Boundary condition at the junction

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May 22, 2006

1 Introduction

Practical calculation of transport properties of quantum networks is often reduced to the scattering problem for a one-dimensional differential operator on a quantum graph, see for instance [1, 2, 3, 4, 5]. Quantum graph plays a role of a solvable model for the 2-d network, see [6, 7, 8]. Basic element of the model is a star-shape graph with a self-adjoint boundary condition at the node. It was commonly expected that the realistic boundary condition is defined by the angles between the wires at the node. For T-junction, [1], the boundary condition is presented in terms of limit values of the wave-function on the wires $\{\psi_i\}_{i=1}^3 := \vec{\psi}$ and the values of the corresponding outward derivative $\{\psi_i'\}_{i=1}^3 := \vec{\psi}'$ at the node:

$$\beta^{-1}\psi_1 = \psi_2 = \psi_3\,, \quad \beta\psi_1' + \psi_2' + \psi_3' = 0\,, \qquad (1)$$

or in the form

$$P_0^{\perp}\bar{\psi} = 0\,, \quad P_0\bar{\psi}' = 0 \qquad (2)$$

with the projection

$$P_0 = \frac{1}{\beta^2+2}\begin{pmatrix} \beta^2 & \beta & \beta \\ \beta & 1 & 1 \\ \beta & 1 & 1 \end{pmatrix},$$

see [9, ?]. The scattering matrix of such a T-junction is $S = I - 2P_0$, see [1, 4, 10]. In [1] β is interpreted as a free parameter which describes "the strength of the coupling" between the leg and the bar of the T-junction. In [11] the condition (2) is used for analysis of spin-dependent transmission across the quantum ring.

Based on [13], we extend the above boundary condition (2) to any junction of equivalent wires and interpret the corresponding parameter P_0.

2 Intermediate Hamiltonian

Consider one body scattering problem on the junction Ω formed by few 2-d equivalent semi-infinite wires Ω_j, $s = 1, 2, \ldots m$, attached to the quantum well Ω_{int} via the orthogonal bottom sections Γ_s, see 1, for simplest case of Y-junction $m = 3$: 3 The corresponding one-body Hamiltonian for the spin-less electron is scaled via replacement of energy E by the spectral parameter $\lambda = \hbar^{-2}2m^*E$ to the standard Schrödinger operator with zero conditions on the boundary $\partial\Omega$, and a constant potential in the wires $q|_{\omega_s} = q_\infty$:

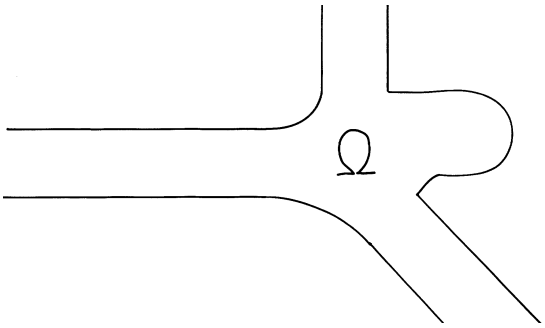

Figure 1: A junction

$$\mathcal{L}\psi = -\triangle\psi + q\psi. \qquad (3)$$

We assume, following [13], that the potential on the vertex domain is defined by the scaled constant electric field $\mathcal{E}$: $q|_{\Omega_{int}} = q_{int}(x) = \langle\mathcal{E}, x\rangle, x \in \Omega_{int}$. The role of the non-perturbed Hamiltonian is played by the Schrödinger operator L_{out} in the wires with zero boundary conditions on the union $\Gamma = \cup_s\Gamma_s$ of the bottom sections of the wires, which play roles of solid walls, separating the vertex domain from the wires:

$$\psi|_\Gamma = 0. \qquad (4)$$

The eigenfunctions of $\mathcal{L}_{out}$ in the wires $\Omega_s : 0 < x_s = x < \infty$, $0 < y_s = y < \delta$ are combined from *running waves*

$$\exp(\pm i\sqrt{\lambda - \pi^2 l^2 \delta^{-2} - q_\infty}x)\ \sqrt{2/\delta}\sin \pi l y/\delta$$

$$:= \exp(\pm i p_l x)\ \ e_s^l$$

Hereafter we used on the wires ω_s the corresponding local coordinates x, y, $0 < x < \infty$, $0 < x < \delta$, and denote $e_s^l\rangle\langle e_s^l := P_s^l$. The eigenfunctions of the operator L_{int} defined by (3,4) in the vertex domain Ω_{int} are standing waves. Replacement of the solid wall condition (4) by the matching condition is a strong perturbation blending the standing waves on the vertex domains with the running waves in the wires. This is a perturbation on the continuous spectrum, so the corresponding analytic perturbation procedure does not converge. In [**?**] we suggested a modified analytic perturbation procedure based on introduction of an Intermediate Hamiltonian obtained via appropriate splitting, see [14], of $\mathcal{L}$.

Assume that the scaled Fermi level in the vires lies, for instance, in the middle f the first spectral band $2m^* E_F \hbar^{-2} := \lambda_F = \pi^2\delta^{-2}5/2 + q_\infty$. In that case all branches of the continuous spectrum with thresholds $\pi^2 l^2 \delta^{-2} + q_\infty$, $l \geq 2$, are closed, that is all exponential solutiLns $\exp \pm i p_l x\ \ e_s^l$, , $l \geq 2$, of the homogeneous equation $-\triangle\psi + q\psi = \lambda\psi$ in the wires are exponentially decreasing. Impose, additionally to (1), the semi-transparent boundary condition on the bottom section:

$$u\big|_\Gamma \perp E_+,\ E_+ = \bigvee_{s=1}^{m} e_s^l,\ P_{E_+} := P_+. \qquad (5)$$

This condition prevents excitations of the first channel $\mathcal{H}_+ = E_+ \times L_2(R_+)$ in the wires from entering into the vertex domain, and, vice versa, exiting from the vertex domain into the wires. However it does not stop the excitations of higher channels $\mathcal{H}_- = [L_2(\Gamma) \ominus E_+] \times L_2(R_+) := E_- \times L_2(R_+)$. The corresponding operator $\mathcal{L}^F$ is split into the orthogonal sum of the trivial operator in the open first channel $\mathcal{H}_+$

$$l^F u = -\frac{d^2u}{dx^2} + [q_\infty + \pi^2\delta^{-2}]u,\ \ ,$$

with zero boundary condition on $\partial\omega_s$, and the *Intermediate Hamiltonian* L^F in the orthogonal complement $\mathcal{H}^F = \{L_2(\Omega) \ominus \mathcal{H}_+\}$. The spectrum $\sigma_a(l^F)$ is just the first spectral branch $[\pi^2/\delta^2 + q_\infty, \infty)$ and the continuous spectrum of L^F is $\cup_{l\geq 2}[l^2\pi^2/\delta^2 + q_\infty, \infty) := \sigma_a(l^F)$. There is a finite number of eigenvalues of L^F on the first spectral band $[\pi^2/\delta^2 + q_\infty, 4\pi^2/\delta^2 + q_\infty] := \Delta_1$ and a countable number of embedded eigenvalues accumulating at infinity.

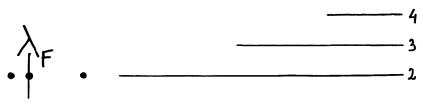

Figure 2: Spectrum of L^F

3 Scattering matrix via Intermediate DN map

Usually the Scattering matrix on the quantum network is obtained via matching exponential solutions in the wires to the solutions of the homogeneous Schrödinger equation inside the vertex domain, see, for instance [15]. This approach requires solving an infinite algebraic system. We consider the boundary problem for the Intermediate equation:

$$-\triangle\psi + q\psi = \lambda\psi,\ \psi \in L_2(\omega),$$

$$\psi|_{\partial\Omega} = 0,\ \psi|_\Gamma = \psi_\Gamma \in E_+,\ \Im\lambda \neq 0. \qquad (6)$$

The solution ψ exists for all complex λ and has normal limit values on the continuous spectrum. We introduce the Dirichlet-to-Neumann map of the intermediate Hamiltonian (DN-map) as

$$\mathcal{DN}^F : \psi_\Gamma \longrightarrow P_+\frac{\partial\psi}{\partial n}\big|_\Gamma. \qquad (7)$$

It is a 3×3 matrix-function which is obtained via differentiation of the resolvent of the intermediate operator with respect to exterior normals, and subsequent restriction onto Γ

$$\mathcal{DN}^F(y,\eta) = -P_+\frac{\partial^2 G_\lambda^F(y,\eta)}{\partial n_y \partial n_\eta}P_+.$$

It has the spectral representation on the complement of the spectrum of $\sigma(L^F)$

$$\mathcal{DN}^F(\lambda) = \sum_r \frac{P_+\frac{\partial\Phi_r^F(\xi)}{\partial n}\rangle\ \langle P_+\frac{\partial\Phi_r^F(\xi')}{\partial n}}{\lambda - \lambda_r} + \mathcal{K}(\lambda), \quad (8)$$

where the summation is extended over the discrete spectrum of L^F and $\mathcal{K}(\lambda)$ contains an integral over continuous spectrum. The Scattering matrix of $\mathcal{L}$ is obtained via matching of the scattering Ansatz in the open channel of the wires with $p = p_1$

$$e^{ip\xi}e_+ + e^{-ip\xi}S(p)e_+ \qquad (9)$$

to the limit values on the spectrum, $\Im\lambda \to 0$, of the solution of the above intermediate boundary problem (7):

$$ip\left[e_+ - S(p)e_+\right] = \mathcal{DN}^F(\lambda)\ \left[e_+ + S(p)e_+\right].$$

Solving this equation we obtain, see [13], we obtain the formula for the scattering matrix of the operator $\mathcal{L}$ on the first spectral band Δ in terms of $\mathcal{L}^F$ by the formula

$$S(p) = \frac{\mathcal{DN}^F(\lambda) + ipP_+}{-\mathcal{DN}^F(\lambda) + ipP_+}. \quad (10)$$

The DN-map $\mathcal{DN}^F$ of the intermediate Hamiltonian $L_{_F}$ is connected with the standard, see [12], DN-map $\mathcal{DN}$ of the operator L_{int} on the quantum well Ω by the formula

$$\mathcal{DN}^F = P_+\mathcal{DN}P_+ - P_+\mathcal{DN}P_- \ \mathbf{D}^{-1}P_-\mathcal{DN}P_+. \quad (11)$$

Here $K_- = -\oplus\sum_{l>1}\sum_s p_l P_s^l := -\oplus\sum_{l>1} p_l P_l$, $|K_-| \geq \pi\delta^{-1}\sqrt{3/2}$, and $P_- := \oplus\sum_{l>1} P_l = I \ominus P_+$ and $\mathbf{D} = P_-\mathcal{DN}P_- - K_-$. Near the eigenvalue λ_0 the DN-map can be represented as

$$\mathcal{DN}(\lambda) = \frac{\phi_{_0}\rangle\langle\phi_{_0}}{\lambda - \lambda_0} + \mathcal{K}_0, \quad (12)$$

where $\phi_{_0} = \frac{\partial\Phi_0}{\partial n}|_\Gamma$ and $\mathcal{K}_0$ - the contribution from other eigenvalues/eigenfunctions. The spacing between the eigenvalues of L_{int} relates to the diameter d_{int} of Ω_{int} as $\rho_0 = \min_{r\neq 0}|\lambda_0 - \lambda_r| = O(d_{int}^{-2}$. Due to the spectral estimate $|\mathcal{K}_0(\lambda_0)| \approx 1/\sqrt{\rho_0}$ it's matrix elements $\mathcal{K}_{\pm,\pm} := P_\pm\mathcal{K}_0P_\pm$ in the decomposition $I = P_+ \oplus P_-$ of the unit operator in $L_2(\Gamma)$ are estimated by $1/d_{int}$. For relatively thin networks the analytic perturbation procedure for $\mathcal{DN}^F$ can be developed based on (11), with the small parameter δ/d_{int}.

Assume that there exist only one eigenvalue λ_0 of L_{int} on the essential spectral interval $\Delta_T := [\lambda^F - 2\hbar^{-2}m^*\kappa T \leq \lambda \leq \lambda^F - 2\hbar^{-2}m^*\kappa T]$ near the scaled Fermi level. Then for $\delta/d_{int} << 1$ the denominator of (11) near λ_0 can be represented, with $P_-\phi^- := \phi_0^- :=$ as

$$\mathbf{D}(\lambda) \approx \frac{\phi_0^-\rangle\langle\phi_0^-}{\lambda - \lambda_0} + \mathcal{K}_{--} - K_- := \frac{\phi_0^-\rangle\langle\phi_0^-}{\lambda - \lambda_0^0} + k$$

and the whole expression (11) can be calculated via analytic perturbation procedure, since $|k^{-1}| \approx \delta[1 + \delta/d_{int}]^{-1} << 1$:

$$\mathcal{DN}^{^F} \approx \phi_{_0}^{^F}\rangle\,(\lambda - \lambda_0^F)^{-1}\,\langle\phi_{_0}^{^F}, \quad (13)$$

with, $\lambda_0^F = \lambda_0 + \langle P_-\phi_0,\, k^{^{-1}}\ P_-\phi_0\rangle \approx \lambda_0$ and $\phi_0^F = P_+\phi_0 - \mathcal{K}_{+-}k^{-1}\ P_-\phi_0 \approx P_+\phi_0$. For low temperature only electrons with energy close to Fermi level E_F contribute to transport phenomena. Hence $\mathcal{DN}^F$ may be substituted by the single resonance term $\frac{P_+\phi_{_0}\rangle\,\langle P_+\phi_{_0}}{\lambda_0 - \lambda}$, thus resulting in the approximate expression for the scattering matrix on Δ_T :

$$S_{approx}(\lambda) = \frac{ipP_+ - \frac{P_0\phi_{_0}\rangle\,\langle P_+\phi_{_0}}{\lambda_0 - \lambda}}{ipP_+ + \frac{P_0+\phi_{_0}\rangle\,\langle P_+\phi_{_0}}{\lambda_0 - \lambda}}. \quad (14)$$

See [13] and more details in [16].

4 Boundary condition at the junction

The approximate scattering matrix can be formally obtained from the energy-dependent boundary condition at the vertex imposed onto the scattering Ansatz (9) in the wires:

$$ip[I - S_{approx}(\lambda)]\vec{\psi} = [I + S_{approx}(\lambda)]\vec{\psi'}. \quad (15)$$

The polar terms in the numerator and in the denominator of (14) have the dimension cm^{-1} and can be represented via the relevant one-dimensional orthogonal projection $P_{_0} := \vec{e}_{_0}\rangle\,\langle\vec{e}_{_0}$ with $\vec{e}_{_0} := (e_0^1, e_0^2, \ldots e_0^n) = \| \vec{\phi}_{_0} \|^{-1}\ \vec{\phi}_{_0} := \alpha^{-1}\vec{\phi}_{_0}$. Then $\vec{\phi}_{_0}\rangle\,\langle\vec{\phi}_{_0} = \alpha^{^2}P_{_0}$. Denoting by $P_{_0}^{^\perp}$ the complementary projection $I - P_{_0}^{^\perp}$ in $L_2(\Gamma)$, we obtain

$$S_{approx}(\lambda) = P_{_0}^{^\perp} + \left[\frac{ip(\lambda - \lambda_0) + \alpha^{^2}}{ip(\lambda - \lambda_0) - \alpha^{^2}}\right]P_{_0} \quad (16)$$

$$\equiv P_{_0}^{^\perp} + \Theta(\lambda)\,P_{_0}.$$

The factor Θ on the essential spectral interval Δ_T, for low temperature $2\pi m * \sqrt{3/2}\kappa T << \delta\alpha^2\hbar^2$ is close to -1. Then, in first approximation, the energy-dependent boundary condition (15) is reduced on Δ_T to $iP_{_0}^{^\perp}\psi - P_{_0}\psi' \approx 0$, or, due to orthogonality of $P_{_0}, P_{_0}^{^\perp}$, to $P_{_0}^{^\perp}\vec{\psi} \approx 0$; $P_{_0}\vec{\psi'} \approx 0$. This condition coincides with the above Datta condition (1) presented in form (2). Our analysis reveals the meaning of the projection P_0: it coincides with the projection onto the one-dimensional subspace defined by the vector $P_+\frac{\partial\phi_0(\xi)}{\partial n}|_\Gamma$ of boundary values of the normal derivatives of the resonance eigenfunction, projected onto E_+.

5 Example

Consider a two-dimensional quantum network 3 constructed as an asymmetric T-junction of three straight quantum wires width $\pi/2$ at the vertex square Ω_{int} : $0 < \xi_{_1} < \pi, 0 < \xi_{_2} < \pi$. The first wire $\omega_{_1} = \{\xi_{_1} < 0,\, \pi/2 < \xi_{_2} < \pi\}$ is attached orthogonally to the left side of the square on $\Gamma_{_1} = \{\xi_{_1} = 0,\, \pi/2 < \xi_{_2} < \pi\}$, the second wire $\omega_{_2}$ is attached in the middle of the upper side on $\Gamma_2 = \{\pi/4 < \xi_1 < 3\pi/4, \xi_2 = \pi,\ \}$, and the third wire $\omega_{_3}$ is attached on the middle part $\Gamma_3 = \{\xi_1 = \pi,\, \pi/4 < \xi_2 < 3\pi/4,\}$ of the right side of Ω_{int}. The first spectral band in the wires is $\Delta_1 = [4, 16]$.

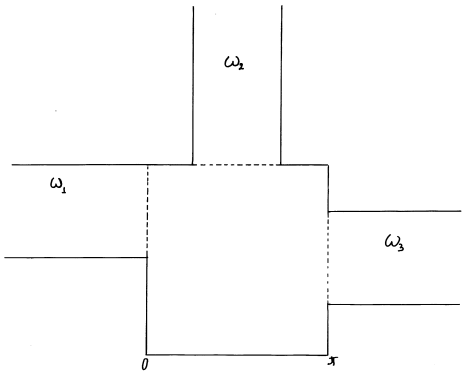

Figure 3: Simplest asymmetric T-junction

The cross-section eigenfunctions in the open channels in the wires are

$$e^1_+\Big|_{\Gamma_1} = \frac{2}{\sqrt{\pi}}\sin 2\xi_2,\ e^2_+\Big|_{\Gamma_2} = \frac{2}{\sqrt{\pi}}\cos 2\xi_1,$$

$$e^3_+\Big|_{\Gamma_3} = \frac{2}{\sqrt{\pi}}\cos 2\xi_2,$$

The Dirichlet Laplacian $-\Delta_{int}$ on Ω_{int} has on Δ_1 the eigenvalues $\lambda_0 = 5$,$\lambda_1 = 8$, $\lambda_2 = 10$ and $\lambda_3 = 13$ with normalized eigenfunctions Ψ_s, $\Phi_0(\xi) = \frac{2}{\pi}\sin\xi_1\ \sin 2\xi_2$. The boundary currents of Φ_0 on Γ_s are :

$$\frac{\partial\Phi_0}{\partial n}\Big|_{\Gamma_1} = -\frac{2}{\pi}\ \sin 2\xi_2,\ \frac{\partial\Phi_0}{\partial n}\Big|_{\Gamma_2} = -\frac{4}{\pi}\ \sin\xi_1,$$

$$\frac{\partial\Phi_0}{\partial n}\Big|_{\Gamma_3} = -\frac{2}{\pi}\ \sin 2\xi_2.$$

Assume that the scaled Fermi level is $\lambda^F = 4.33\ cm^{-2}$. The corresponding eigenfunction of $-\Delta_{int}$ is $\Phi_0(\xi) = \frac{2}{\pi}\sin\xi_1\ \sin 2\xi_2$. Consider the Scattering problem for the network Ω. The electrons are supplied in the first spectral band from the second wire across the bottom section Γ_2 and exit across Γ_1, Γ_3. Due to orthogonality of the cross-section eigenfunction of the open channel to the boundary currents of the eigenfunctions Φ_0', Φ_3', the corresponding modes are not excited. An essential link to the closed channels is supplied only by Φ_0, the contribution from other eigenfunctions either vanish, or we neglect them due to the factors $(\lambda_0 - \lambda_s)$ in the denominator. Taking into account only the link to $\mathcal{H}_-|_{\omega_3}$ we obtain the equation for the eigenvalue λ_0^F of the Intermediate Hamiltonian:

$$\frac{1}{\lambda_0 - 5}\int_{\Gamma_3}\left|P_-\frac{\partial\Phi_0}{\partial n}\right|^2 d\Gamma_3 + \sqrt{16-5} := \mathbf{D}_-(\lambda_0) =$$

$$\sqrt{11}\ [0.67 + \lambda_0 - 5], \qquad (17)$$

and find $\lambda_0^F = 4.33 = \lambda^F$. The boundary current of the corresponding eigenfunction essentially coincides with one of Ψ_0. Projections of the resonance boundary current onto $E_+|_{\Gamma_{1,2,3}}$ are:

$$\hat{\phi}_0^1 = \int_{\Gamma_1}\frac{\partial\Phi_0}{\partial n}\Big|_{\Gamma_1} e^1_+\Big|_{\Gamma_1} d\xi_2 = -\frac{1}{\sqrt{\pi}} = -0.56,$$

$$\hat{\phi}_0^2 = \int_{\Gamma_2}\frac{\partial\Phi_0}{\partial n}\Big|_{\Gamma_2} e^2_+\Big|_{\Gamma_2} d\xi_1 = 0.43,\ \hat{\phi}_0^3 = 0.$$

Then the normalized vector of the boundary current is $e_0 = (-0.8,\ 0.6,\ 0)$, and the boundary conditions at the junction for low temperatures are represented by the formulae (2) with $P_0 = e_0\rangle\langle e_0$, which is different from the boundary condition for a symmetric T-junction in [1]. For the higher temperatures the boundary condition is energy dependent and can be represented in form (15), with the approximate scattering matrix

$$S_{appr}(p) = \frac{i\sqrt{\lambda-4}P_+ - 0.15\frac{P_0}{\lambda-4.33}}{i\sqrt{\lambda-4}P_+ + 0.15\frac{P_0}{\lambda-4.33}}.$$

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