Two particle scattering on pencil of rays

Igor Lobanov\textsuperscript{1}, Igor Popov\textsuperscript{2}
\textsuperscript{1,2} Saint Petersburg State University of Information Technologies, Mechanics and Optics, 197101, Saint-Petersburg, Str. Sablinskaya 14
E-mail: lobanov.igor@gmail.com
E-mail: popov@mail.ifmo.ru

Abstract. We consider the scattering problem for the two particle Schrödinger operator on the star graph, which can be considered as an explicitly solvable model of the many electron Hamiltonian on a nanotubes junction. For inverse square interaction potential, the Green function and the scattering matrix are obtained.

1. Motivation
There are few known explicitly solvable models, which therefore are especially valuable tools to study qualitative properties of quantum systems. In many-particle theory, the Sutherland-Calogero systems [6] become most widely known explicitly solvable models having unfortunately very simple one-dimensional configuration spaces. One the other hand, in single particle theory the quantum graphs prove their usability as simple model of complex networks [1]. In the present work, we study an explicit many-particle model of a quantum network, namely of a pencil of rays or a star graph. The star graph is of special interest, since it can be considered as very simple model of a carbon nanotubes junction. The one particle problem for the graph was analyzed in details in [4]. Two particle problem on star graph was recently partially investigated in [3] for δ-type particle interaction. The aim of the present work is to obtain explicit solution of the two particles scattering problem on the star graph for inverse square particle interaction potential.

2. Model
We assume that the considered charged particles are restricted to pencil of rays (star graph) X consisting of N rays $\mathbb{R}_n$, $n \in \tilde{N} = \{1, \ldots, N\}$, glued at origins, i.e. particle motion is one-dimensional. The corresponding two particle Hamiltonian $H$, $D(H) \subset L^2(X^2)$, has the form

$$H = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + V(\rho(x, y)),$$

for $x, y \neq 0$ and is subjected to Kirchhoff boundary conditions

$$f_{1k}(0, \tau) = f_{jk}(0, \tau), \quad f_{j1}(\tau, 0) = f_{jk}(\tau, 0), \forall \tau \in \mathbb{R}, \ j, k \in \tilde{N},$$

$$\sum_{n=1}^{N} \partial_1 f_{nk}(0, \tau) = 0, \quad \sum_{n=1}^{N} \partial_2 f_{jn}(\tau, 0) = 0, \forall \tau \in \mathbb{R}, \ j, k \in \tilde{N},$$
where \(f_{jk}\) denotes the restriction of a wave function \(f\) to \(\mathbb{R}_j \times \mathbb{R}_k\). The proposed method is suitable also for arbitrary particle number; we consider two particles only to shorten formulae. To obtain an explicitly solvable model we consider inverse square potential \(V(r) = \frac{1}{r^2}\). The distance \(\rho\) on \(X\) is the distance on metric graph, i.e.

\[
\rho((j,x),(k,y)) = \begin{cases} |x - y|, & j = k, \\ |x + y|, & j \neq k. \end{cases}
\]

The obtained model is explicitly solvable, in the sense that the resolvent of \(H\) can be written explicitly. Our aim is to calculate the resolvent and the scattering matrix for \(H\).

3. Decoupling

Our first step is to decouple edges of the graph; this is possible due to the high symmetry. The wave functions can be considered as functions on \(\bar{\mathbb{N}}\), that is \(\mathcal{D}(H) \subset L(\bar{\mathbb{N}} \times \bar{\mathbb{N}}, L^2(\mathbb{R}_+ \times \mathbb{R}_+))\). Since the Hamiltonian \(H\) is invariant under rays permutations, the following theorem is applicable:

**Theorem.** Let \(\bar{\mathbb{N}}\) be a finite set, \(\mathcal{H}\) be a Hilbert space. Let \(T\) be a linear representation of the transpositions group \(S\) of the set \(\mathbb{N}\) on \(l(M, \mathcal{H})\) defined by \(T \sigma f(m,n) = f(\sigma^{-1}m, \sigma^{-1}n)\), \(m,n \in \bar{\mathbb{N}}\), \(\sigma \in S\), \(f \in L(\bar{\mathbb{N}} \times \bar{\mathbb{N}}, \mathcal{H})\). Suppose \(H, \mathcal{D}(H) \subset L(\bar{\mathbb{N}} \times \bar{\mathbb{N}}, \mathcal{H})\), is a densely defined linear operator commuting with \(T\). Then

\[
H = (P \otimes P \otimes H_1) \oplus (P \otimes (1 - P) \otimes H_2) \oplus ((1 - P) \otimes P \otimes H_3) \oplus ((1 - P) \otimes (1 - P) \otimes H_4),
\]

for some operators \(H_k, \mathcal{D}(H_k) \subset \mathcal{H}\), where \(P\) is the orthoprojector on the subspace of symmetric vectors, \((P)_{jk} = |\mathbb{N}|^{-1}\).

For the considered Hamiltonian, \(H_k\) are self-adjoint operators on quarter plane \(\mathbb{R}_+ \times \mathbb{R}_+\) defined by the differential expression

\[
H_k = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + N^{-1}V(x - y) + (1 - N^{-1})V(x + y),
\]

with boundary conditions

\[
\begin{cases}
(\delta_{k1} + \delta_{k2})\partial_1 f(0,y) + (\delta_{k3} + \delta_{k4}) f(0,y) = 0 & \forall y, \\
(\delta_{k1} + \delta_{k3})\partial_2 f(x,0) + (\delta_{k2} + \delta_{k4}) f(x,0) = 0 & \forall x,
\end{cases}
\]

where \(\delta_{jk}\) is the Kronecker \(\delta\)-symbol.

4. Green functions for quarter plane

The spectral and scattering properties of \(H\) can be recovered from the Green functions of \(H_k\). Unfortunately, the variables in \(H_k\) do not separate, and the mirror method can be applied only for the trivial case \(N = 2\). We propose the following approach based on restriction-extension method to obtain the Green function for a subdomain if the Green function for the whole domain is known.

Consider the operator \(H_0, \mathcal{D}(H) \subset L^2(\mathbb{R} \otimes \mathbb{R})\), of the form

\[
H_0 = -\frac{\partial^2}{\partial \zeta^2} - \frac{\partial^2}{\partial \eta^2} + N^{-1}V(\zeta) + (1 - N^{-1})V(\eta) = H_\zeta \otimes I + I \otimes H_\eta.
\]

Changing the coordinates \(\zeta = x - y, \quad \eta = x + y\), we obtain

\[
H_0 = -2\frac{\partial^2}{\partial \zeta^2} - 2\frac{\partial^2}{\partial \eta^2} + N^{-1}V(\zeta) + (1 - N^{-1})V(\eta) = H_\zeta \otimes I + I \otimes H_\eta.
\]
Then the Green function of $H_0$ has the form

$$G_0(x, y; x', y'; z) = \int_{\text{spec } H_\zeta} \int_{\text{spec } H_\eta} (z - E - E')^{-1} \times$$

$$\times \phi_\zeta (x - y, E) \phi_\eta (x + y, E') \phi_\zeta (x' - y', E) \phi_\eta (x' + y', E') dE' dE,$$

where $\phi_\zeta$, $\phi_\eta$ are generalized eigenfunction of $H_\zeta$, $H_\eta$, respectively.

Consider the restriction $S_0$ of the operator $H_0$ to the functions vanishing on lines $\eta = 0$, $\zeta = 0$. The operator $H_0$ is the self-adjoint extension of $S_0$ corresponding to Kirchhoff boundary conditions, and the operators $H_k$, to Dirichlet and Neumann boundary conditions in various combinations. To describe the extension of $S_0$ we use Krein resolvent formula in term of boundary triples $(\mathcal{G}, \Gamma_1, \Gamma_2)$. The defect space $\mathcal{N}_z = \ker (S_0^* - z)$ is isomorphic to $\mathcal{G} = \mathcal{G}_x \oplus \mathcal{G}_x \oplus \mathcal{G}_y \oplus \mathcal{G}_y$. The operators $\Gamma_k$ must satisfy $\langle S^* f | g \rangle - \langle f | S^* g \rangle = \langle \Gamma_1 f | \Gamma_2 g \rangle - \langle \Gamma_2 f | \Gamma_1 g \rangle$, and can be chosen of the form

$$\Gamma_1 f (\tau) = \begin{pmatrix} f(+0, \tau) - f(-0, \tau) \\ \partial_1 f(-0, \tau) - \partial_1 f(+0, \tau) \\ f(\tau, +0) - f(\tau, -0) \\ \partial_2 f(\tau, -0) - \partial_2 f(\tau, +0) \end{pmatrix}, \quad \Gamma_2 f (\tau) = \begin{pmatrix} \partial_1 f(+0, \tau) + \partial_1 f(-0, \tau) \\ f(-0, \tau) + f(+0, \tau) \\ \partial_2 f(\tau, +0) + \partial_2 f(\tau, -0) \\ f(\tau, -0) + f(\tau, +0) \end{pmatrix}.$$ 

The extensions of $S_0$ are parametrized by couple of operators $A, B$: $\mathcal{G} \to \mathcal{G}$, such that $AB^* = BA^*$ and the rank of $(A | B)$ is maximal. The extension $H_{A,B}$ of $S_0$ corresponding to $(A, B)$ has the domain

$$\mathcal{D}(H_{A,B}) = \{ f \in \mathcal{D}(S^*) : A \Gamma_1 f = B \Gamma_2 f \}.$$ 

Therefore, the operators $H_k$ correspond to boundary conditions $A_k \Gamma_1 f = B_k \Gamma_2 f$, where

$$A_1 = B_0 \oplus B_0, \quad A_2 = A_0 \oplus B_0, \quad A_3 = B_0 \oplus A_0, \quad A_4 = A_0 \oplus A_0,$$

$$B_1 = A_0 \oplus A_0, \quad B_2 = B_0 \oplus A_0, \quad B_3 = A_0 \oplus B_0, \quad B_4 = B_0 \oplus B_0.$$

$$A_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad B_0 = \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix}.$$

The resolvent of the extension $H_{A,B}$ is given by the Krein formula:

$$(H_{A,B} - z)^{-1} = (H_0 - z)^{-1} + \gamma(z) [A Q(z) - B]^{-1} A \gamma^*(z),$$

where $H_0$ is the self-adjoint extension with domain $\{ f \in \mathcal{D}(S_0^*) : \Gamma_1 f = 0 \}$, $\gamma(z) = (\Gamma_1 |_{\mathcal{N}_z})^{-1}$ is a Krein $\Gamma$-field, $Q(z)$ is a Krein $Q$-function. In the explicit form: $\gamma(z) = \gamma_x (z) + \gamma_y (z)$,

$$\gamma_x (z) (f_1, f_2)^T (x, y) = \lim_{\epsilon \to +0} \int_{\mathbb{R}} G_0 (x, y; \tau, 0; z) \times$$

$$\times [ (\theta(x) - \partial_2 G_0(\tau, \epsilon; \tau, 0; z)) G_0^{-1}(\tau, \epsilon; \tau, 0; z) a(\tau) - b(\tau) ] d\tau,$$

$$\gamma_y (z) (f_1, f_2)^T (x, y) = \lim_{\epsilon \to +0} \int_{\mathbb{R}} G_0 (x, y; 0, \tau; z) \times$$

$$\times [ (\theta(x) - \partial_2 G_0(\epsilon, \tau; 0, \tau; z)) G_0^{-1}(\epsilon, \tau; 0, \tau; z) a(\tau) - b(\tau) ] d\tau.$$

By definition $Q(z) = \Gamma_2 \gamma (z)$. Since all integral kernels of operators in the Krein resolvent formula are known, the Green functions of $H_k$ are obtained.
5. Scattering matrix for quarter plane

The generalized eigenfunctions of $H_0$ are given by

$$\psi_{jk}(p, E) = \frac{1}{2} \sqrt{\kappa} H^j(\sqrt{E} \sin p) H^k(\sqrt{E} \cos p), \quad \lambda = \sqrt{1 + \lambda},$$

where $H^k$ are Hankel functions. In virtue of the Krein resolvent formula, the scattering states $\phi(E)$ of $H_k$ can be written in the form

$$\phi(z) = \psi(z) + \gamma_+ (z)[AQ_+(z) - B]^{-1} \Gamma_1 \psi(z),$$

where $\psi(E)$ are scattering states of $H_0$. The scattering matrices $S_k$ are calculated by inspecting asymptotic behaviour of the functions $\psi$ as $\zeta, \eta \to \infty$:

$$\psi_{jk}(p, E) \sim \frac{1}{E \pi} \sqrt{\frac{2}{\sin 2p}} [i(((-1)^k + (-1)^j)(\frac{\lambda \pi}{2} + \frac{\pi}{4}) - \sqrt{E((-1)^j \zeta \sin p + (-1)^k \eta \cos p))}].$$

6. Scattering

Due to the symmetry properties, the scattering matrix for $H$ is decomposed to

$$S = (P \otimes P \otimes S_1) \oplus (P \otimes (1 - P) \otimes S_2) \oplus ((1 - P) \otimes P \otimes S_3) \oplus ((1 - P) \otimes (1 - P) \otimes S_4),$$

where $S_k$ is the scattering matrix for $H_k$. Therefore there are only four scattering channels with distinct reflection and transition amplitudes, $j \neq j', k \neq k'$:

- both particles are reflected:
  $$T_1(E) = S_{j,kj,k}(E) = S_1(E),$$

- only one particle is reflected:
  $$T_2(E) = S_{j,kj,k'}(E) = S_1(E) - S_2(E),$$
  $$T_3(E) = S_{j,kj',k}(E) = S_1(E) - S_3(E),$$

- both particles are not reflected:
  $$T_4(E) = S_{j,kj',k'}(E) = S_1(E) - S_2(E) - S_3(E) + S_4(E).$$

7. Conclusion

An approach to solve many particle scattering problem on star graph for wide class of particle interaction potential and gluing conditions is proposed. Due to the symmetry of the graph, the transmission coefficients does not depend on the choice of ray, therefore parameters of the problem allow to control only ratio of transition and reflection probabilities. It is worth noting that the reflection of one particle change the reflection probability of another particle; this gives a chance to construct a complex network serving as a quantum gate.

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