Available online at www.sciencedirect.com
ScienceDirect
Surface Science 601 (2007) 2712–2716
SURFACE SCIENCE
www.elsevier.com/locate/susc

Standing waves and resonance transport mechanism in quantum networks

Boris Pavlov [a,*], Adil Yafyasov [b]

[a] *Department of Mathematics, The University of Auckland, New Zealand*
[b] *Institute for Physics, St-Petersburg University, Russia*

Available online 16 December 2006

Abstract

One-electron spin-dependent scattering problem is considered on the star-shaped 2-d quantum network consisting of a quantum well and few relatively thin leads attached to it. The resonance nature of transmission coefficients is revealed based on accurate analysis of interaction between the running spin-waves in the leads and the standing spin-waves in the quantum well. Modeling of the transport problem on the two-dimensional junction by the 1-d scattering problem on the corresponding quantum graph is discussed.

Keywords: Quantum well; Quantum wire; Resonance

1. Transport in networks as a scattering problem

Spin-dependent transport problem for a single electron with an effective mass m^* is studied on a star-shaped quantum network – a junction $\Omega \cup \omega$ – constructed on a surface of a semi-conductor of a vertex domain Ω (a quantum well of an arbitrary shape), and a few straight semi-infinite leads $\omega = \cup_{m=1}^{M} \omega^m$ (quantum wires, of a constant width δ) attached to Ω at the bottom sections $\Gamma = \cup_{m=1}^{M} \gamma^m$. In strong normal electric field the dynamic of the electron on the network is described by the Schrödinger equation which is transformed, after separation of time and scaling of energy $E \to \lambda = 2m^* E\hbar^{-2}$, to the spectral problem for the Schrödinger operator

$$\mathscr{L}\psi = -\triangle\psi + H_R\psi + V_\delta\psi = \lambda\psi,$$

for 2-spinor ψ, with the spin–orbital interaction defined the symmetrized Rashba term

$$H_R = \alpha(x)[\sigma, p] + [\sigma, p]\alpha(x), \quad p = i\nabla,$$

containing the Rashba – factor α, see [1], defined by the magnitude of the normal component of electric field and vanishing near the boundary $\partial\Omega$ and on the wires. We assume that the temperature is low and the Fermi level $\Lambda = 2\, m^* E_F \hbar^{-2}$ lies deep enough to assume that ψ vanishes on the boundary of the network. The electrostatic potential V_δ is constant on the wires, and magnetic field is absent. We consider also the Schrödinger equation $L\psi = \lambda\psi$, on the quantum well Ω with L defined by the same potential and Rashba term as $\mathscr{L}$. The above one-electron Hamiltonian $\mathscr{L}$ is self-adjoint in the Hilbert space $L_2(\Omega \cup \omega)$ of all square-integrable functions. The transport properties of the junction are defined by the structure of the corresponding eigenfunctions of continuous spectrum of $\mathscr{L}$ – scattered waves. The scattered waves are obtained via matching on Γ of solutions of the Schrödinger equation $L\psi = \lambda\psi$ in Ω with the scattering Ansatz $\vec{\psi}(x,\lambda) = \{\psi_l^m(x,\lambda)\}$ in the wires $\omega^m = (x : 0 < x^\parallel < \infty, 0 < x^\perp < \delta)$. The Ansatz is combined of oscillating modes, or exponentially decreasing modes in the wires

$$\chi_\pm^l(x) := \exp\left(\pm i\sqrt{\lambda - V_\delta - \pi^2 l^2 \delta^{-2}} x^\parallel\right) e_l(x^\perp), \quad \lambda > \pi^2 l^2 \delta^{-2},$$

$$\xi^l(x) := \exp\left(-\sqrt{\pi^2 l^2 \delta^{-2} + V_\delta - \lambda x^\parallel}\right) e_l(x^\perp), \quad \lambda < \pi^2 l^2 \delta^{-2}$$

* Corresponding author.
E-mail addresses: pavlov@math.auckland.ac.nz (B. Pavlov), yafyasov@bk.ru (A. Yafyasov).

0039-6028/$ - see front matter
doi:10.1016/j.susc.2006.12.023

with cross-section eigen-spinors $e_l(x^{\perp}) = \sqrt{2/\delta}e^l \sin \pi l x^{\perp}/\delta$, $l = 1, 2, \ldots$

$$\psi_l^m(x) = \begin{cases} \chi_+^l(x) + \sum_{\pi^2 r^2/\delta^2<\lambda} S_{l,r}^{m,m}\chi_-^r(x) \\ \quad + \sum_{\pi^2 r^2/\delta^2>\lambda} s_{l,r}^{m,m}\xi^r(x), \quad x \in \omega^m, \\ \sum_{\pi^2 r^2/\delta^2<\lambda} S_{l,r}^{m,n}\chi_-^r(x) \\ \quad + \sum_{\pi^2 r^2/\delta^2>\lambda} s_{l,r}^{n,m}\xi^r(x), \quad x \in \omega^n, \ n \neq m. \end{cases} \tag{1}$$

Matching of the scattering ansatz $\vec{\psi}$ to the solution of the Schrödinger equation $L\psi = \lambda\psi$ on the bottom sections γ^m of the wires gives an infinite linear system for the coefficients $S_{l,r}^n, s_{l,r}^n$, see for instance [2]. Formally this system can be solved, if the Green 2×2 matrix-function G_Ω of the Schrödinger equation on Ω with zero boundary condition is constructed. Really, according to general theory of second order linear equations, see [3], the solution u and the boundary current of the boundary problem with data $u|_\Gamma = u_\Gamma$ is represented by the integral map with the Poisson kernel $\mathscr{P}_\Omega(x,\gamma) = -\frac{\partial G_\Omega(x,\gamma)}{\partial n}$

$$u(x) = \int_\Gamma \mathscr{P}_\Omega(x,\gamma)u_\Gamma(\gamma)\mathrm{d}\gamma, \quad \frac{\partial u}{\partial n}\bigg|_\Gamma = -\int_\Gamma \frac{\partial^2 G_\Omega(x,\gamma)}{\partial n_x \partial n_\gamma}u_\Gamma(\gamma)\mathrm{d}\gamma\bigg|_\Gamma := \mathscr{D}\mathscr{N}_\Omega u_\Gamma.$$

The integral operator $\mathscr{D}\mathscr{N}_\Omega$ with 2×2 matrix kernel is called "Dirichlet-to-Neumann map", see [4,5]. It depends on λ and is analytic with poles at the eigenvalues of the Schrödinger operator L_Ω on the quantum well with zero boundary conditions. The coefficients of the scattering Ansatz can be, in principle, found from the infinite linear system:

$$\frac{\partial\psi}{\partial n}\bigg|_\Gamma = \mathscr{D}\mathscr{N}_\Omega\psi|_\Gamma. \tag{2}$$

The difficulty of this problem is defined by the fact, that the above matching is a strong perturbation of the problem with the quantum wires ω and the quantum well Ω separated by the "solid wall" Γ with zero boundary condition on it. Removing of this wall causes breeding of the standing waves in the quantum well with the running waves in the wires, creating resonance states, which define resonance singularities of the transmission across the junction. The influence of these singularities was observed in numerical experiments, see for instance [6].

2. Scattering matrix via intermediate DN map

Note that our transport problem contains a small parameter δ so that it can be solved via analytic perturbation procedure in form of power series over δ^n. Standard methods of analytic perturbation technique are developed for problems with discrete spectrum. Generally, the perturbation series for the eigenvalue λ_1^δ of a perturbed operator $\mathscr{L}_\delta = \mathscr{L}_0 + \delta B$ is convergent if the perturbation is dominated by the half-spacing $\|\delta B\| < \rho_0/2$ at the corresponding eigenvalue λ_1^0 of the non-perturbed operator $\mathscr{L}_0 : \rho_0 = \min_{s\neq 1}|\lambda_1^0 - \lambda_s^0|$. This requirement is too restrictive for operators with dense discrete spectrum and generally useless for operators with continuous spectrum. Nobel prize 1972 winner I. Prigogine [7] suggested an idea of a two-step modification of the conventional analytic perturbation technique with an "intermediate operator" $\mathscr{L}^\delta$

$$\mathscr{L}_0 \to \mathscr{L}^\delta \to \mathscr{L}_\delta, \tag{3}$$

assuming that there exist a function $\mathscr{L}^\delta$ of the unperturbed operator $\mathscr{L}_0$ such that the standard analytic perturbation series connecting the eigenvalues $\mathscr{L}^\delta$ to ones of $\mathscr{L}_\delta$, on the second step, is convergent. Search of the intermediate operator with these properties was not successful, and the idea was finally abandoned. We revitalize this idea, assuming that the role of the intermediate operator may be played by an operator which differs from the unperturbed one $\mathscr{L}_0$ by a finite-dimensional perturbation. In case of the junction this modification corresponds to replacement of the hard perturbation defined by erection or removal of the solid wall, associated with the zero boundary condition on Γ:

$$\mathscr{L} \overset{\text{erect}}{\to} L_\Omega \oplus l_\omega \overset{\text{remove}}{\to} \mathscr{L}$$

by a "softer" – finite-dimensional – perturbation we describe below, following [9,10].

The continuous spectrum of $\mathscr{L}$ consists of a countable system of branches $\cup_{l=1}^\infty[\pi^2 l^2\delta^{-2} + V_\delta, \infty)$, separated by the thresholds $\pi^2 l^2\delta^{-2} + V_\delta$ inherited from the unperturbed operator l_ω in the wires. For low temperature the scattering processes in the junction are observed only on an essential spectral interval $\Delta_T = (\Lambda - 2m^*\kappa \quad T\hbar^{-2} < \lambda < \Lambda + 2m^*\kappa T\hbar^{-2})$ near the Fermi level Λ. The spectral band Δ_Λ between the upper threshold $\lambda_{\max} < \Lambda$ of open channels and lower threshold $\lambda_{\min} > \Lambda$ of closed channels is the conductivity band, see [8]. We assume that Δ_T is a part of the conductivity band. Linear combinations of all cross-section spinors which correspond to the thresholds below the Fermi level constitute $\sum_{\pi^2 l^2\delta^{-2}+V_\delta<\Lambda} \oplus \{e_l\} := \sum_{\text{open}} \oplus \{e_l\} := E_+$. We denote by P_+ the orthogonal projection onto E_+ in $L_2(\Gamma)$. The subspace $E_+ \in L_2(\Gamma)$ plays a role of the entrance subspace of open channels in scattering processes. Restrict the full Hamiltonian $\mathscr{L} \to L_\Lambda \oplus l_\Lambda$ via imposing on Γ the partial zero boundary condition in open channels, see [9]:

$$P_+ u|_\Gamma = 0. \tag{4}$$

This boundary condition defines a semi-transparent wall at Γ which neither admits to the quantum well the waves from the open channels in the wires, nor releases the waves from the quantum well, shaped on Γ to fit open channels, to exit from Ω to ω. We refrain here from a discussion of a physical realization of this boundary condition, but we remark, that, due to the finite dimension of E_+, the perturbation in $\mathscr{L}$ introduced by the additional boundary condition (4) is finite-dimensional. It splits $\mathscr{L} \to \mathscr{L}_\Lambda$ into two