases} (qy, px, 0)\,, & \sqrt{x^2+y^2} < R\,, \\ 0 & \text{otherwise}\,, \end{cases} \qquad p, q = \text{const}\,. \tag{9}$$

Thus, the magnetic field is directed orthogonally to the plane containing all generatrices. The field is uniform inside the cylinder $x^2 + y^2 < R^2$ and vanishes outside it. In other words, $\mathcal{H} = -\Delta^{\mathcal{D}}$

[2]Special care is necessary for threshold energies. We do not dwell on these details, assuming that E does not coincide with a threshold. The interested reader is addressed to [8–10] and the references therein.

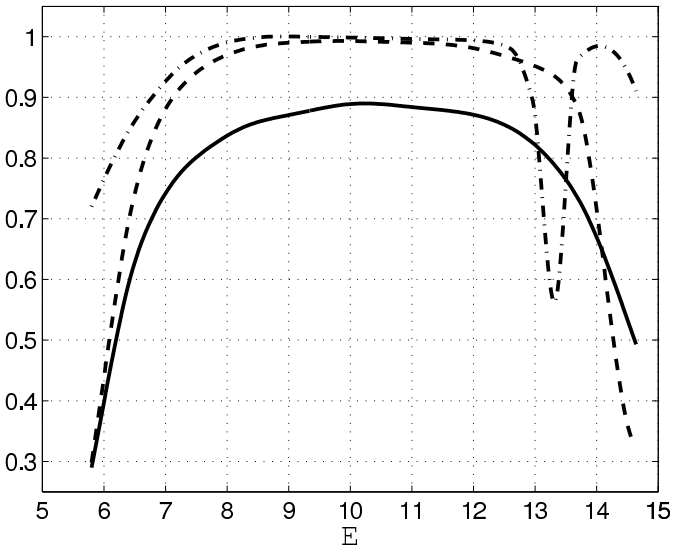

Fig. 2. Total conductance $|S_{12}|^2 + |S_{13}|^2$ versus energy E for Y-junction with various opening angles φ: $\varphi = \pi/3$ (solid line), $\varphi = \pi/6$ (dashed line), and $\varphi = \pi/12$ (dash-dot line).

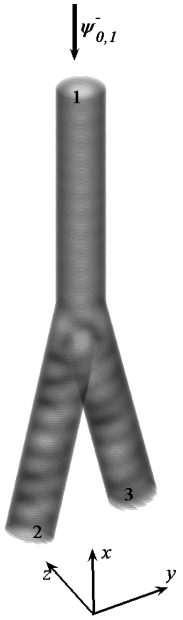

Fig. 3. Scattering of nonrotational mode ($m = 0$) incoming from the first channel ($j = 1$). Opening angle of the junction is $\pi/12$.

(the Dirichlet Laplacian) outside the cylinder. The Dirichlet eigenfunctions for the circular cross-section of radius $d = 1$ are known to be

$$\Phi_m(\rho) := \Phi_{m,p}(r,\alpha) = \mathrm{e}^{\mathrm{i}m\alpha}\frac{\mathrm{J}_m(\zeta_{m,p}r)}{\sqrt{\pi}d\mathrm{J}_{m+1}(\zeta_{m,p})},$$

where $\zeta_{m,p}$, $p = 1, \ldots,$ stands for the pth zero of the Bessel function J_m and d for the radius of the cross-section. Provided that $d = 1$ is fixed, the corresponding eigenvalues (and thus the energy thresholds) are $\lambda_{m,p} = \zeta_{0,1}^2 < \zeta_{0,2}^2 < \zeta_{1,1}^2 < \cdots$. The energy range between the first two thresholds corresponds to nonrotational modes.

3.2. *Scattering in the Absence of a Magnetic Field*

In this subsection, we assume that $p = q = 0$, i.e., the transport of a free electron will be examined. We consider first the scattering of nonrotational modes, i.e., for the energy levels $\zeta_{0,1}^2 < E < \zeta_{0,2}^2$. For such energies, each open channel supports exactly one (up to inversion of the propagation direction) propagating mode ($M = 3$).

In Fig. 2, we focus on the total conductance through a junction from one channel, say, j, to others $j_{1,2} \neq j$. This term is usually understood as the sum (up to some non-important constant factor) $|S_{jj_1}|^2 + |S_{jj_2}|^2$ ($\|S_{jk}\|$ is the scattering matrix). We compare the conductance for various mutual orientations of generatrices of the merged half-cylinders. In all cases, the conductance exhibits a maximum, not strictly pronounced, around the middle of the energy interval between the first and second thresholds. At the same time, the variation of the opening angle of the junction causes not only qualitative but also quantitative differences.

For energy levels between $\zeta_{0,2}^2$ and $\zeta_{1,1}^2$, the scattering picture is more complicated, since both nonrotational and rotational modes are involved, $M = 6$. In Fig. 3, the scattering of nonrotational mode ($m = 0$) incoming from channel $j = 1$ is shown. It is seen that rotational modes are excited in channels $j = 2$ and $j = 3$.

The conductance for $\zeta_{0,2}^2 < E < \zeta_{1,1}^2$ is shown in Fig. 4. We focus both on the total conductance and nonrotational and rotational parts of conductance. It can be seen that the conductance to nonrotational modes is much stronger.

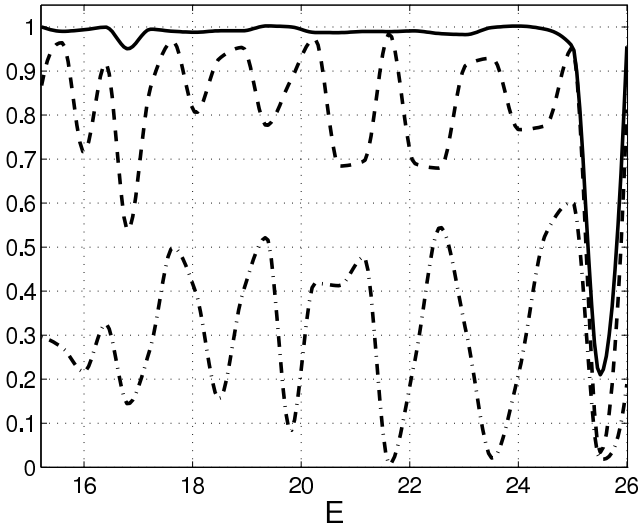

Fig. 4. Conductance versus energy varying in the range $\zeta_{0,2}^2 < E < \zeta_{1,1}^2$: the solid line shows the total conductance $|S_{13}|^2 + |S_{14}|^2 + |S_{15}|^2 + |S_{16}|^2$ of the nonrotational mode incoming from the first channel, the dashed line, that of the nonrotational part $|S_{13}|^2 + |S_{15}|^2$ of the conductance, and the dash-dot line, that of the rotational part $|S_{24}|^2 + |S_{26}|^2$ of the conductance. The opening angle of the junction is $\varphi = \pi/12$.

3.3. *Controlling of Electron Transport through the Junction by the Magnetic Field*

In this subsection, we study the influence of the magnetic field on electron transport. It can be seen in Fig. 5 that a sufficiently strong magnetic field thoroughly changes the conductance properties of the junction. For example, starting from $q \gtrsim 1.75$, the channel $j = 1$ is almost excluded from the conductance: neither electrons coming from this channel can propagate to others nor electrons from channels $j = 2, 3$ can reach the first channel. This observation can be applied for practical constructing of electron switches.

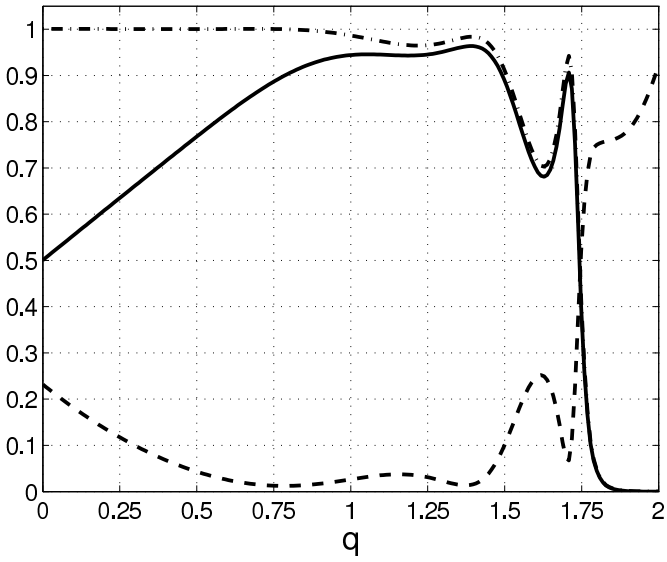

Fig. 5. Conductance through a Y-junction of opening angle $\varphi = \pi/12$ versus strength q ($p = 0$ is fixed to reduce the number of parameters) of the magnetic field: the solid line shows $|S_{21}|^2$ (from the second to the first channel), the dashed line shows $|S_{23}|^2$ (from the second to the third channel), and the dash-dot line shows $|S_{12}|^2 + |S_{13}|^2$ (the total conductance from the first channel). The energy is fixed in the middle of the range of nonrotational modes: $E = 9$.

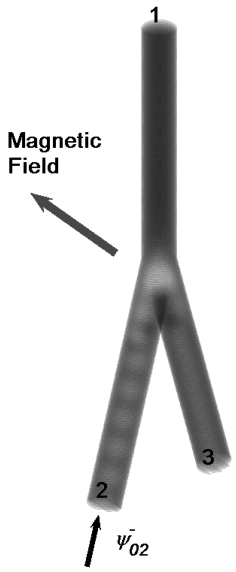

Fig. 6. Switching of the mode incoming from the channel $j = 2$ to the channel $j = 3$ by a sufficiently strong ($q = 2$) magnetic field. The geometry of Y-junction is the same as in Fig. 3 and $E = 9$.

4. ON "GLUING" CONDITIONS FOR QUANTUM GRAPHS

A quantum graph is sometimes regarded as a limiting model for a thin (nano) wire or tube. Such a model is rather natural and promising because of its one-dimensional character. Moreover, for some cases, the direct and inverse scattering problems on a graph can be solved explicitly.

Many studies [13–21] have been devoted to the investigation of the limiting procedure as $d \to 0$ from different points of view, where d is the parameter defining the thickness of a wire. In particular, the problem of adequate formulation of the *gluing condition* at a graph-junction has attracted much attention. However, this question is still not completely clear.

We suggest identifying the scattering matrix on the graph (*graph-matrix*) with the *S-matrix* for the nano-junction. The latter can be computed numerically by the technique given in Section 2 (no gluing condition is required). This suggestion is based on the following motivations.

First, we note that the scattering problem (1)–(5) is invariant with respect to simultaneous scaling of coordinates $x \rightsquigarrow x/d$ and the energy $E \rightsquigarrow Ed^2$. Moreover, the S-matrix is invariant under this scaling as well. The second observation deals with the composition rules for graph-matrices. As was discussed in [22], the whole (*on-shell*) scattering matrix for a graph with several vertices can be obtained from *elementary* scattering matrices related to each vertex. It was numerically verified in [1] that the S-matrix for the wire's structure with several junctions asymptotically (if the wire's longitudinal scale is much larger than the transverse one) behaves in the same way: it can be computed by means of the same composition rules as in [22], provided that the scattering matrices for each junction are known.

By accepting the above identifications, we apply the scattering theory on graphs (which is briefly reviewed in Appendix 1; see also the references there). In particular, we explore the gluing condition in (the most general) form (2)–(3) and use explicit direct and inverse relations (5) and (6) between the scattering matrix and the coefficients in (2). As a consequence, the matrices A and B in (2) are obtained.

These matrices were computed in accordance with the above procedure for various junctions and energy levels. Since, for all examined cases, the matrix A turned out to be invertible, we focus on $A^{-1}B$ (the latter matrix is defined uniquely by the scattering matrix). Numerical results characterizing this matrix are shown in Fig. 7.

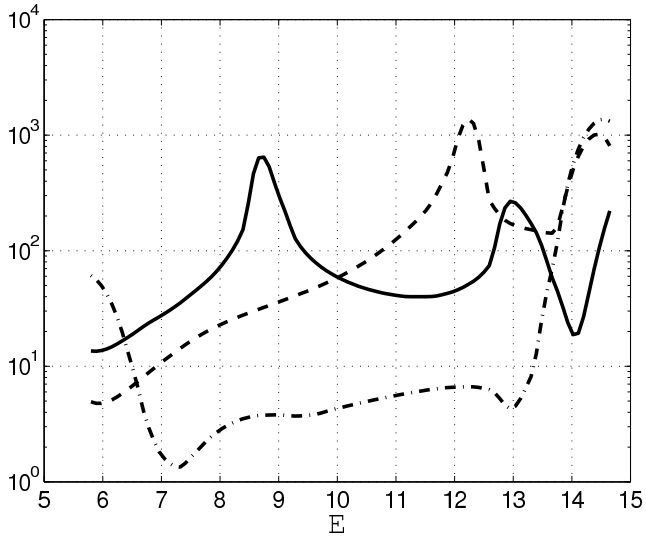

Fig. 7. Condition number of matrix $A^{-1}B$ versus energy E for the same junctions as in Fig. 2.

In these results, we control the condition number of $A^{-1}B$ because of the following considerations. Note that condition (7) was discussed by many authors as an appropriate graph model for reliable junctions. It follows from (8) that rank $\left(A^{-1}B\right) = 1$, and thus the condition number is singular. Our results are in contradiction with this inference: the condition number exhibits peaks only for some energy values (unfortunately, the authors have no natural explanation for these specific energies). Thus, condition (7) could hardly be applicable. Moreover, (7) also leads to the energy-independent matrices (8). This independence does not confirm by numerical results shown in Figs. 2 and 7.

CONCLUSION AND ACKNOWLEDGMENTS

The approach to the computation of the scattering properties of Y-type junctions of three-dimensional metallic nanotubes was suggested and illustrated by various examples. In particular, we showed the possibility to control electronic transport through a Y-junction by the magnetic field. The research was also applied to arrive at the appropriate gluing condition when modeling nanostructures by graphs.

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APPENDIX. INVERSE SCATTERING FOR QUANTUM GRAPHS

In this appendix, we briefly represent (with minor modifications) some results of the series of papers [22–24] dealing with scattering properties of quantum graphs. First, we define an *elementary graph* as the direct sum

$$\mathbb{H} = \bigoplus_{m=1}^{M} H_m\,, \qquad H_m = -\frac{\mathrm{d}^2}{\mathrm{d}x_m^2} + \lambda_m, \tag{A.1}$$

of Schrödinger operators acting on half-lines $x_m \in (0,\infty)$[3] with the *gluing* condition

$$Au + Bu'\Big|_{x=0} = 0\,, \tag{A.2}$$

where $u = \{u_1(x1), \dots, u_M(x_M)\}^T$, $H_m u_m = EU_m$. Here A and B are $M \times M$ matrices such that

$$AD_\nu B^\dagger \quad \text{is Hermitian}, \quad D_\nu = \operatorname{diag}\|\nu_m\|\,, \quad \nu_m = \sqrt{E-\lambda_m} \tag{A.3}$$

(the inequality $E > \lambda_m$ is assumed for all $m \leqslant M$).

Let the set of solutions to $\mathbb{H}u = Eu$,

$$u_n^- + \sum_{m=1}^{M} \mathcal{S}_{nm} u_m^+\,, \qquad n = 1, \dots M\,, \tag{A.4}$$

where $u_m^\pm = \exp\{\pm \mathrm{i}\nu_m x_m\}/\sqrt{\nu_m}$, satisfy condition (A.2). Then $\mathcal{S} = \|\mathcal{S}_{nm}\|$ is called the scattering matrix of an elementary graph. It can be obtained explicitly as

$$\mathcal{S} = -\left(A + \mathrm{i}BD_\nu\right)^{-1}\left(A - \mathrm{i}BD_\nu\right)\,. \tag{A.5}$$

The inverse scattering problem is to determine the matrices A and B in (A.2) when the scattering matrix $\mathcal{S}$ is given. The solution to this problem is not unique, and these matrices can be found up to left multiplication by an arbitrary nondegenerate matrix. By omitting this uncertainty, one arrives at

$$A = \frac{1}{2}\left(\mathbb{I}_M - \mathcal{S}\right)\,, \quad B = \frac{1}{2\mathrm{i}}\left(\mathbb{I}_M + \mathcal{S}\right) D_\nu^{-1}\,, \tag{A.6}$$

where $\mathbb{I}_M$ is the $M \times M$ identity matrix.

Note that, if A^{-1} exists, then condition (A.2) (end hence the scattering matrix (A.5)) is defined by a single matrix $A^{-1}B$. In turn, this matrix can be restored uniquely from $\mathcal{S}$.

The following gluing condition is commonly used in the analysis on graphs:

$$u_1(0) = u_2(0) = \dots = u_M(0)\,, \qquad u_1'(0) + u_2'(0) + \dots + u_M'(0) = \gamma u_M(0)\,. \tag{A.7}$$

(It is said that γ models the strength of δ-potential at $x = 0$; (A.7) is referred to as the *Kirchhoff's condition* for $\gamma = 0$.) Conditions (A.7) lead to the following relations:

$$A^{-1}B = \frac{1}{\gamma}\begin{pmatrix} 1/\nu_1 & \dots & 1/\nu_M \\ \dots & \dots & \dots \\ 1/\nu_1 & \dots & 1/\nu_M \end{pmatrix}\,, \qquad \mathcal{S} = \frac{2}{M - \mathrm{i}\gamma}\begin{pmatrix} 1 & \dots & 1 \\ \dots & \dots & \dots \\ 1 & \dots & 1 \end{pmatrix} - \mathbb{I}_M\,. \tag{A.8}$$

Thus, the gluing condition (A.7) results in the scattering matrix, and the matrix $A^{-1}B$ is independent of the energy E.

[3] The case of more general operators is studied in [25].

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