

The relativistic inverse scattering problem for quantum graphs

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In this paper, we treat the inverse scattering problem for the Dirac equation on metric graphs. Using the known scattering data, we recover the potential in the Dirac equation. The Gel'fand-Levitan-Marchenko integral equation is derived and potential is explicitly obtained for the case of a primary star graph.

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1. Introduction

The study of particle and wave transport in branched structures and networks is of fundamental and practical importance in different topics of contemporary physics. In particular, transport in such nanoscale systems as quantum networks, molecular chains, networks of carbon nanotubes or quantum wires and the problem of charge transport in a DNA double helix can be successfully modeled by quantum mechanical wave equations on metric graphs. Initially, the concept of quantum graphs was introduced by Pauling more than half a century ago to describe electron transport in complex molecular chains of organic molecules. The difference between the usual graph and the quantum graph (both from the mathematical term) is that the dynamics of particles in such systems are described with quantum-mechanical wave equations. Quantum graphs can be considered as a class of confined quantum systems where the dynamics strongly depends on the topology of a graph. The topology of the graph can be given in terms of adjacency matrix:

$$C_{i,j} = C_{j,i} = \begin{cases} 1, & \text{if } i, j \text{ are connected,} \\ 0, & \text{otherwise.} \end{cases}$$

Direct spectral and scattering problems on quantum graphs have been studied earlier in the context of quantum chaos theory (see reviews [1,2] and references therein). The inverse problem for quantum graphs can be divided into two types: the problem of the recovering the potential in the wave equation and the problem of finding the topology of a graph using the given spectral data. The latter is a more difficult problem because of possible isospectrality of graphs for different topologies [3]. In this paper, we solve the inverse scattering problem for the massless Dirac equation, given on the graph of the simplest topology, the so-called star graph. The importance of this problem is a result of its application for modeling charge, information and spin transport in branched nanostructures (e.g., networks of graphene nanoribbons, carbon nanotubes (CNT) and quantum wires). The dynamics of quasi-particles in such systems are described by the massless Dirac equation. In this paper, we propose an

algorithm for reconstructing the potential of the Dirac equation using the available elements of the scattering matrix.

2. Formulation of the problem

Consider a star graph consisting of three semi-infinite edges connected at one point (see. Fig. 1). On each edge, we b_j determine the coordinates $x_j \in [0, \infty)$ where $x_j = 0$ corresponds to the vertex of the graph. The Dirac equation on the each edge b_j is given as:

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \frac{d}{dx} f_j(x_j) + \begin{pmatrix} 0 & q_j(x_j) \\ -p_j(x_j) & 0 \end{pmatrix} f_j(x_j) = i\zeta f_j(x_j), \quad (1)$$

where $f_j(x_j) = \begin{pmatrix} f_{j,1}(x_j) \\ f_{j,2}(x_j) \end{pmatrix}$, $j = 1, 2, 3$. The following boundary conditions are imposed at the branching point:

$$\begin{aligned} f_{1,1}(0) &= f_{2,1}(0) = f_{3,1}(0), \\ f_{1,2}(0) + f_{2,2}(0) + f_{3,2}(0) &= 0. \end{aligned} \quad (2)$$

Let us define scattering matrices on each bond as:

$$S_j(\zeta) = \begin{pmatrix} a_j(\zeta) & b_j(\zeta) \\ \bar{b}_j(\zeta) & -\bar{a}_j(\zeta) \end{pmatrix}, j = 1, 2, 3. \quad (3)$$

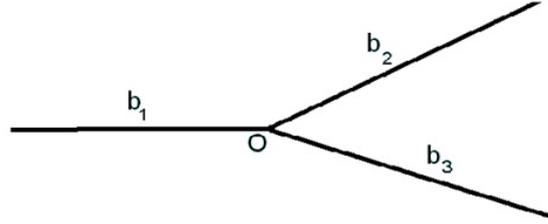


FIG. 1. Star graph

3. The direct scattering problem

We find three solutions $f^{(m)}(x, \zeta) = \{f_1^{(m)}(x_1, \zeta), f_2^{(m)}(x_2, \zeta), f_3^{(m)}(x_3, \zeta)\}$, $m = 1, 2, 3$ for the problem given by Eqs. (1)–(3). Furthermore, we define the functions $\psi_j(x_j, \zeta)$, $\bar{\psi}_j(x_j, \zeta)$ as solutions of the following integral equations:

$$\begin{aligned} \psi_{j,1}(x_j, \zeta) &= \int_{x_j}^{+\infty} q_j(t) e^{-i\zeta(x_j-t)} \psi_{j,2}(t, \zeta) dt, \\ \psi_{j,2}(x_j, \zeta) &= e^{i\zeta x_j} + \int_{x_j}^{+\infty} \int_t^{+\infty} p_j(t) q_j(z) e^{-i\zeta(2t-x_j-z)} \psi_{j,2}(z, \zeta) dz dt, \end{aligned} \quad (4)$$

$$\begin{aligned} \bar{\psi}_{j,1}(x_j, \zeta) &= e^{-i\zeta x_j} + \int_{x_j}^{+\infty} \int_t^{+\infty} q_j(t) p_j(z) e^{i\zeta(2t-x_j-z)} \bar{\psi}_{j,1}(z, \zeta) dz dt, \\ \bar{\psi}_{j,2}(x_j, \zeta) &= \int_{x_j}^{+\infty} p_j(t) e^{i\zeta(x_j-t)} \bar{\psi}_{j,1}(t, \zeta) dt. \end{aligned} \quad (5)$$

Also, we introduce the solutions $\varphi_j(x_j, \zeta)$, $\bar{\varphi}_j(x_j, \zeta)$ obeying the following integral equations:

$$\begin{aligned} \varphi_{j,1}(x_j, \zeta) &= e^{-i\zeta x_j} + \int_0^{x_j} \int_0^t q_j(t) p_j(z) e^{i\zeta(2t-x_j-z)} \varphi_{j,1}(z, \zeta) dz dt, \\ \varphi_{j,2}(x_j, \zeta) &= \int_0^{x_j} p_j(t) e^{i\zeta(x_j-t)} \varphi_{j,1}(t, \zeta) dt, \end{aligned} \quad (6)$$

$$\begin{aligned}\bar{\varphi}_{j,1}(x_j, \zeta) &= \int_0^{x_j} q_j(t) e^{-i\zeta(x_j-t)} \bar{\varphi}_{j,2}(t, \zeta) dt, \\ \bar{\varphi}_{j,2}(x_j, \zeta) &= -e^{i\zeta x_j} + \int_0^{x_j} \int_0^t p_j(t) q_j(z) e^{-i\zeta(2t-x_j-z)} \bar{\varphi}_{j,2}(z, \zeta) dz dt.\end{aligned}\quad (7)$$

It is easy to see that if $q_j, p_j \in L_1$, then the functions $e^{i\zeta x_j} \varphi_j(x_j, \zeta)$, $e^{-i\zeta x_j} \psi_j(x_j, \zeta)$ are analytic on the upper plane $Im\zeta > 0$, $e^{-i\zeta x_j} \bar{\varphi}_j(x_j, \zeta)$, $e^{i\zeta x_j} \bar{\psi}_j(x_j, \zeta)$ are analytic on the lower plane $Im\zeta < 0$.

Since the functions $\psi_j(x_j, \zeta)$, $\bar{\psi}_j(x_j, \zeta)$ obey the boundary conditions:

$$\left. \begin{aligned}\psi_j(x_j, \zeta) &\sim \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\zeta x_j} \\ \bar{\psi}_j(x_j, \zeta) &\sim \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\zeta x_j}\end{aligned}\right\} \text{ at } x_j \rightarrow +\infty, \quad (8)$$

the solutions $\psi_j(x_j, \zeta)$, $\bar{\psi}_j(x_j, \zeta)$ are linearly independent. This follows from the condition for the Wronskian: $W(\psi_j, \bar{\psi}_j) = -1$. Therefore we have:

$$\begin{aligned}\varphi_j &= a_j(\zeta) \bar{\psi}_j + b_j(\zeta) \psi_j, \\ \bar{\varphi}_j &= -\bar{a}_j(\zeta) \psi_j + \bar{b}_j(\zeta) \bar{\psi}_j.\end{aligned}\quad (9)$$

It follows from Eqs. (6)–(7) that functions $\varphi_j(x_j, \zeta)$, $\bar{\varphi}_j(x_j, \zeta)$ satisfy conditions:

$$\begin{aligned}\varphi_j(0, \zeta) &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \\ \bar{\varphi}_j(0, \zeta) &= \begin{pmatrix} 0 \\ -1 \end{pmatrix}.\end{aligned}\quad (10)$$

Furthermore, from $W(\varphi_j, \bar{\varphi}_j) = -1$ we have:

$$a_j \bar{a}_j + b_j \bar{b}_j = 1, \quad (11)$$

which implies that:

$$\begin{aligned}\psi_j(0, \zeta) &= \begin{pmatrix} \bar{b}_j \\ a_j \end{pmatrix}, \\ \bar{\psi}_j(0, \zeta) &= \begin{pmatrix} \bar{a}_j \\ -b_j \end{pmatrix}.\end{aligned}\quad (12)$$

The solutions $f^{(m)}(x, \zeta) = \{f_1^{(m)}(x_1, \zeta), f_2^{(m)}(x_2, \zeta), f_3^{(m)}(x_3, \zeta)\}$, $m = 1, 2, 3$ can be written as:

$$\begin{aligned}f_j^{(m)}(x_j, \zeta) &= t_j^{(m)}(\zeta) \bar{\psi}_j(x_j, \zeta), \quad m \neq j, \quad j = 1, 2, 3, \\ f_m^{(m)}(x_m, \zeta) &= \varphi_m(x_m, \zeta) + r_m^{(m)}(\zeta) \psi_m(x_m, \zeta) e^{-2i\zeta x_m}, \quad m = 1, 2, 3.\end{aligned}\quad (13)$$

The coefficients $r_m^{(m)}$, $t_j^{(m)}$ ($m \neq j$, $m, j = 1, 2, 3$) can be found from the boundary conditions for $f^{(m)}(x, \zeta)$. For example, at $m=1$ we have:

$$\begin{aligned}\varphi_{1,1}(0, \zeta) + r_1^{(1)}(\zeta) \psi_{1,1}(0, \zeta) &= t_2^{(1)}(\zeta) \bar{\psi}_{2,1}(0, \zeta) = t_3^{(1)}(\zeta) \bar{\psi}_{3,1}(0, \zeta), \\ \varphi_{1,2}(0, \zeta) + r_1^{(1)}(\zeta) \psi_{1,2}(0, \zeta) + t_2^{(1)}(\zeta) \bar{\psi}_{2,2}(0, \zeta) + t_3^{(1)}(\zeta) \bar{\psi}_{3,2}(0, \zeta) &= 0.\end{aligned}\quad (14)$$

Using Eqs. (11)-(12), one can obtain:

$$\begin{aligned} r_1^{(1)}(\zeta) &= \frac{\bar{a}_2 b_3 + b_2 \bar{a}_3}{a_1 \bar{a}_2 \bar{a}_3 - b_1 \bar{a}_2 b_3 - b_1 b_2 \bar{a}_3}, \\ t_2^{(1)}(\zeta) &= \frac{a_1 \bar{a}_3}{a_1 \bar{a}_2 \bar{a}_3 - b_1 \bar{a}_2 b_3 - b_1 b_2 \bar{a}_3}, \\ t_3^{(1)}(\zeta) &= \frac{a_1 \bar{a}_2}{a_1 \bar{a}_2 \bar{a}_3 - b_1 \bar{a}_2 b_3 - b_1 b_2 \bar{a}_3}. \end{aligned} \quad (15)$$

The above analysis is usually called the direct scattering problem. In the following, we will treat the inverse scattering problem.

4. The inverse scattering problem

Using the following integral representations for the functions $\psi_j(x_j, \zeta)$, $\bar{\psi}_j(x_j, \zeta)$:

$$\psi_j(x, \zeta) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\zeta x_j} + \int_{x_j}^{+\infty} K_j(x_j, s) e^{i\zeta s} ds, \quad (16)$$

$$\bar{\psi}_j(x, \zeta) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\zeta x_j} + \int_{x_j}^{+\infty} \bar{K}_j(x_j, s) e^{-i\zeta s} ds, \quad (17)$$

where $K_j(x_j, s) = \begin{pmatrix} K_{j,1}(x_j, s) \\ K_{j,2}(x_j, s) \end{pmatrix}$, $\bar{K}_j(x_j, s) = \begin{pmatrix} \bar{K}_{j,1}(x_j, s) \\ \bar{K}_{j,2}(x_j, s) \end{pmatrix}$ are two-component vectors.

To obey the boundary conditions (8), we assume that $K_j(x_j, s) = 0$ at $x_j > s$. Now, we will prove the existence of representations (16)–(17). To do that, it is enough to insert Eqs. (16)–(17) into (1). Then, from Eq. (16) we obtain:

$$\begin{aligned} &\int_{x_j}^{+\infty} e^{i\zeta s} [(\partial_{x_j} - \partial_s) K_{j,1}(x_j, s) - q_j(x_j) K_{j,2}(x_j, s)] ds - \\ &- [q_j(x_j) + 2K_{j,1}(x_j, x_j)] e^{i\zeta x_j} + \lim_{s \rightarrow \infty} [K_{j,1}(x_j, s) e^{i\zeta s}] = 0 \end{aligned} \quad (18)$$

$$\begin{aligned} &\int_{x_j}^{+\infty} e^{i\zeta s} [(\partial_{x_j} + \partial_s) K_{j,2}(x_j, s) - p_j(x_j) K_{j,1}(x_j, s)] ds - \\ &- \lim_{s \rightarrow \infty} [K_{j,2}(x_j, s) e^{i\zeta s}] = 0 \end{aligned} \quad (19)$$

Thus, for the existence of representations (16)–(17), it is necessary and sufficient that functions $K_j(x_j, s)$ obey the following equations:

$$\begin{aligned} (\partial_{x_j} - \partial_s) K_{j,1}(x_j, s) - q_j(x_j) K_{j,2}(x_j, s) &= 0, \\ (\partial_{x_j} + \partial_s) K_{j,2}(x_j, s) - p_j(x_j) K_{j,1}(x_j, s) &= 0, \end{aligned} \quad (20)$$

with the boundary conditions:

$$\begin{aligned} K_{j,1}(x_j, x_j) &= -\frac{1}{2} q_j(x_j), \\ \lim_{s \rightarrow +\infty} K_j(x_j, s) &= 0. \end{aligned} \quad (21)$$

Solutions for problems (20)–(21) (the Goursah problem) exist and are unique. The above treatment can be done for the function $\bar{K}_j(x_j, s)$, as well.

Let given C_j contour that begins from $-\infty + i0^+$, rounds above all zeros of $a_j(\zeta)$ and poles of $r_j^{(j)}(\zeta)$, and ends at $+\infty + i0^+$. We introduce the following function:

$$g_1^{(1)}(x_1, \zeta) = \varphi_1(x_1, \zeta) + r_1^{(1)}(\zeta) \psi_1(x_1, \zeta) e^{-2i\zeta x_1} \quad (22)$$

Then, from Eq. (9) we have:

$$\begin{aligned} g_1^{(1)}(x_1, \zeta) &= \varphi_1(x_1, \zeta) + r_1^{(1)}(\zeta) \psi_1(x_1, \zeta) e^{-2i\zeta x_1} = \\ &= a_1(\zeta) \bar{\psi}_1(x_1, \zeta) + \left\{ b_1(\zeta) + r_1^{(1)}(\zeta) e^{-2i\zeta x_1} \right\} \psi_1(x_1, \zeta). \end{aligned} \quad (23)$$

The last equation can be rewritten as:

$$\begin{aligned} \frac{g_1^{(1)}(x_1, \zeta)}{a_1(\zeta)} &= \bar{\psi}_1(x_1, \zeta) + \left\{ \frac{b_1(\zeta)}{a_1(\zeta)} + \frac{r_1^{(1)}(\zeta)}{a_1(\zeta)} e^{-2i\zeta x_1} \right\} \psi_1(x_1, \zeta) = \\ &= \bar{\psi}_1(x_1, \zeta) + R_1^{(1)}(x_1, \zeta) \psi_1(x_1, \zeta). \end{aligned} \tag{24}$$

where $R_1^{(1)}(x_1, \zeta) = \frac{b_1(\zeta)}{a_1(\zeta)} + \frac{r_1^{(1)}(\zeta)}{a_1(\zeta)} e^{-2i\zeta x_1}$. Inserting Eqs. (16) and (17) into (24):

$$\begin{aligned} \frac{g_1^{(1)}(x_1, \zeta)}{a_1(\zeta)} &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} e^{-i\zeta x_1} + \int_{x_1}^{+\infty} \bar{K}_1(x_1, s) e^{-i\zeta s} ds + \\ &+ R_1^{(1)}(x_1, \zeta) \left(\begin{pmatrix} 0 \\ 1 \end{pmatrix} e^{i\zeta x_1} + \int_{x_1}^{+\infty} K_1(x_1, s) e^{i\zeta s} ds \right), \end{aligned} \tag{25}$$

multiplying Eq. (25) by $\frac{1}{2\pi} e^{i\zeta y} d\zeta$ and integrating along the contour C_1 at $y > x_1$, by taking into account the representation $\delta(x) = \frac{1}{2\pi} \int_{C_1} e^{i\zeta x} d\zeta$ the Dirac- δ function we have:

$$\begin{aligned} \frac{1}{2\pi} \int_{C_1} \frac{g_1^{(1)}(x_1, \zeta)}{a_1(\zeta)} e^{i\zeta y} d\zeta &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \delta(y - x_1) + \int_{x_1}^{+\infty} \bar{K}_1(x_1, s) \delta(y - s) ds + \\ &+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \left[\frac{1}{2\pi} \int_{C_1} R_1^{(1)}(x_1, \zeta) e^{i\zeta(x_1+y)} d\zeta \right] + \int_{x_1}^{+\infty} K_1(x_1, s) \left[\frac{1}{2\pi} \int_{C_1} R_1^{(1)}(x_1, \zeta) e^{i\zeta(y+s)} d\zeta \right] ds. \end{aligned} \tag{26}$$

Since the functions $e^{i\zeta x_j} \varphi_j(x_j, \zeta)$, $e^{-i\zeta x_j} \psi_j(x_j, \zeta)$ are analytic on the upper half of the plane $Im\zeta > 0$, $y > x_1$ and the contour C_1 round above zeros of $a_1(\zeta)$ and poles of $r_1^{(1)}(\zeta)$, the integral of the left hand side of equality (26) is equal to zero. Therefore we get:

$$\bar{K}_1(x_1, y) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} F_1(x_1, x_1 + y) + \int_{x_1}^{+\infty} K_1(x_1, s) F_1(x_1, y + s) ds = 0, \tag{27}$$

where $F_1(x, y) = \frac{1}{2\pi} \int_{C_1} R_1^{(1)}(x, \zeta) e^{i\zeta y} d\zeta$.

Repeating the same procedure for the function $\bar{f}_1^{(1)}(x, \zeta)$, we obtain:

$$K_1(x_1, y) - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \bar{F}_1(x_1, x_1 + y) - \int_{x_1}^{+\infty} \bar{K}_1(x_1, s) \bar{F}_1(x_1, y + s) ds = 0, \tag{28}$$

where $\bar{F}_1(x, y) = \frac{1}{2\pi} \int_{\bar{C}_1} \bar{R}_1^{(1)}(x, \zeta) e^{-i\zeta y} d\zeta$ and \bar{C}_1 is the same contour as C_1 , but rounds below the zeros of $\bar{a}_1(\zeta)$ and poles of $\bar{r}_1^{(1)}(\zeta)$.

Similarly, one can obtain the following equations for the functions K_2 and K_3 :

$$\begin{aligned} \bar{K}_j(x_j, y) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} F_j(x_j, x_j + y) + \int_{x_j}^{+\infty} K_j(x_j, s) F_j(x_j, y + s) ds &= 0, \\ K_j(x_j, y) - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \bar{F}_j(x_j, x_j + y) - \int_{x_j}^{+\infty} \bar{K}_j(x_j, s) \bar{F}_j(x_j, y + s) ds &= 0, \end{aligned} \tag{29}$$

where

$$\begin{aligned} F_j(x, y) &= \frac{1}{2\pi} \int_{C_j} R_j^{(j)}(x, \zeta) e^{i\zeta y} d\zeta, \bar{F}_j(x, y) = \frac{1}{2\pi} \int_{\bar{C}_j} \bar{R}_j^{(j)}(x, \zeta) e^{-i\zeta y} d\zeta, \\ R_j^{(j)}(x, \zeta) &= \frac{b_j(\zeta)}{a_j(\zeta)} + \frac{r_j^{(j)}(\zeta)}{a_j(\zeta)} e^{-2i\zeta x_j}, \bar{R}_j^{(j)}(x, \zeta) = \frac{\bar{b}_j(\zeta)}{\bar{a}_j(\zeta)} + \frac{\bar{r}_j^{(j)}(\zeta)}{\bar{a}_j(\zeta)} e^{2i\zeta x_j}, j = 2, 3. \end{aligned}$$

From Eq. (21), we obtain:

$$q_j(x_j) = -2K_{j,1}(x_j, x_j). \quad (30)$$

Using the same approach used for Eqs. (18) and (19), we get the following formula for the potential $p_j(x_j)$:

$$p_j(x_j) = -2\bar{K}_{j,2}(x_j, x_j). \quad (31)$$

5. Conclusions

In this paper, we developed a procedure for finding the unknown potential in the Dirac equation on metric graphs using a given scattering matrix. In this case, the solutions for the inverse scattering problem were obtained by solving Gelfand-Levitan-Marchenko integral equations. The above results can be used in different practically important problems for emerging nanotechnologies. In addition, they can be useful for solving some nonlinear evolution equations on metric graphs such as nonlinear Schrodinger and KdV equations.

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