EXACTLY SOLVABLE MODEL OF ELECTRON SCATTERING BY AN INHOMOGENEITY IN A THIN CONDUCTOR

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A simple explicitly solvable model of electron propagation in a thin conductor in a three-dimensional space is considered. Resonance scattering by a point inhomogeneity possessing internal structure is analyzed by the methods of the theory of extensions.

The motion of an electron in a one-dimensional conductor in a free space is modeled on the basis of the methods of the theory of extensions of symmetric operators [1,2,3]. It is shown how the interaction of the "interior" and "exterior" parts of the energy operator leads to the appearance of a waveguide channel. The behavior of the electrons in this channel is described by a certain pseudodifferential operator with an "energy-dependent" potential. In the framework of the proposed model allowance is also made for inhomogeneities, the occurrence of which leads to nontrivial scattering into the exterior space and reflection in the waveguide channel. It is also shown that there exist values of the inhomogeneity parameters for which total reflection or total transmission of the electrons occurs.

Electron propagation in a thin conductor can be modeled as follows. Let $H_{ex} = -\Delta$ be the energy operator of a free electron in three-dimensional space; $H_{in} = -d^2/dl^2 + \hat{A}$ is an operator defined on $L_2(R, E)$, the space of square-summable vector functions with values in a certain auxiliary Hilbert space E; $\hat{A}$ is an abstract operator that acts on E. The operator H_{in} can be regarded as a model operator for the description of electron states in the semiconductor L. We model the interaction in the momentum representation.

We consider the operator $\overset{0}{H}=\overset{0}{H}_1\oplus H_2$, where $\overset{0}{H}_1$ is the Fourier transform of the operator E_{ex} restricted to the set of functions that vanish on the line L (the methods for such restriction are described in [3]),

$$\overset{0}{H}_1 = p^2\big|_{D(\overset{0}{H}_1)}; \quad D(\overset{0}{H}_1) = \left\{u_0\colon \iint u_0 dp_\perp = 0\right\}.$$

Here, $p = (p_L, p_\perp)$, where p_L is the momentum conjugate to the coordinate $l \in L$, and $p_\perp$ is the part of the momentum p orthogonal to p_L. Further, let A_0 be the restriction of A with deficiency element θ in E, i.e., the operator A considered on the set

$$D(A_0)=\{v_0\in E : \langle (A-i)v_0,\ \theta\rangle_E=0\}.$$

Then $\overset{0}{H}_2=p_L{}^2+A_0$ is the restriction of H_2, the Fourier transform of H_{in}. We describe the conjugate operator $\overset{0}{H}{}^*$. The element u_1 of $D(H_1{}^*)$ admits the representation [3,4]

$$u_1=u_0+\frac{p^2\eta^+(p_L)}{p^4+1}+\frac{\eta^-(p_L)}{p^4+1}, \tag{1}$$

where u_0 belongs to $D(\overset{0}{H}_1)$; $\eta^\pm(p_L)$ are functions defined on L and satisfying the conditions

$$\int|\eta^+(p_L)|^2dp_L<+\infty; \quad \int|\eta^-(p_L)|^2\operatorname{arcctg}(p_L{}^2)dp_L<\infty.$$

For the second operator $\overset{0}{H}_2{}^*$ the domain of definition has the form

$$D(\overset{0}{H}_2{}^*) = \left\{u_2 = u_0 + \xi^+\frac{A}{A-i}\theta + \xi^-\frac{1}{A-i}\theta\right\}, \tag{2}$$

where the coefficients $\xi^\pm$, like the deficiency element θ, can in the general case depend on the variable p_L. Finally, the domain of definition of $\overset{0}{H}{}^*$ can be expressed as follows:

$$D(\overset{0}{H}{}^*) = \left\{u = \begin{pmatrix}u_1\\u_2\end{pmatrix};\quad u_{1,2}\in D(\overset{0}{H}{}^*_{1,2})\right\}.$$

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The boundary form

$$J(u, v) = \langle \overset{0}{H}{}^* u, v\rangle - \langle u, \overset{0}{H}{}^* v\rangle$$

on elements u, v belonging to $D(\overset{0}{H}{}^*)$ can be calculated directly with allowance for the fact that the deficiency elements are labeled by the continuous symbol p_L:

$$J(u, v) = \int (-\eta_u^+ \tilde{\eta}_v^- + \tilde{\eta}_u^- \eta_v^+) dp_L + \int (-\xi_u^+ \xi_v^- + \xi_u^- \xi_v^+) dp_L, \tag{3}$$

where $\tilde{\eta}^-(p_L) = \eta^-(p_L) \cot^{-1}(p_L^2)$.

The self-adjoint extensions of the operator $\overset{0}{H}$ distinguished by the Lagrangian planes on which the boundary form (3) vanishes can be defined in various ways, since the deficiency indices of $\overset{0}{H}$ are infinite. We consider the simplest form of homogeneous interaction, for which the self-adjoint operator H_γ is distinguished by the condition

$$\begin{pmatrix} \xi^- \\ \tilde{\eta}^- \end{pmatrix} = \begin{pmatrix} 0 & \bar{\gamma} \\ \gamma & 0 \end{pmatrix} \begin{pmatrix} \xi^+ \\ \eta^+ \end{pmatrix}, \tag{4}$$

i.e., H_γ is the operator determined by the differential expressions H_1 and H_2 on the set of functions in $D(\overset{0}{H}{}^*)$ whose coefficients $\xi^\pm$, $\eta^\pm$ satisfy the condition (4).

1. The eigenfunctions Ψ_γ of H_γ, determined by the equation $H_\gamma \Psi_\gamma = \lambda \Psi_\gamma$, can be calculated explicitly in terms of the known eigenfunctions of the operators H_1, H_2. Namely, let $\Psi_{1,2}(\lambda, p)$ be the eigenfunctions of $H_{1,2}$; if it is borne in mind that the interior and exterior parts of $\Psi_\gamma(\lambda, p)$ have the representations (1) and (2), respectively, and that the coefficients $\xi^\pm$, $\eta^\pm$ satisfy the conditions (4), we obtain a simple system for determining ξ^+, η^+:

$$\begin{pmatrix} -D_1(\lambda) & \bar{\gamma} \\ \gamma & -D_2(\lambda) \end{pmatrix} \begin{pmatrix} \xi^+ \\ \eta^+ \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}. \tag{5}$$

In the system (5), we have used the notation

$$f_1(p_L) = \iint \Psi_1(\lambda, p) dp_\perp; \quad f_2(p_L) = \langle (A - i)\Psi_2(p_L), \theta\rangle_E,$$

$$D_1(\lambda, p_L) = \iint \frac{1 + \lambda p^2}{(p^2 - \lambda)(p^4 + 1)} dp_\perp = -2\pi \ln \frac{p_L^2 - \lambda}{\sqrt{p^4 + 1}}, \quad D_2(\lambda, p_L) = \left\langle \frac{1 + \lambda A - p_L^2 A}{A - \lambda + p_L^2} \theta, \theta \right\rangle_E.$$

The solution of Eqs. (5) is readily found:

$$\eta^+ = \frac{-\gamma f_1 - D_1 f_2}{-|\gamma|^2 + D_1 D_2} + \eta_0^+, \quad \xi^+ = \frac{-\bar{\gamma} f_2 - D_2 f_1}{-|\gamma|^2 + D_1 D_2} + \xi_0^+,$$

where η_0^+ satisfy the equation

$$\{|\gamma|^2 - D_1(p_L) D_2(p_L)\} \eta_0^+(p_L) = 0, \quad \xi_0^+ = \frac{\gamma}{D_2} \eta_0^+. \tag{6}$$

Substituting the obtained solution ξ^+, η^+ in the representation for the eigenfunctions, we finally obtain

$$(\Psi_\gamma(\lambda, p))_1 = \Psi_1(\lambda, p) + \frac{\eta^+(p_L)}{p^2 - \lambda}, \quad (\Psi_\gamma(\lambda, p))_2 = \Psi_2(\lambda, p_L) + \xi^+(p_L) \frac{A + i}{A - \lambda + p_L^2} \theta.$$

Of course, the spectrum of the operator H_γ contains several components. Naturally, it contains parts of the spectrum generated solely by the exterior or the interior part of H_γ. The greatest interest is in the existence of "waveguide" eigenfunctions generated by the described perturbation of the operator $H_1 \oplus H_2$. They have the form

$$(\Psi_w(\lambda, p))_1 = \frac{\eta_0^+(p_L)}{p^2 - \lambda}, \quad (\Psi_w(\lambda, p_L))_2 = \xi_0^+(p_L) \frac{A + i}{A - \lambda + p_L^2} \theta. \tag{7}$$

We recall that the densities η_0^+, ξ_0^+ satisfy the relation (6). If the operator A: $E \to E$ has a single eigenvalue α, Eq. (6) is an equation of Schrödinger type with energy-dependent potential:

$$\left\{ p_L^2 + \alpha + \pi \frac{1 + \alpha^2}{|\gamma|^2 + \alpha} \ln \frac{p_L^2 - \lambda}{\sqrt{p_L^4 + 1}} \right\} \eta_0^+(\lambda, p_L) = \lambda \eta_0^+(\lambda, p_L). \tag{8}$$

The solutions of Eq. (8) are conveniently described in terms of the corresponding momentum $\varkappa$, which solves the algebraic equation

$$\varkappa^2+\alpha-\lambda=\frac{1+\alpha^2}{|\gamma|^2+\alpha}\pi\ln\frac{\sqrt{\varkappa^4+1}}{\varkappa^2-\lambda}. \tag{9}$$

It is the values of λ for which there exist real solutions of (9) that form the "waveguide" spectrum σ_w of the operator H_γ, which contains two continuous branches. Note that the asymptotic behavior $\varkappa(\lambda) = \sqrt{\lambda} + O(\ln \lambda)$ differs from that of the standard momentum only in the rate of growth of the second term. Besides the dependence $\varkappa = \varkappa(\lambda)$, we shall also use the inverse function $\lambda(\varkappa)$, which is specified implicitly by the same equation (9).

2. The S matrix for the pair of operators H, H_γ can be calculated by the standard methods [1,5], but for homogeneous boundary condition (4) the transmission coefficient in the waveguide channel is equal to unity. We also model the inhomogeneity on which nontrivial scattering occurs by means of extension theory.

We consider first the operator H_γ only in the subspace of eigenfunctions of the "waveguide" spectrum. Let

$$E_w=\overline{\mathscr{L}\{\Psi_w(\lambda,l)\}}$$

be the closed linear hull of the eigenfunctions $\Psi_w(\lambda, l)$, which are related by Fourier transformation to the functions $\Psi_w(\lambda, p_L)$ (7); $H_w=H_\gamma|_{E_w}$ is the operator H_γ restricted to E_w. Its action can be calculated explicitly:

$$(H_wu)(l)=\int_{\sigma_w}\lambda(\varkappa)\Psi_w(\varkappa,l)\langle u,\Psi_w(\varkappa)\rangle_{E_w}d\rho(\varkappa), \tag{10}$$

where the measure $d\rho(\varkappa)$ is determined from the representation of the spectral projector by means of the Riesz integral

$$\mathscr{P}_w=-\frac{1}{2\pi i}\oint_{\gamma}\frac{H+iI}{H-\lambda I}P\begin{pmatrix}D_1(\lambda) & \bar\gamma\\ \gamma & D_2(\lambda)\end{pmatrix}^{-1}P\frac{H-iI}{H-\lambda I}d\lambda=$$

$$-\int_{\sigma_w}\frac{H+iI}{H-\lambda I}P\begin{pmatrix}D_1'(\lambda(\varkappa)) & 0\\ 0 & D_2'(\lambda(\varkappa))\end{pmatrix}^{-1}P\frac{H-iI}{H-\lambda I}d\varkappa. \tag{11}$$

Here, P is the projector onto the deficiency subspace of $\overset{0}{H}$. Applying the projector $\mathscr{P}_w$ (11) to the eigenfunction and making a comparison with the result obtained from the representation (10), we finally obtain

$$d\rho(\varkappa)=-\begin{pmatrix}D_1'(\lambda(\varkappa)) & 0\\ 0 & D_2'(\lambda(\varkappa))\end{pmatrix}^{-1}d\varkappa.$$

Further, we separate the eigenfunctions $\Psi_S(\lambda, x)$ which derive from the eigenfunctions $\Psi_1(\lambda, x)$ of the exterior operator H_1. Their Fourier transforms are

$$(\hat\Psi_S(\lambda,p))_1=\Psi_1(\lambda,p)+\frac{1}{p^2-\lambda}\frac{\gamma}{|\gamma|^2-D_1D_2}\iint\Psi_1(\lambda,p)dp_\perp,$$

$$(\hat\Psi_S(\lambda,p))_2=\frac{D_2}{|\gamma|^2-D_1D_2}\iint\Psi_1(\lambda,p)dp_\perp\frac{A+i}{A-\lambda+p_L^2}\theta.$$

Let H_S be the operator H_γ restricted to E_S, the closed linear hull of the functions $\Psi_S(\lambda, x)$. The kernel of the resolvent of the operator $\mathscr{H}=H_S\oplus H_w$ consists of two blocks $G_S(x, x')$, $G_w(l, l')$, representations for which are, respectively,

$$G_S(x,x')=\int\frac{1}{\lambda-k^2}\Psi_S(k,x)\Psi_S^*(k,x')dk,\quad G_w(l,l')=\int_{\sigma_w}\frac{1}{\lambda-\lambda(\varkappa)}\Psi_w(\varkappa,l)\Psi_w^*(\varkappa,l')d\rho(\varkappa).$$

We consider the restriction of the operator $\mathscr{H}$ to the set of vector functions

$$D_0=\{\varphi_0:\langle(\mathscr{H}-i)\varphi_0,\theta^i\rangle_{E_S\oplus E_w}=0\},$$

where

$$\theta^i=\begin{pmatrix}\theta_S^i\\ \theta_w^i\end{pmatrix};\quad \theta_w^i=\int_{\sigma_w}\frac{1}{\lambda(\varkappa)+i}\Psi_w^N(\varkappa,l)e^{i\varkappa l_0}d\varkappa,\quad \theta_S^i=\int\frac{1}{k^2+i}\Psi_S(k,x)e^{i(k,l_0)}dk;$$

$\Psi_w^N(\varkappa, l)=[\rho'(\varkappa)]^{-1/2}\Psi_w(\varkappa, l)$ are normalized eigenfunctions of the waveguide spectrum. Then the conjugate operator $\mathscr{H}_0^*$ will have domain of definition

$$D(\mathcal{H}_0^*)=\left\{\varphi=\varphi_0+\sum_{\alpha=S,w}\left(\xi_\alpha^+\frac{H_\alpha}{H_\alpha-i}\theta_\alpha+\xi_\alpha^-\frac{1}{H_\alpha-i}\theta_\alpha\right)\right\}.$$

Let B be some self-adjoint operator describing the internal structure of an inhomogeneity at the point l_0. We denote by g the deficiency element of the restriction B_0 and write down in the standard manner the domain of definition of the conjugate operator:

$$D(B_0^*)=\left\{v=v_0+\xi_{in}^+\frac{B}{B-i}g+\xi_{in}^-\frac{1}{B-i}g\right\}.$$

Then for the orthogonal operator sum $\mathcal{H}_0\oplus B_0$ the self-adjoint extensions $\mathcal{H}_\Gamma$ are parametrized by an Hermitian matrix Γ, which relates the coefficients ξ^- and ξ^+:

$$D(\mathcal{H}_\Gamma)=\left\{\begin{pmatrix}\varphi\\ v\end{pmatrix};\ \begin{matrix}\varphi\in D(\mathcal{H}_0^*)\\ v\in D(B_0^*)\end{matrix}\ :\ \xi^+=\Gamma\xi^-\right\}.$$

Here $\xi^\pm=(\xi_S^\pm,\ \xi_w^\pm,\ \xi_{in}^\pm)^T$; the off-diagonal elements of Γ characterize the interaction of the internal structure of the inhomogeneity with the exterior and waveguide channels. To determine the scattering data, we shall seek an eigenfunction of the operator $\mathcal{H}_\Gamma$ satisfying the radiation conditions $\mathcal{H}_\Gamma\Psi_\Gamma=\lambda\Psi_\Gamma$,

$$(\Psi_\Gamma)_w=\Psi_w^N(\varkappa,l)+f_w(\lambda)\int_{\sigma_w}\frac{1}{\lambda(\varkappa)-\lambda}\Psi_w^N(\varkappa,l)e^{i\varkappa l_0}d\varkappa=\Psi_w^N(\varkappa,l)+f_w(\lambda)\Psi_w^{\text{out}}(\varkappa,l-l_0),$$

$$(\Psi_\Gamma)_S=f_S(\lambda)\int\frac{1}{k^2-\lambda}\Psi_S(k,x)e^{i\langle k l_0\rangle}dk=f_S(\lambda)\Psi_S^{\text{out}}(\lambda,x-l_0). \tag{12}$$

From the condition that Ψ_Γ belong to the domain of definition of $\mathcal{H}_\Gamma$, we obtain a system of equations for the coefficients ξ^+:

$$\{\Gamma^{-1}-D(\lambda)\}\,\xi^+=\begin{pmatrix}\langle(H_w-i)\,\Psi_w^N,\theta_w\rangle_{E_w}\\ 0\\ 0\end{pmatrix}, \tag{13}$$

where $D(\lambda)$ is a diagonal 3×3 matrix function with diagonal elements D_w, D_S, D_{in}:

$$D_w(\mu)=\left\langle\frac{1+\mu H_w}{H_w-\mu}\theta_w,\theta_w\right\rangle_{E_w}=\int_{\sigma_w}\frac{(1+\lambda(\varkappa)\mu)d\varkappa}{(\lambda(\varkappa)-\mu)(\lambda^2(\varkappa)+1)},$$

$$D_S(\mu)=\left\langle\frac{1+\mu H_S}{H_S-\mu}\theta_S,\theta_S\right\rangle_{E_S}=4\pi\sqrt{\mu}+C,\qquad D_{in}(\mu)=\left\langle\frac{1+B\mu}{B-\mu}g,g\right\rangle_{E_{in}}.$$

Let $Q(\lambda)$, a matrix with elements $q_{ik}(\lambda)$, be the inverse of the matrix of the system (13). Then the scattering amplitude $f_S(\lambda)$ of the outgoing spherical wave $\Psi_S^{\text{out}}(\lambda,x-l_0)$ will have the form

$$f_S(\lambda)=q_{21}(\lambda)e^{i\varkappa(\lambda)l_0}. \tag{14}$$

We recall that $\varkappa$ can be found from the dependence $\varkappa=\varkappa(\lambda)$ determined by Eq. (9). To determine the transmission coefficient t and the reflection coefficient r in the waveguide channel, we represent the solution (12) as a combination of eigenfunctions $\Psi_w^N(\varkappa,l)$:

$$(\Psi_\Gamma)_w=\begin{cases}\Psi_w^N(\varkappa,l)+r(\lambda)\Psi_w^N(-\varkappa,l), & l<l_0,\\ t(\lambda)\Psi_w^N(\varkappa,l), & l>l_0.\end{cases}$$

With allowance for the representation for the Green's function G_w of the waveguide channel,

$$G_w(l,l_0)=\begin{cases}2\pi i\dfrac{\Psi_w^N(\varkappa,l)\Psi_w^{N*}(\varkappa,l_0)}{\lambda'(\varkappa)}, & l>l_0,\\ G_w^*(l_0,l), & l<l_0,\end{cases}$$

and using the solution of the system (13), we obtain explicit expressions for the reflection and transmission coefficients:

$$r(\lambda)=2\pi i\frac{q_{11}(\lambda)}{\lambda'(\varkappa_\lambda)}e^{2i\varkappa l_0},\qquad t(\lambda)=1+2\pi i\frac{g_{11}(\lambda)}{\lambda'(\varkappa_\lambda)}, \tag{15}$$

where $\varkappa_\lambda$ is found from λ using the dependence (9).

We consider in more detail the reflection coefficient (15) and the scattering coefficient (14) in the special case of λ values near the eigenvalue λ_S of the operator B of the internal structure. Then the quadratic form $D_{\text{in}}(\lambda)$ increases unboundedly and admits the representation

$$D_{\text{in}}(\lambda)=\frac{b_S}{\lambda-\lambda_S}+O(1).$$

We denote by Γ_{ik}^{-1} the elements of the matrix Γ^{-1} and by $\Delta(\lambda)$ the determinant

$$\det\begin{vmatrix} \Gamma_{11}^{-1}-D_S(\lambda) & \Gamma_{12}^{-1} \\ \Gamma_{21}^{-1} & \Gamma_{22}^{-1}-D_w(\lambda) \end{vmatrix}.$$

In the neighborhood of the point λ_S, the elements of $Q(\lambda)$ have finite limits:

$$q_{12}(\lambda)\xrightarrow[\lambda\to\lambda_S]{}\frac{\Gamma_{21}^{-1}}{\Delta(\lambda_S)},\quad q_{11}(\lambda)\xrightarrow[\lambda\to\lambda_S]{}\frac{\Gamma_{22}^{-1}-D_S(\lambda_S)}{\Delta(\lambda_S)}.$$

Using the arbitrariness in the choice of the matrix Γ, we can give it a structure such that the element $(\Gamma^{-1})_{21}$ of its inverse is zero while the relation $\Gamma_{22}^{-1} = D_S(\lambda_S)$ also holds. Then in the limit $\lambda \to \lambda_S$ the reflection and scattering coefficients are equal to zero and, thus, the transmission coefficient $t(\lambda_S)$ will be equal to unity.

In conclusion, we note that our model of electron motion through a thin conductor is both exactly solvable and quite nontrivial. First, the model takes into account the position of the conductor in the three-dimensional space (the parameter γ is a coupling constant) and, second, the model includes a possible inhomogeneity of the type of a zero-range potential possessing internal structure. In the framework of the model the scattering data can be calculated almost explicitly (apart from solution of an algebraic equation). It is also found that there exist values of the parameters for which reflectionless transmission of electrons can occur in the waveguide channel at a definite energy λ_S.

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