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Fitting Parameters for a Solvable Model of a Quantum Network

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Fitting Parameters for a Solvable Model of a Quantum Network

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Abstract

A solvable model corresponding to a given quantum network is described in [22] without an explicit description of how to fit the parameters of the solvable model. Here we give a procedure to fit these parameters so that the solvable model reproduces the important features, viz. the scattering matrix for the physically relevant energies, of the quantum network, subject to the non-vanishing of a determinant.

1 Introduction

The current interest in quantum networks is motivated by the design of electronic devices at quantum scales with the objective of manufacturing networks with prescribed transport properties. The literature in this area is extensive with many studies into the mathematical aspects of such problems [1, 2, 5, 6, 7, 8, 9, 12, 15, 16, 13, 14, 18, 19, 20, 22, 23, 26, 25, 24, 27] as well as explicit attempts at the actual design of networks with given scattering properties [3, 4, 10, 11, 17, 21, 28]. We do not make any claim for completeness of our bibliography.

In [22] the authors describe how to associate with a given quantum network a solvable model with the same scattering properties at physically relevant energies. However, it is not shown that the desired solvable model exists, rather some conditions are found which this solvable model has to satisfy. Here we show (subject to the non-vanishing of a determinant) that the desired solvable model can always be constructed and give the explicit construction. We start with a brief description of the quantum network and associated solvable model proposed in [22]. Our notation is the same as, or a simplified version of, the notation in [22].

2 The Quantum Network

The quantum network consists of a connected set of compact domains $\{\Omega_i\}$ and finite and semi-infinite channels $\{\omega^j\}$ lying in the plane $\Omega = \bigcup_i \Omega_i \bigcup_j \omega^j \subset \mathbb{R}^2$. The channel ω^j has straight edges and constant width δ_j and is connected to one compact domain (if it is semi-infinite) or two compact domains (if it is finite). The boundary arc γ_i^j between Ω_i and ω^j is linear and at right angles to the edges of ω^j. We denote by $\Gamma = \bigcup_{i,j} \gamma_i^j$ the set of boundaries.
We consider the spectral problem on the network

$$\begin{aligned} \mathcal{L}\psi \equiv -\Delta\psi + V\,\psi &= \lambda\psi \\ \psi|_{\partial\Omega} &= 0 \end{aligned}$$

where the potential $V : \Omega \mapsto \mathbb{R}$ is real and assumed constant on the channels $V|_{\omega^j} \equiv V_j = \text{const}$.
By the Glazman splitting technique we see that the continuous spectrum, regardless of the form of the compact part of the network, consists of an infinite union of semi-infinite intervals, one for each mode transverse to the channel, and of multiplicity equal to the number of semi-infinite channels. It is assumed that the Fermi energy Λ is in the continuous spectrum. The authors of [22] define the 'intermediate operator' $\mathcal{L}_\Lambda$ in terms of special boundary conditions at Γ which depend on the Fermi energy.
Then the Dirichlet to Neumann map for this intermediate operator $\mathcal{DN}^\Lambda(\lambda)$ is calculated and it is shown that the scattering matrix is given in terms of this operator by ([22], equation (24))

$$\mathbf{S}(\lambda) = -\left(\mathcal{DN}^\Lambda - \frac{i}{2\mu^\parallel}K_+\right)^{-1}\left(\mathcal{DN}^\Lambda + \frac{i}{2\mu^\parallel}K_+\right). \tag{1}$$

Here $\mu^\parallel$ is a constant and K_+ is a simple function of the spectral parameter. For the purposes of approximation by a solvable model the authors use the so called 'essential part' $\mathcal{DN}_T^\Lambda$ of the Dirichlet to Neumann map obtained by only considering eigenvalues in a band around the Fermi energy of width proportional to the temperature. This operator has kernel ([22], equation (48), although there is some discrepancy with equation (35))

$$\mathcal{DN}_T^\Lambda = \sum_{l=1}^{N_T} \frac{1}{\lambda_l - \lambda}\left|P_+\frac{\partial\varphi_l}{\partial n}\right\rangle\left\langle P_+\frac{\partial\varphi_l}{\partial n}\right|.$$

Here the φ_l and λ_l are the eigenfunctions and eigenvalues on the compact part of the network, $\partial\cdot/\partial n$ is the normal derivative and P_+ is a projection onto a finite dimensional subspace on Γ, related to the finite multiplicity of

the continuous spectrum at the Fermi energy. Consequently, this 'essential part' of the Dirichlet to Neumann operator is a finite dimensional operator, ie. a matrix.
Consider an approximation to the scattering matrix obtained by using this simpler operator $\mathcal{DN}_T^\Lambda$ in (1). One of the aims of [22] is to construct a solvable model which has the same scattering matrix as this approximate scattering matrix. Some conditions are found for this construction to proceed but it is not shown that it is always possible to construct the desired solvable model. Here we will show (modulo the non-vanishing of a determinant) that it is always possible to construct a solvable model with the desired properties.

3 The Solvable Model and Fitting Parameters

In [22] the authors approximate the quantum network by a (one-dimensional) graph consisting of n semi-infinite rays and a single vertex with a finite dimensional operator A at the vertex. The set of finite dimensional vectors and eigenvalues

$$\left\{ P_+ \frac{\partial \varphi_l}{\partial n}\,, \quad \lambda_l\,; \quad l = 1, \ldots, N_T \right\} \tag{2}$$

are regarded as given data from the quantum network. Following [22] the vectors $P_+ \partial \varphi_l / \partial n$ are defined to be elements of the n-dimensional[1] vector space E_+.
We denote by $\ell = \bigoplus^n - \frac{d^2}{dx^2}$ the 'Schrödinger' operator on the rays of the graph acting on the Hilbert space $H = \bigoplus^n \mathrm{L}^2[0,\infty)$. We denote by $E_A = \mathbb{C}^N$ the 'abstract' finite dimensional Hilbert space at the vertex on which the self-adjoint matrix $A = A^*$ acts. These are clearly both self-adjoint operators in their respective Hilbert spaces.
We restrict ℓ to a *symmetric* operator $\ell_0 = \ell|_{\mathcal{D}_0}$ acting on functions disappearing near the 'origins' (of the $\mathrm{L}^2[0,\infty)$).
We also restrict A to the domain $D_0 \equiv (A - i\mathbb{I})^{-1} E_A \ominus N_i$ where N_i, the deficiency subspace with $\dim(N_i) = d$, is chosen in the construction of the solvable model. A technical requirement is that $N_{-i} \cap N_i = \emptyset$ where

$$N_{-i} = \frac{A+i}{A-i} N_i\,,$$

ie. the deficiency subspaces do not intersect. For this to hold we need at least $2d \le N$.
Our aim is to find a self-adjoint extension of the symmetric operator

$$\mathbf{A}_0 = \ell_0 \oplus A_0 \tag{3}$$

[1] From [22] we see that the dimension of these vectors is *at least* the number of semi-infinite channels of the network.

which has the same scattering matrix as the network in the desired energy range.
This procedure of restricting then extending the operator to a self-adjoint operator with desired properties is described in some detail in [27, 22]. In summary the scattering ansatz for the solvable model ([22], after equation (43)) takes the form

$$\Psi = \begin{pmatrix} e^{-iK_+\mathbf{x}}\nu + e^{iK_+\mathbf{x}}\mathbf{S}\nu \\ \frac{A+i}{A-\lambda}\xi \end{pmatrix}$$

where ξ are the components of Ψ in the deficiency subspace. We denote by β the self-adjoint boundary conditions for the extension $\mathbf{A}_\beta$ of (3) (to be precise, in this report β is used to denote the off diagonal part of the boundary condition matrix). These boundary conditions relate Ψ and its derivative at the origin allowing the authors of [22] to solve for the scattering matrix in terms of β, A and the deficiency subspaces. This gives theorem 5.1 of [22] which describes the solvable model in terms of the set (2) of given data from the quantum network. Our formulation of this theorem follows the formulation in [22] closely although we have omitted the last two sentences as they are not strictly relevant to our discussion.

Theorem 5.1 *The constructed operator $\mathbf{A}_\beta$ is a solvable model of the quantum network on the essential interval of energy iff: the dimension of the space E_A coincides with the number of eigenvalues on the essential interval of energy $N = N_T$; the eigenvalues λ'_l of A coincide with the eigenvalues of the intermediate operator on the essential interval of energy $\lambda'_l = \lambda_l$ so that*

$$A = \sum_{l=1}^{N_T} \lambda_l \left|e_l\right\rangle \left\langle e_l\right| \;;$$

and there exists a deficiency subspace N_i of A_0, the associated orthogonal projection P_i onto N_i, and an operator $\beta : N_i \mapsto E_+$ such that for the orthonormal basis of eigenvectors e_l of A

$$P_+ \frac{\partial \varphi_l}{\partial n} = \beta P_i e_l \tag{4}$$

for $l = 1, \ldots, N_T$.

Note: the matrix β, although associated with the self-adjoint boundary conditions, is not necessarily self-adjoint because it is the off diagonal block of the boundary condition matrix.
Note: as noted above the dimension of N_i has to be less that or equal half the dimension of E_A, $2d \leq N_T$, otherwise there is no possibility that the intersection of the deficiency subspaces is null. The condition of null intersection is expressed below as the non-vanishing of a determinant; however, if

this determinant vanishes our procedure fails[2].
Really, this theorem defines the solvable model up to the condition (4). We show that it is always possible to choose P_i (and thence N_i) and β to satisfy this condition. We start by defining the n-dimensional vector

$$\Phi_l = P_+ \frac{\partial \varphi_l}{\partial n} \,.$$

Considering the Φ_l as columns of a $n \times N_T$ matrix Φ we can write the condition (4) in matrix form $\Phi = \beta P_i$ where we have implicitly assumed that $\{e_l\}$ is the standard basis (so A is a diagonal matrix in this basis). We diagonalise the self-adjoint matrix

$$\Phi\Phi^* = U^* D U \tag{5}$$

and define the $n \times N_T$ matrix

$$\Upsilon = U\Phi \,. \tag{6}$$

Consequently condition (4) becomes

$$\Upsilon = U\beta P_i \tag{7}$$

and we claim that this has solution

$$\beta = U^* D^{\frac{1}{2}} \tag{8}$$
$$P_i = D^{-\frac{1}{2}} \Upsilon \tag{9}$$

where we take the real non-negative square root of D—it follows easily from (5) that the components of D are non-negative. When D has zeroes on the diagonal we make sense of (9) by defining $D^{-\frac{1}{2}}$ to have zeroes at the corresponding positions in the diagonal.
Clearly (8,9) formally satisfies (4) or (7) and we will show that this holds even when D has zeroes. As we pointed out above β can take any form so the choice of β needs no further discussion. We just need to show that P_i is an orthogonal projection for suitable bases.
Assuming for now that D has no zeroes we consider following set

$$\eta_k = \sum_{l=1}^{N_T} \left(D^{-\frac{1}{2}} \Upsilon \right)_{k,l} e_l \tag{10}$$

of vectors in E_A. Since $\{e_l\}$ is orthonormal, and since (5) and (6) give us

$$\Upsilon\Upsilon^* = D \,, \tag{11}$$

we see that $\{\eta_k\}_{k=1}^n$ is also an orthonormal set in E_A. Now we claim that this is the basis of N_i. In consequence

$$P_i = \sum_{k=1}^{n} \left|\eta_k\right\rangle \left\langle\eta_k\right| \,,$$

[2]Although it appears that the condition of null-intersection may be relaxed.

with domain in the basis $\{e_l\}$ and range in the basis $\{\eta_k\}$, just takes the desired form (9). We note that in this case (D having no zeroes) the deficiency index is $d = n$.
In the case where D has zeroes on the diagonal we easily see from (11) that the corresponding rows of Υ are *identically zero.* Consequently, using the given definition of $D^{-\frac{1}{2}}$ we see that $D^{\frac{1}{2}}D^{-\frac{1}{2}}$ has ones on the diagonal except at those positions corresponding to the zero rows of Υ so that

$$D^{\frac{1}{2}}D^{-\frac{1}{2}}\Upsilon = \Upsilon$$

and (8,9) continues to satisfy (4), (7). Furthermore the definition of the basis (10) continues to make sense as does the demonstration that P_i is an orthogonal projection. We note that in this case the deficiency index is $d = \text{rank}(D) < n$.

The condition for the non-intersection $N_{-i} \cap N_i = \emptyset$ can be written in terms of the non-vanishing of a determinant involving $D^{-\frac{1}{2}}\Upsilon$ and the eigenvalues λ_l. Really, working in the basis $\{e_l\}$ of E_A we see that N_i has orthonormal basis given by the rows of $D^{-\frac{1}{2}}\Upsilon$. Since the Cayley trasform $(A+i)(A-i)^{-1}$ is unitary, N_{-i} has orthonormal basis given by the rows of $D^{-\frac{1}{2}}\Upsilon \,\text{diag}\left((\lambda_l + i)/(\lambda_l - i)\right)$. Consequently, the deficiency subspaces have null intersection iff

$$\det \begin{pmatrix} D^{-\frac{1}{2}}\Upsilon \\ D^{-\frac{1}{2}}\Upsilon \,\text{diag}\left(\frac{\lambda_l+i}{\lambda_l-i}\right) \end{pmatrix} \neq 0 \tag{12}$$

where of course we omit any zero rows in the matrix $D^{-\frac{1}{2}}\Upsilon$.

In summary, given the data (2) we find D, U and Υ from equations (5) and (6). The boundary condition for the desired solvable model is then given by equation (8) and the deficiency subspace is given by (9,10) where the deficiency index is $d = \text{rank}(D) \leq n$. We note that there are no free parameters to ensure that the condition for the null intersection of the deficiency subspaces (12) is satisfied.

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