Two-body scattering on a graph and application to simple nanoelectronic devices

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The two-body system on a graph with one junction is considered. The effective three-body scattering problem turns out to be exactly solvable for pointwise interactions. Additional degrees of freedom corresponding to a dynamics of some structure (e.g., an atomic cluster) located in the junction (point of common contact) of three thin electrodes are considered. These degrees of freedom bring effective energy-dependent interaction into the effective Schrödinger equation in the scattering channel. The wave function of the system is constructed in the explicit form using the extension theory methods. The obtained results are applied to the qualitative description of a simple three-electrode nanoelectronic device. The perturbation theory approach based on the analysis of the Liouville equation is suggested for calculation of the conductivity for such a device in terms of the obtained wave function. © *1995 American Institute of Physics.*

I. INTRODUCTION

Investigation of the so-called one-electron device[1,2] is usually based on some models representing their basic properties. Special interest is related to the study of conductivity of such devices, because they can probably serve as an element base for nanoelectronic circuits.

Complete description of a many-body quantum system is a hardly solvable problem, so the usual way to construct the correspondent model is the following. First, one can study the one-electron problem for the considered quantum system and calculate the correspondent wave function. Next, using methods of statistical physics, one can apply the obtained results to calculate the macrocharacteristics, e.g., the conductivity. However, this approach gives no opportunity to consider few-body effects in the quantum system. Effects of resonance scattering generated by simultaneous location of several electrons in the device cannot be considered without a preliminary solution of the few-electron problem. At the same time these effects can be crucial for nanoelectronic systems. Really, because of the sizes of nanoelectronic devices, an individual act of interaction between quantum particles in the device is significant. An example is given by the electron pairing effect in superconductivity. That is why one-electron models can be considered as a zero-order approximation only, and the next step is to solve the similar two-electron problem at least. However, because of the nontrivial topology of the device (i.e., of the correspondent graph) in the general case this problem has all the difficulties of a three-body problem.

Our first aim is to construct an exactly solvable model of a two-electron system in a simple nanoelectronic device in order to have an opportunity to estimate qualitatively some possible effects. From the mathematical point of view the problem is related to scattering on graphs.[3,4] The obtained formulas are the base for calculation of the conductivity in frames of the mentioned model.
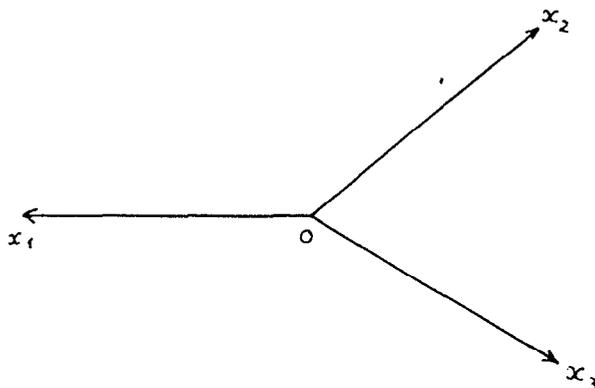
FIG. 1. Y graph Γ.

II. MODEL OF A THREE-ELECTRODE DEVICE WITH ATOMIC CLUSTER IN THE JUNCTION

Let us consider a system of three thin (quasi-one-dimensional) long conductors with one junction (point of common contact). We suppose the presence of some atomic cluster with fixed energy levels in this point of junction. We are going to study the dynamics of the system of two electrons which spread along the conductors and can be captured by the atomic cluster in the junction. Special attention is paid to the process with one free electron in the initial state and two free electrons in the final state (the electron bounded by the atomic cluster is knocked out by the incoming electron), because these process cannot be described in frames of any one-electron model.

The system of three thin conductors is simulated by the Y graph (see Fig. 1). In the description of the atomic cluster we restrict ourselves to the consideration of two-electron resonances. We suppose that $n-1$ lowest energy levels are occupied at every moment. The value of the energy $E=0$ is assigned to the state with no other electrons bounded by the cluster, and the state with one additional electron on the nth level is supposed to have energy $E=-h^2$, where $h>0$ is the parameter of the model.

The scheme of two-electron states of the isolated atomic cluster is shown in Fig. 2. The set of the energy levels $\{\lambda_s\}$ marked by the crosses on the interval $[-2h^2,0)$ we denote as $\sigma(H^{ad})=\{\lambda_s\}$. We interpret this set as the spectrum of some (finite-dimensional) self-adjoint operator (Hermitian matrix) H^{ad}. Concrete representation of the operator H^{ad} is not essential in frames of the used
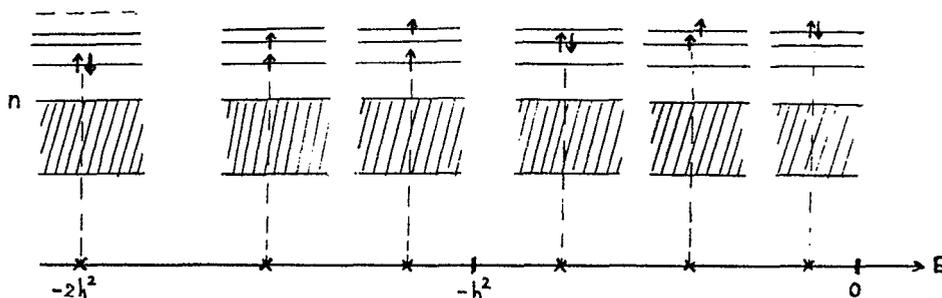
FIG. 2. Two-electron states of the isolated atomic cluster.

technique[5,6] and without lost of generality one can take for H^{ad} the diagonal real-valued matrix $H^{ad} = \mathrm{diag}\{\lambda_s\}$. The operator H^{ad} models the internal dynamics of the isolated atomic cluster.

It is well known[7] that in a solid the effective interelectron interaction decreases exponentially (like the Yukawa potential), so in some approximation we can simulate it by a contact pointwise interaction (zero-range potential). An example is given by the so-called exchange forces generated by the spin components of the wave functions. Namely, the system of two electrons with parallel (antiparallel) spins is antisymmetric (symmetric) with respect to the permutation of particles, and the correspondent problems can be solved separately. Here we restrict our consideration to the pointwise interaction in order to obtain an exactly solvable model.

III. ONE-ELECTRON PROBLEM ON Y GRAPH

In frames of our model the configuration space for one electron in the system of three conductors is the Y graph Γ (see Fig. 1). The phase space is

$$L^2(\Gamma) = \sum_{j=1}^{3} \oplus L^2(\mathbf{R}_+^1)$$

and its elements are three-component functions $u(x) = \{u_j(x_j)\}_{j=1}^{3}$. The component u_j describes the the distribution of the electron density on the jth branch of the graph.

We use the system of units $\hbar = c = 2m = 1$, where m stands for the effective mass of the electron in the conductor. We choose the Hamiltonian of the system in the form

$$\hat{h} = -\frac{d^2}{dx^2} \otimes I,$$

where I is the matrix 3×3 unit operator. The domain of the operator $\hat{h}$ is

$$D(\hat{h}) = \sum_{j=1}^{3} \oplus W_2^2(\mathbf{R}_+^1) \cap Q_1,$$

where Q_1 is the set of three-component functions satisfying the relations

$$u_1(0) = u_2(0) = u_3(0) = -\frac{1}{3h} \sum_{j=1}^{3} \frac{du_j}{dx_j}\bigg|_{x_j=0}.$$

Here $W_2^2(\mathbf{R}_+^1)$ is Sobolev space of twice-differentiable distributions on $\mathbf{R}_+^1$, square integrable together with their first and second derivatives. The parameter of the model $h > 0$ was introduced in the previous section; one can calculate that the Hamiltonian $\hat{h}$ described above has the single bound state with the energy $E = -h^2$. So, the operator $\hat{h}$ models the contact interaction between the electron and the junction. This operator is self-adjoint on its domain $D(\hat{h})$ and describes the simplest dynamics of the electron on the Y graph with no complicated structure (atomic cluster) in the junction.

The wave functions of the Hamiltonian $\hat{h}$ can be easily calculated. The electron incoming from infinity along the jth branch of the graph with the energy k^2 is described by the wave function with the components

$$u_j(x_j; k) = e^{-ikx_j} + R(k)e^{ikx_j}, \quad u_l(x_l; k) = T(k)e^{ikx_l}, \quad l \neq j, \tag{1}$$

where

$$R(k) = -\frac{3h+ik}{3h+3ik}, \quad T(k) = \frac{2ik}{3h+3ik}$$

are the reflection and transition coefficients, respectively. The normalized eigenfunction of the bound state corresponds to the energy $E = -h^2$ and has three identical components

$$u_j^b(x_j) = (2h/3)^{-1/2} e^{-hx_j}, \quad j = 1,2,3.$$

Below we need the explicit expression for the resolvent $g(k^2)$ of the Hamiltonian $\hat{h}$

$$(\hat{h} - k^2)^{-1} g(k^2) f = f, \quad f \in L^2(\Gamma), \quad g(k^2) f \in D(\hat{h}). \tag{2}$$

The components of the kernel of the resolvent $g(k^2)$ are

$$g_{jl}(x_j, x_l'; k^2) = a(k) e^{ik(x_j + x_l')} + g_D(x_j, x_j'; k^2) \delta_{jl}, \tag{3}$$

where

$$a(k) = -(3h + 3ik)^{-1} \tag{4}$$

and

$$g_D(x, x'; k^2) = k^{-1}(e^{ikx} \sin kx'|_{x' < x} + e^{ikx'} \sin kx|_{x' > x}).$$

IV. TWO-ELECTRON PROBLEM ON Y GRAPH WITHOUT INTERELECTRON INTERACTION

The configuration space for the two-electron system on the graph Γ is the Cartesian product $B = \Gamma \times \Gamma = \cup_{i,j=1}^{3} \Omega_{ij}$, $\Omega_{ij} = \mathbf{R}_+^2 = \{(x_i, y_j) : x_i \geq 0, y_j \geq 0\}$ and the phase space is

$$\mathscr{H}^{sc} = L^2(B).$$

The elements of the space $\mathscr{H}^{sc}$ are nine-component functions $\mathscr{U} = \{\mathscr{U}_{ij}(x_i, y_j)\}_{i,j=1}^{3}$. Let us notice that the index of the first (second) argument of the component $\mathscr{U}_{ij}(x_i, y_j)$ always coincides with the first (second) index of $\mathscr{U}_{ij}$ and henceforth we will not supply the arguments x, y by the subindices, using the shorter notation $\mathscr{U}_{ij}(x, y)$.

If there is no complex atomic cluster in the junction and no interelectron interaction the dynamics of the system is given by the Hamiltonian

$$H = (-\partial_x^2 - \partial_y^2) \otimes \mathscr{I},$$

where $\mathscr{I}$ is the 9×9 unit matrix. This operator is self-adjoint on the domain

$$D(H) = \sum_{i,j=1}^{3} \oplus W_2^2(\mathbf{R}_+^2) \cap Q_2,$$

where Q_2 is the set of the nine-component functions satisfying the following conditions:

(i) $\mathscr{U}_{i,j}(x,0) = \mathscr{U}_{i,j'}(x,0)$, for any x, i, j, j';

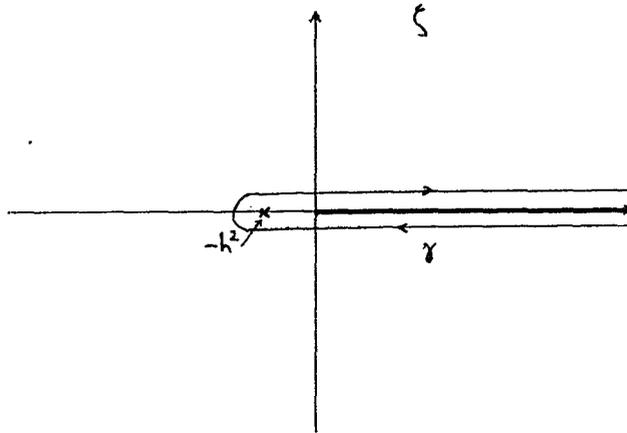(ii) $\mathscr{U}_{i,j}(0,y) = \mathscr{U}_{i',j}(0,y)$, for any y, i, i', j;

FIG. 3. Contour γ in the complex plane.

(iii) $\displaystyle\sum_{i=1}^{3} \partial_x \mathscr{U}_{ij}(x,y)|_{x=0} = -3h\mathscr{U}_{ij}(0,y)$,   for any y,j;

(iv) $\displaystyle\sum_{j=1}^{3} \partial_y \mathscr{U}_{ij}(x,y)|_{y=0} = -3h\mathscr{U}_{ij}(x,0)$,   for any x,i.

Obviously the Hamiltonian H can be represented in the form

$$H = \hat{h}_x \otimes \mathbf{1}_y + \mathbf{1}_x \otimes \hat{h}_y,$$

where $\hat{h}_x$ and $\hat{h}_y$ stand for the one-electron operator $\hat{h}$ acting over the variables x and y, respectively; $\mathbf{1}$ stand for the correspondent unit operators. Wave functions of the operator H are the products of one-electron wave functions described above

$$\mathscr{U}_{ij}(x,y;E) = u_i(x,k)u_j(y,p), \quad p^2 + k^2 = E. \tag{5}$$

The separation of variables allows to calculate the resolvent of the operator H using the contour integral method

$$(H-\lambda)^{-1} = \frac{1}{2\pi i} \oint_{\gamma} (\hat{h}_x - \zeta)^{-1}(\hat{h}_y - \lambda + \zeta)^{-1} \, d\zeta. \tag{6}$$

Contour γ encircles in the complex plane the spectrum of the operator $\hat{h}$ (see Fig. 3). This formula results in the following expression for the components of the Green function G [the kernel of the resolvent $((H-\lambda)^{-1})$]

$$G_{iji'j'}(x,y,x',y';\lambda) = \frac{1}{2\pi i} \int_0^{\infty} g_{jj'}(y,y';\lambda-\zeta)(g_{ij'}(x,x';\zeta+i0) - g_{ii'}(x,x';\zeta-i0))d\zeta$$

$$+ \frac{2h}{3} e^{-h(x+x')} g_{jj'}(y,y';\lambda+h^2). \tag{7}$$

V. TWO-ELECTRON PROBLEM ON Y GRAPH WITH EXCHANGE CONTACT INTERACTION

The spin-induced exchange interaction is related to the additional condition of symmetry (for the antiparallel spins) or antisymmetry (for the parallel spins) of the wave function with respect to the permutation of the electrons.

The antisymmetric wave function $\mathcal{U}^{(a)}$ has the components

$$\mathcal{U}_{ij}^{(a)}(x,y) = -\mathcal{U}_{ji}^{(a)}(y,x),$$

which gives $\mathcal{U}_{jj}^{(a)}(t,t) \equiv 0$ and can be calculated as

$$\mathcal{U}_{ij}^{(a)}(x,y) = \mathcal{U}_{ij}(x,y) - \mathcal{U}_{ji}(y,x).$$

Obviously, $\mathcal{U}^{(a)}$ satisfies the Schrödinger equation and boundary conditions (i)–(iv). The Green function of the correspondent Hamiltonian $H^{(a)}$ has the components

$$G_{iji'j'}^{(a)}(x,y,x',y';\lambda) = \tfrac{1}{2}(G_{iji'j'}(x,y,x',y';\lambda) - G_{jii'j'}(y,x,x',y';\lambda)). \qquad (8)$$

One can see that the Hamiltonian $H^{(a)}$ has no eigenvalues.

In a similar way the condition of symmetry of the wave function gives

$$\mathcal{U}_{ij}^{(s)}(x,y) = \mathcal{U}_{ij}(x,y) + \mathcal{U}_{ji}(y,x),$$

$$G_{iji'j'}^{(s)}(x,y,x',y';\lambda) = \tfrac{1}{2}(G_{iji'j'}(x,y,x',y';\lambda) + G_{jii'j'}(y,x,x',y';\lambda)) \qquad (9)$$

and the correspondent Hamiltonian $H^{(s)}$ has the eigenvalue $E = -h^2$, as well as H.

VI. TWO-ELECTRON PROBLEM ON Y GRAPH WITH ADDITIONAL SINGULAR INTERACTION IN THE JUNCTION

The above described simple model cannot reproduce processes with one free electron in the initial state and two ones in the final state. Also it does not consider the complex structure (atomic cluster) in the junction. In order to make the model more realistic (and still exactly solvable) we introduce some additional pointwise potential simulating the interaction of the electrons in the vicinity of the junction. The construction presented below in this section is an intermediate step for consideration of the influence of the complex atomic cluster.

In the limit case the mentioned interaction is localized in the "triple point" (the common origin of all nine sectors Ω_{ij} in the configuration space B), i.e., it is the zero-range potential. Zero-range potentials have been successfully used in various problems of quantum mechanics.[5,6,8–10] Their rigorous mathematical interpretation and tools for investigation are based on the extension theory for the symmetric operators. Classical description of the method can be found in Refs. 8 and 9. A more subtle and developed version of the method used in the present article is based on the ideas discussed in Refs. 5 and 6. In this section we present only the necessary brief description of the classical method.

In order to construct a zero-range potential, the original self-adjoint Hamiltonian (in our case $H^{(s)}$ or $H^{(a)}$) should be restricted to the set of functions vanishing in the vicinity of some point (in general case, in the vicinity of a manifold of junior dimension), that is, the point of localization of the zero-range potential. Then one should find the deficiency subspaces of the obtained symmetric operator (for the differential operators that are the square-integrable solutions of the Schrödinger equation having some singularities in the mentioned point). Next, following the von Neumann scheme[11] one can construct the family of self-adjoint extensions of the restricted symmetric operator. Every extension differs from the original Hamiltonian (which also belongs to the family)

only because of the zero-range potential localized in the point of the restriction. The parameter of the extension (which fixes the concrete self-adjoint operator in the family) is the parameter of the zero-range potential; usually it is equal to the zero for the original Hamiltonian.

Following this scheme, first let us construct the above-mentioned restriction and find its deficiency elements. Let us notice, that this procedure has no sense for the operator $H^{(a)}$, because the antisymmetric wave function *a priori* vanishes in the origin, so the restricted operator is essentially self-adjoint (has no deficiency elements). Thus, we shall proceed for the Hamiltonian $H^{(s)}$.

We denote as H_0 the operator $H^{(s)}$ restricted to the set

$$D(H_0) = D(H) \cap \{ \mathcal{U} : \mathcal{U}_{ij}(0,0) = 0 \quad \text{for any} \quad i,j \}.$$

Deficiency element $\mathcal{U}^d(\mu)$ of the operator H_0 in the point μ, Im $\mu \neq 0$, is given by the solution of the conjugated Schrödinger equation

$$(H_0^* - \mu) \mathcal{U}^d(\mu) = 0$$

and coincides with the Green function of the operator $H^{(s)}$ in the point $x' = y' = 0$

$$\mathcal{U}_{ij}^d(x,y;\mu) = G^{(s)}_{iji'j'}(x,y,0,0;\mu), \quad \text{for any} \quad i',j'.$$

One can calculate that in the point $x' = y' = 0$ the functions $G_{iji'j'}$ do not depend on the indices i,j,i',j', namely,

$$\mathcal{U}^d(x,y;\mu) = \mathcal{U}_{ij}^d(x,y;\mu) = G_{iji'j'}(x,y,0,0;\mu)$$

$$= \frac{1}{2\pi i} \int_0^\infty \exp\{iy\sqrt{\mu-\zeta}\} a(\sqrt{\mu-\zeta})$$

$$\times (a\sqrt{\zeta+i0} \exp\{ix\sqrt{\zeta+i0}\} - a\sqrt{\zeta-i0} \exp\{ix\sqrt{\zeta-i0}\}) d\zeta$$

$$+ \frac{2h}{3} e^{-hx} a(\sqrt{\mu+h^2}) \exp\{iy\sqrt{\mu+h^2}\},$$

where $f(\zeta \pm i0) = \lim_{\epsilon \to 0} f(\zeta \pm i\epsilon)$ and the function $a(k)$ was defined above in Eq. (4). Thus the deficiency indices (the number of linear independent deficiency elements) are (1,1).

Using the von Neumann scheme[11] and the proven below asymptotic representation of the deficiency element in vicinity of the origin, $r = \sqrt{x^2+y^2} \to 0$

$$\mathcal{U}^d(x,y;\mu) = \xi_s \ln r + \xi_r(\mu) + o(1) \tag{10}$$

one can show that all the self-adjoint extensions H_η of the symmetric operator H_0 are parametrized by one real parameter η. The differential expression for H_η coincides with that for the original operator $H^{(s)}$, $H_\eta = (-\partial_x^2 - \partial_y^2) \otimes \mathscr{I}$, and the domain of the operator H_η is the union

$$D(H_\eta) = D(H_0) \cup \mathscr{O}_\eta.$$

Here $\mathscr{O}_\eta$ stands for the set of the functions lying in the orthogonal sum of nine Hilbert spaces

$$\mathscr{O}_\eta \subset \sum_{i,j=1}^{3} \oplus W_2^2(\mathbf{R}_+^2 \setminus \{0\})$$

and having the following asymptotical behavior in the vicinity of the common origin in every sector $\Omega_{ij} = \mathbf{R}_+^2$:

$$\mathcal{O}_\eta \ni \Psi = \text{Const}(\eta \ln r + 1) + \mathcal{A}(1), \quad r \to 0. \tag{11}$$

Obviously, for $\eta = 0$ we have the original operator $H^{(s)}$.

The description of the operator H_η given above allows to immediately calculate its wave functions. The wave function correspondent to the energy E is the linear combination of the plane wave $\mathcal{U}$ given by formula (5) and the deficiency element $\mathcal{U}^d$ in the correspondent point

$$\Psi_{ij}^{(\pm)}(x,y;E) = \mathcal{U}_{ij}(x,y;E) + A_{ij}^{(\pm)}(E)\,\mathcal{U}_{ij}^d(x,y;E \pm i0). \tag{12}$$

The amplitudes $A_{ij}^{(\pm)}(E)$ can be calculated with the help of the representation (11)

$$A_{ij}^{(\pm)}(E) = \frac{\eta \mathcal{U}_{ij}(0,0;E)}{\xi_s - \eta \xi_r(E \pm i0)}, \tag{13}$$

where ξ_s, ξ_r are the coefficients in the asymptotical representation of the deficiency element $\mathcal{U}^d(x,y;E \pm i0)$ in the vicinity of the origin, $r = \sqrt{x^2 + y^2} \to 0$

$$\mathcal{U}^d(x,y;E \pm i0) = \xi_s \ln r + \xi_r(E \pm i0) + \mathcal{A}(1). \tag{14}$$

Thus, in order to calculate the amplitudes $A_{ij}^{(\pm)}$ one should prove the asymptotical representation (14) and calculate the coefficients ξ_s, ξ_r. The calculations are rather cumbersome and here we write down the result for $A_{ij}^{(+)}$, i.e., for the spectral parameter $E + i0$

$$\xi_s = -\frac{2}{9\pi};$$

$$-\frac{9\pi}{2}\,\xi_r(E+i0) = \frac{\pi h^2}{2h^2+E} - \int_0^{\sqrt{E}} \frac{h}{h^2+E-k^2}\,\frac{k^2}{h^2+k^2}\,dk + \int_0^{2h}\left(\frac{k\sqrt{E+k^2}}{h^2+E+k^2} - \frac{h\sqrt{E+k^2}}{2h^2+E}\right)\frac{dk}{k-h}$$

$$+ \int_{2h}^\infty\left(\frac{k\sqrt{E+k^2}}{(k-h)(h^2+E+k^2)} - \frac{1}{k}\right)dk + \int_0^1 \frac{1-e^{-k}}{k}\,dk + \int_1^\infty \frac{e^{-k}}{k}\,dk - \ln(2h)$$

$$- i\int_0^{\sqrt{E}} \frac{\sqrt{E-k^2}}{h^2+E-k^2}\,\frac{k^2}{h^2+k^2}\,dk. \tag{15}$$

Different functions $\mathcal{U}_{ij}$ given by the formula (5) determine different initial states, and Eq. (13) gives the correspondent amplitudes. As $\eta \in \mathbf{R}$, Eqs. (13) and (15) demonstrate that the amplitude $A_{ij}^{(+)}(E)$ has no singularities at $E > 0$.

Equations (12), (13), and (15) determine the components $\Psi_{ij}^{(+)}(x,y;E)$ of the wave function $\Psi^{(+)}(E)$. We have calculated the asymptotical behavior of these components as $r = \sqrt{x^2 + y^2} \to \infty$

$$\Psi_{ij}^+(r,\varphi;E) = \mathcal{F}_{ij}(\varphi,E)\,\frac{e^{ir\sqrt{E}}}{\sqrt{r}} + \mathcal{O}(r^{-1}), \tag{16}$$

where the scattering amplitude is

$$\mathcal{F}_{ij}(\varphi,E) = \sqrt{\pi/2}\,E^{3/4}\,\frac{\eta \mathcal{U}_{ij}(0,0;E)}{1+9\pi\eta\xi_r(E+i0)/2}\,\frac{\sin\varphi\,\cos\varphi}{(h+i\sqrt{E}\,\sin\varphi)(h+i\sqrt{E}\,\cos\varphi)}. \tag{17}$$

Here $x = r \cos \varphi$, $y = r \sin \varphi$.

VII. TWO-ELECTRON PROBLEM ON Y GRAPH WITH COMPLEX STRUCTURE IN THE JUNCTION

Now we are going to construct and study the model considering a complex structure of the atomic cluster located in the junction. In Sec. II we have announced the model using some self-adjoint matrix H^{ad} with fixed spectrum in order to describe spectral properties of the mentioned cluster and have suggested a way to construct H^{ad}. In order to consider this information in frames of our model we should extend the phase space. Namely, from the mathematical point of view the description of the correspondent singular electron-junction interaction is based on the extension theory in a pair of Hilbert spaces[5,6] generalizing the classical extension theory methods.[8,9] Here we give only a brief description of the approach; detailed consideration of both its mathematical and physical aspects is given in Refs. 5 and 6.

We use here a new total Hilbert space $\mathscr{H} = \mathscr{H}^{sc} \oplus \mathbf{C}^N$ which is the orthogonal sum of the original Hilbert space $\mathscr{H}^{sc} = L^2(B)$ and the additional N-dimensional space $\mathbf{C}^N$, where N stands for the number of the considered atomic cluster energy levels. The operator given by the Hermitian matrix $H^{ad} = \text{diag}\{\lambda_s\}_{s=1}^N$ described in Sec. II acts in $\mathbf{C}^N$. The idea is to consider the operator $H_{(0)}^{tot} = H^{(s)} \oplus H^{ad}$ in the space $\mathscr{H}$ as the unperturbed operator. Next, we restrict both the operators $H^{(s)}$ and H^{ad} to the symmetric operators H_0 and H_0^{ad}, respectively. Finally, we construct the family of the self-adjoint extensions of the symmetric operator $H_0 \oplus H_0^{ad}$ in the total Hilbert space $\mathscr{H}$. Each operator in this family can be interpreted as the total perturbed operator H_η^{tot} and every concrete self-adjoint operator in this family corresponds to concrete electron-junction interaction.

In the previous section the restriction H_0 of the operator $H^{(s)}$ is described. We also need a way to restrict the operator H^{ad} which is not given in the differential form. The general scheme of restriction of an abstract self-adjoint operator has been described in detail in various articles (see e.g., Refs. 5 and 6). Here we shall not discuss all the mathematical aspects and details of the general theory and single out only some necessary results and relations.

Using the results of the general extension theory[5,6] for our model, we can say that the extra channel $\mathscr{H}^{ad}$ brings the following changes in the construction of the extension H_η described in the previous section. For the operator H_η^{tot} the parameter η turns out to be not a real constant, but a function of special form (R-function[5,6]) depending on the spectral parameter. In the most simple case this function has the form

$$\eta(E) = -\frac{\tau}{\Delta(E)}, \tag{18}$$

where $\Delta(E)$ is the Schwarz integral with respect to the spectral measure of the operator H^{ad} (Refs. 5 and 6)

$$\Delta(E) = \sum_{s=1}^N \frac{\mu^2 + \lambda_s E}{\lambda_s - E} \Pi_s, \tag{19}$$

and $\tau, \mu, \Pi_s \in \mathbf{R}$ are the parameters of the model; $\Sigma_{s=1}^N \Pi_s \leq 1$. The parameter τ is the coupling constant; obviously at $\tau = 0$ the channels are not linked and we have the original operator $H_{(0)}^{tot} = H^{(s)} \oplus H^{ad}$.

All the formulas obtained in the previous section for the operator H_η are still valid for the operator H_η^{tot} with the only change $\eta \rightarrow \eta(E) = -\tau/\Delta(E)$. In particular, the expression (17) for the scattering amplitude turns into
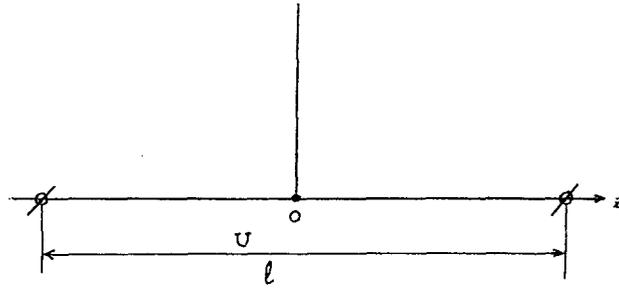
FIG. 4. Simple three-electrode device.

$$\mathscr{F}_{ij}^{\text{tot}}(\varphi,E) = -\sqrt{\pi/2}\,E^{3/4}\,\frac{\tau\mathscr{U}_{ij}(0,0;E)}{\Delta(E)-9\pi\tau\xi_r(E+i0)/2}\,\frac{\sin\varphi\,\cos\varphi}{(h+i\sqrt{E}\,\sin\varphi)(h+i\sqrt{E}\,\cos\varphi)}. \quad (20)$$

The singularities of the amplitude $\mathscr{F}_{ij}^{\text{tot}}(\varphi,E)$ [except the angular ones $E=-h^2/\sin^2\varphi$, $E=-h^2/\cos^2\varphi$ which are out of our consideration because asymptotic representation (16) is valid only for $E>0$] coincide with solutions of the dispersion equation

$$\Delta(E)=9\pi\tau\xi_r(E+i0)/2. \quad (21)$$

Similar formulas can be obtained for the amplitudes of processes with one free electron in both initial and final states. In order to do it one should construct the asymptotic representation of the wave function $\Psi^{(+)}$ in the regions of the configuration space where one of the coordinates is bounded.

Thus our consideration results in the construction of the wave function $\Psi^{(+)}$ of the two-electron system on the Y graph with complex atomic cluster in the junction in the absence of external fields. This is the final result of the microscopic study of the model and now we are going to apply the obtained results to the calculation of some macrocharacteristics of simulated nanoelectronic devices.

VIII. DENSITY MATRIX AND CONDUCTIVITY

In this section we describe briefly the way to calculate conductivity in a simple three-electrode device in frames of the two-electron approximation for the microscopic problem. These calculations are based on the above solution of the quantum scattering problem and differs from the usual scheme.[12] Our aim is to obtain the functional dependence $\mathscr{I}_\rho(U)$, where U is voltage and $\mathscr{I}_\rho$ stands for the current form the correspondent to some electron density matrix ρ.

In this section we consider the dynamics of the electron on a line and introduce a new variable $z\in\mathbf{R}$ (see Fig. 4). At the first step we do not consider the voltage on the third electrode and make calculations with the wave function averaged both over the component of the wave function correspondent to the third electrode and over the location of the second electron. Namely, we use the following procedure for the calculation of the density matrix:

$$\Phi(z;k)=\int_\Gamma dy \int_0^\infty dx_3\,\Psi^{(+)}(x,y;k)+\int_\Gamma dx \int_0^\infty dy_3\,\Psi^{(+)}(x,y;k), \quad (22)$$

where $x = \{x_1, x_2, x_3\}$, $y = \{y_1, y_2, y_3\}$; in the first integral $z \equiv -x_1$ at $z < 0$, $z \equiv x_2$ at $z > 0$, and in the second integral $z \equiv -y_1$ at $z < 0$, $z \equiv y_2$ at $z < 0$. Then the density matrix depending on the variables x, x', t is

$$\rho(z, z'; t) = \int \sigma(k, t) \Phi(z; k) \bar{\Phi}(z'; k) dk, \qquad (23)$$

where the function $\sigma(k, t)$ describes the energetic distribution of the electrons at the moment of time t. The detailed discussion of this procedure and more accurate calculations will be presented elsewhere.

Introduce the current operator

$$\mathscr{J} = -ie \frac{d}{dz},$$

where e and m are the effective electron charge and mass, respectively. The correspondent current form looks like

$$\mathscr{J}_\rho = \mathrm{Re} \int \sigma(k, t) \langle \Phi(z; k) | \mathscr{J} | \Phi(z; k) \rangle dk. \qquad (24)$$

For the fixed distribution $\sigma(k, t)$ and known function $\Phi(z; k)$ Eqs. (23), (24) allow to calculate $\mathscr{J}_\rho$ in terms of density matrix ρ

$$\mathscr{J}_\rho = \mathrm{Re} \int \langle \Phi(z; k) | \rho \mathscr{J} | \Phi(z; k) \rangle dk. \qquad (25)$$

Thus, the next problem is to obtain ρ using the Liouville equation

$$i \frac{\partial \rho}{\partial t} = [L, \rho], \qquad (26)$$

where $[\cdot, \cdot]$ stands for the commutator and the operator L generates the dynamics of the electrons in the device in the external field

$$L = L_0 + V(z), \quad L_0 = -\frac{\hbar^2}{2m} \partial_z^2$$

and $V(z)$ is the potential described below.

It is convenient to introduce the notation $A^\times$ for the superoperator acting as

$$A^\times B = [A, B].$$

We denote

$$W = \exp\{it\hbar^{-1} L_0^\times\} \rho \qquad (27)$$

and rewrite Eq. (26) in the form

$$i\hbar \partial_t W = \exp\{it\hbar^{-1} L_0^\times\} V^\times \exp\{-it\hbar^{-1} L_0^\times\} W. \qquad (28)$$

Let Λ and T stand for the characteristic scales of length and time of the process under consideration. We introduce the parameter

$$\chi = \frac{T\hbar}{2m\Lambda^2}$$

and restrict our consideration to the case $\chi \ll 1$. In the first order approximation with respect to χ we have

$$\exp\{\pm it\hbar^{-1}L_0^\times\} = I \mp i\hbar(2m)^{-1}t(\partial_z^2)^\times + \mathcal{O}(\chi^2)$$

hence

$$\exp\{it\hbar^{-1}L_0^\times\}V^\times \exp\{-it\hbar^{-1}L_0^\times\} = V^\times - i\hbar(2m)^{-1}t(\partial_z^2)^{\times\times}V^\times + \mathcal{O}(\chi^2). \tag{29}$$

Let us suppose the following properties of the potential $V(z)$:

$$V(z) = \frac{eUz}{l} + \tilde{V}(z), \quad |\partial_z(\tilde{V}(z))| + |\partial_z^2(\bar{V}(z))| \ll \frac{eU}{l}, \tag{30}$$

where U is voltage and $l \gg \Lambda$ is distance between the "input" and the "output" points of the device (see Fig. 4). Using Eqs. (28)–(30) and obvious relations

$$A^{\times\times}B^\times = [A, B]^\times, \quad [\partial_z^2, V] = \partial_z^2 V + 2\partial_z V \partial_z$$

one can obtain the following equation:

$$i\hbar\partial_t W = eUl^{-1}(z - i\hbar tm^{-1}\partial_z)^\times W + \mathcal{O}(\chi^2).$$

The latter equation can be written in terms of the kernel $w(z,z',t)$ of the operator W

$$i\hbar\partial_t w(z,z',t) = eUl^{-1}[(z-z')w(z,z',t) - i\hbar tm^{-1}(\partial_z + \partial_{z'})w(z,z',t)] + \mathcal{O}(\chi^2). \tag{31}$$

We introduce new variables $s = (z+z')/2$, $q = (z-z')/2$ and rewrite Eq. (31) with the accuracy up to $\mathcal{O}(\chi)$ as

$$i\hbar\left(\partial_t + \frac{eUt}{lm}\partial_s - \frac{2eUq}{l}\right)\tilde{w}(s,q,t) = 0, \tag{32}$$

where $\tilde{w}(s,q,t) = w(s+q,s-q,t)$. Equation (32) can be exactly solved; the solution is

$$\tilde{w}(s,q,t) = \exp\left\{-\frac{2ieUq}{\hbar l}t\right\}f\left(t^2 - \frac{2ml}{eU}s\right),$$

where the function $f(p)$ is determined by the initial density matrix

$$w(z,z',0) = \rho(z,z',t) = \rho_0(z+z') = f\left(-\frac{ml}{eU}(z+z')\right)$$

hence

$$w(z,z',t) = \exp\left\{-\frac{ieU}{\hbar l}(z-z')t\right\}\rho_0\left(-\frac{eU}{ml} + z + z'\right) + \mathcal{O}(\chi^2). \tag{33}$$

Collecting the information of Eqs. (27)–(33) we obtain

$$\rho(z,z',t)=\exp\left\{-\frac{ieU}{\hbar l}(z-z')t\right\}\tau_0\left(-\frac{eU}{ml}t^2+z+z',t\right)+\mathcal{O}(\chi^2),\tag{34}$$

where

$$\tau_0(p,t)=\left(1-\frac{3ie^2U^2t^3}{2l^2m\hbar}\right)\rho_0(p)+\frac{eUt^2}{ml}\partial_p\rho_0(p)-\frac{i\hbar t}{2m}\partial_p^2\rho_0(p).$$

Substituting the expression (34) for ρ into Eq. (25) and using the wave function calculated in the previous section one can obtain in frames of the considered approximation the current form $\mathcal{T}_\rho$ as a function of the voltage U, i.e., calculate the conductivity of the device.

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[1] A. M. Elyashevich, A. A. Kiselev, A. V. Liapzev, and G. P. Miroshnichenko, Phys. Lett. **156**, 111 (1991).
[2] B. S. Pavlov and A. V. Strepetov, Theor. Math. Phys. **90**, 202 (1992).
[3] N. I. Gerasimenko and B. S. Pavlov, Theor. Math. Phys. **74**, 170 (1988).
[4] N. I. Gerasimenko, Theor. Math. Phys. **74**, 304 (1988).
[5] B. S. Pavlov, Russ. Math. Surv. **42**, 230 (1988).
[6] Yu. A. Kuperin and S. P. Merkuriev, Am. Methods Soc. Transl. **150**, 141 (1992).
[7] K. C. Kao and W. Huang, *Electron Transport in Solids* (Pergamon, New York, 1981).
[8] R. Werner, J. Math. Anal. Appl. **70**, 131 (1979).
[9] F. A. Berezin and L. D. Faddeev, Sov. Math. Dokl. **2** (1961).
[10] S. Albeverio, F. Gesztezy, R. Hoeg-Krohn, and H. Holden, *Solvable Models in Quantum Mechanics* (Springer-Verlag, Berlin, 1988).
[11] N. I. Akhiezer and I. M. Glazman, *The Theory of Linear Operators in Hilbert Space* (Pitman, Boston, 1981).
[12] R. Landauer, Phys. Lett. A **85**, 91 (1981).