Boundary Conditions at the Junction

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ABSTRACT

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 a two-dimensional network, see [6], [7], [8]. Basic detail of the model is a star-shape element with a self-adjoint boundary condition at the node. It was commonly expected that the realistic boundary condition is defined by the local geometry of the graph, that is by the angles between the wires at the node. For instance the boundary conditions for the T-junction, [1], is presented in terms of limit values of the wave-function on the wires $\{\psi_i\}_{i=1}^3$ and the values of the corresponding outward derivative $\{\psi_i'\}_{i=1}^3$ at the node:

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

Here β is a free parameter which describes "the strength of the coupling" between the leg and the bar of the T-junction. These boundary conditions can be represented, see [9], in the form

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

where $\bar{\psi}$ and $\bar{\psi}'$ are vectors of values of the wave-function at the vertex, with the projection

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

The scattering matrix of such a junction is $S = I - 2P_0$, see [1], [4], [10]. In [11] the condition (2) is used for analysis of spin-dependent transmission across the quantum ring. In fact the projection $P_0 = P_0(\beta)$ can also play a role of the free parameter of the model junction.

In our talk we extend, based on [12], the above boundary condition (2) to any junction of equivalent wires and interpret the corresponding free parameter P_0. Consider the junction Ω formed by few 2-d semi-infinite wires Ω_j, $j = 1, 2, \dots n$, attached to the quantum well Ω_{int} via the orthogonal bottom sections Γ_j. The transport properties of Ω are defined by the one-electron scattering in Ω. We consider the resonance case when the scaled Fermi level E_F coincides with the resonance eigenvalue $\hbar^{-2}2mE_F = \lambda_0$ of the corresponding Schrödinger operator in $L_2(\Omega)$, with effective mass m and "partial" Dirichlet boundary condition at $\partial\Omega_{int}$. We will show that the parameter P_0 is defined by the shape of the resonance eigenfunction Ψ_0, but not by the angles between the wires at the node, as an example shows.

Assume that all wires have the same width δ, the potential on the vires vanishes, and the Fermi level is situated on the first spectral band $[\pi^2\,\delta^{-2},\, 4\pi^2\,\delta^{-2}] := [\mu_1, \mu_2]$. The cross-section eigenfunctions in the first (open) channel are $\sin\frac{\pi y_j}{\delta} = e_j$. Denote by $E_+ := \bigvee_{j=1}^n e_j$ the subspace spanned by cross-section eigenfunctions of the open channel, and introduce the boundary current $\vec{\phi}_0 = P_+ \frac{\partial \Psi_0}{\partial n}|_\Gamma$ of the normalized resonance eigenfunction Ψ_0 via projection $P_+ : L_2(\Gamma) \to E_+$ on the union $\Gamma = \cup_j \Gamma_j$ of the bottom sections. If the network is relatively thin on Fermi level, $\delta\,\max_{s=1,2}|\lambda_0 - \mu_s| << 1$, the temperature is low, $2m\kappa T << \hbar^2 \min_{s=1,2}|\lambda_0 - \mu_s|$, and there exist only one simple resonance eigenvalue λ_0 of the Schrödinger operator on the well on the essential spectral interval $\Delta_T := [\lambda_0 - 2\hbar^{-2}m\kappa T \leq \lambda \leq \lambda_0 - 2\hbar^{-2}m\kappa T] \subset [\mu_1,\, \mu_2]$, then we are able to derive, based on [12], an approximate expression

ISBN 3-901578-16-1

for the scattering matrix on Δ_T :

$$S_{approx}(\lambda) = \left[i\sqrt{\lambda - \mu_1} I + \frac{\vec{\phi}_0\rangle\langle\vec{\phi}_0}{\lambda_0 - \lambda} \right] \times \left[i\sqrt{\lambda - \mu_1} I - \frac{\vec{\phi}_0\rangle\langle\vec{\phi}_0}{\lambda_0 - \lambda} \right]^{-1} . \quad (3)$$

The corresponding energy-dependent boundary condition at the node of the model graph is written down in terms of the limit values of the wave function and the outward derivatives, $\vec{\psi} = (\psi_1(0), \psi_2(0), \dots \psi_n(0))$, $\vec{\psi}' = (\psi_1'(0), \psi_2'(0), \dots \psi_n'(0))$ at the node:

$$i\sqrt{\lambda - \mu_1}[I - S_{approx}(\lambda)]\vec{\psi} = [I + S_{approx}(\lambda)]\vec{\psi}'. \quad (4)$$

The polar terms in the numerator and in the denominator of (3) 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 $\vec{e}_0 := (e_0^1, e_0^2, \dots e_0^n) = \parallel \vec{\phi}_0 \parallel^{-1} \vec{\phi}_0 := \alpha^{-1}\vec{\phi}_0$. Then $\vec{\phi}_0\rangle\langle\vec{\phi}_0(\lambda - \lambda_0)^{-1} = \alpha^2(\lambda - \lambda_0)^{-1}P_0$. Denoting by $P_0^{\perp}$ the complementary projection $I - P_0^{\perp}$ in $L_2(\Gamma)$, we obtain

$$S_{approx}(\lambda) = P_0^{\perp} + \left[\frac{i\sqrt{\lambda - \mu_1}(\lambda - \lambda_0) + \alpha^2}{i\sqrt{\lambda - \mu_1}(\lambda - \lambda_0) - \alpha^2} \right] P_0 \equiv P_0^{\perp} + \Theta(\lambda)\, P_0. \quad (5)$$

In particular, for *even lower* temperature and appropriate α the factor Θ in front of P_0 is estimated on Δ_T as $|\Theta(\lambda) + 1| << 4\kappa T\, m\sqrt{\lambda_0 - \mu_1}\alpha^{-2}\hbar^{-2}$. Then, in first approximation, the corresponding boundary condition (4) 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 $P_0^{\perp}\vec{\psi} \approx 0$; $P_0\vec{\psi}' \approx 0$. The results are applied to design of the resonance quantum switch and spin-filter based on standing waves in a 2-d quantum well.

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