INVERSE SCATTERING ON THE QUANTUM GRAPH FOR GRAPHENE

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Abstract. We consider the inverse scattering on the quantum graph associated with the hexagonal lattice. Assuming that the potentials on the edges are compactly supported and symmetric, we show that the S-matrix for all energies in any given open set in the continuous spectrum determines the potentials.

1. Introduction

In this paper, we are concerned with a family of one-dimensional Schrödinger operators $-d^2/dz^2 + q_e(z)$ defined on the edges of the hexagonal lattice assuming the Kirchhoff condition on the vertices. Here, $z$ varies over the interval $(0, 1)$ and $e \in \mathcal{E}$, $\mathcal{E}$ being the set of all edges of the hexagonal lattice. The following assumptions are imposed on the potentials.

(Q-1) $q_e(z)$ is real-valued, and $q_e \in L^2(0, 1)$.

(Q-2) $q_e(z) = 0$ on $(0, 1)$ except for a finite number of edges.

(Q-3) $q_e(z) = q_e(1 - z)$ for $z \in (0, 1)$.

Under these assumptions, the Schrödinger operator

$$\hat{H}_{\mathcal{E}} = \left\{ -\frac{d^2}{dz^2} + q_e(z); \ e \in \mathcal{E} \right\}$$

is self-adjoint with essential spectrum $\sigma_e(\hat{H}_{\mathcal{E}}) = [0, \infty)$. There exists a discrete (but infinite) subset $\mathcal{T} \subset \mathbb{R}$ such that $\sigma_e(\hat{H}_{\mathcal{E}}) \setminus \mathcal{T}$ is absolutely continuous. We can then define Heisenberg’s S-matrix $S(\lambda)$ for $\lambda \in (0, \infty) \setminus \mathcal{T}$. The following two theorems are the main purpose of this paper.

Theorem 1.1. Assume (Q-1), (Q-2) and (Q-3). Then, given any open interval $I \subset (0, \infty) \setminus \mathcal{T}$, and the S-matrix $S(\lambda)$ for all $\lambda \in I$, one can uniquely reconstruct the potential $q_e(z)$ for all $e \in \mathcal{E}$.

Under our assumptions (Q-1), (Q-2), (Q-3), $S(\lambda)$ is meromorphic in the complex domain $\{\text{Re}\lambda > 0\}$ with possible branch points at $\mathcal{T}$. Therefore, the assumption of Theorem 1.1 is equivalent to the condition that we are given $S(\lambda)$ for all $\lambda \in (0, \infty) \setminus \mathcal{T}$. One can also deal with perturbation of periodic edge potentials.

Date: January 4, 2022.
2000 Mathematics Subject Classification. Primary 81U40, Secondary 47A40.
Key words and phrases. Schrödinger operator, lattice, quantum graph, S-matrix, inverse scattering.
Theorem 1.2. Assume (Q-1) and (Q-3). Assume that we are given a real $q_0(z) \in L^2(0,1)$ satisfying $q_0(z) = q_0(1-z)$ and $q_e(z) = q_0(z)$ on $(0,1)$ except for a finite number of edges $e \in E$. Given an open interval $I \subset \sigma_c(\tilde{H}_G) \setminus \mathcal{T}$ and the S-matrix $S(\lambda)$ for all $\lambda \in I$, one can uniquely reconstruct the potential $q_e(z)$ for all edges $e \in E$.

It is well-known that there is a close connection between the Laplacian on the quantum graph and that on the associated vertex set (see e.g. [9], [10], [36], [43], [15]). Therefore, the basic results on the spectral theory for the quantum graph are derived from those for the associated discrete Laplacian. Sections 2, 3 and 4 are devoted to this transfer. In particular, we show that the S-matrix for the whole quantum graph determines the Dirichlet-to-Neumann map in a finite region on which perturbations are confined (Theorem 1.3). The inverse problem is solved in §5 by using the classical theorem of Borg [13].

The monographs [21], [22], [18], [46], [10] are expositions of the graph spectra and related problems from algebraic, geometric, physical and functional analytic view points with slight different emphasis on them. The present situation of the study of quantum graph is well explained in the above mentioned books, especially in Chapter 7 of [10] together with an abundance of references therein. See also [25], [42] for more recent results. Plenty of deep results for the inverse problem on the quantum graph have been presented. See e.g. [9], [44], [26], [2], [27], [3], [4], [23], [17], [7], [50], [40], [53], [12] and other papers cited in the above books. We must also mention [19], [20] on inverse problem for the planar discrete graph. There are also many recent works on the spectral and (inverse) scattering theory for discrete Schrödinger operators on perturbed periodic structures [31], [32], [33], [20], [49], [41], [20], [2], [27], [3], [4], [23]. In this paper, we use our previous results [3], [4] in the transfer from the discrete Laplacian to the quantum graph. Many parts of this paper, especially the part dealing with the the forward problem, can be generalized to more general lattices, which can be seen in [6].

For a measure space $(M, d\mu)$, let $L^2(M; C^n; d\mu)$ be the space of the $C^n$-valued functions on $M$. It is often denoted by $L^2(M; C^n)$ or $L^2(M)$ when $n = 1$. For Banach spaces $X$ and $Y$, let $\mathcal{B}(X; Y)$ be the set of all bounded operators from $X$ to $Y$, and $\mathcal{B}(X) = \mathcal{B}(X; X)$.

2. Quantum graph

2.1. Vertex Laplacian. We follow the standard formulation of metric graph (see e.g. [36] or [43]). In $\mathbb{R}^2$, let $p^{(1)} = (1, 0)$, $p^{(2)} = (2, 0)$, $v_1 = \left(\frac{3}{2}, -\sqrt{\frac{3}{2}}\right)$, $v_2 = \left(\frac{3}{2}, \sqrt{\frac{3}{2}}\right)$, and $v(n) = n_1v_1 + n_2v_2$ for $n = (n_1, n_2)$. We define the vertex set $V$ by

$$V = \bigcup_{i=1}^{2} V_i, \quad V_i = \{p^{(i)} + v(n) : n \in \mathbb{Z}^2\}.$$ 

Let $I_2 : L^2_{loc}(V; \mathbb{C}) \to L^2_{loc}(\mathbb{Z}^2; \mathbb{C}^2)$ be defined by

$$I_2 : \hat{f}(v) \to (I_2 \hat{f})(n) = \left(\hat{f}_1(n), \hat{f}_2(n)\right) = \left(\hat{f}(p^{(1)} + v(n)), \hat{f}(p^{(2)} + v(n))\right).$$

For the figure of hexagonal lattice, see e.g. [36] or [6].
We often write \( \hat{f}(n) \) instead of \((I_2 \hat{f})(n)\). The Laplacian is defined by
\[
(\hat{\Delta_v} \hat{f})(n) = \frac{1}{3} \left( \hat{f}_2(n_1, n_2) + \hat{f}_2(n_1 - 1, n_2) + \hat{f}_2(n_1, n_2 - 1) \right),
\]
which is self-adjoint on \( L^2(\mathcal{V}) \) equipped with the inner product
\[
(\hat{f}, \hat{g}) = 3 \sum_{n \in \mathbb{Z}^2} \hat{f}(n) \cdot \overline{\hat{g}(n)}.
\]
Define the discrete Fourier transform \( \mathcal{U}_V : L^2(\mathbb{Z}^2; \mathbb{C}^2) \to L^2(\mathbb{T}^2; \mathbb{C}^2) \) by
\[
(\mathcal{U}_V \hat{f})(x) = \sqrt{3} (2\pi)^{-1} \sum_{n \in \mathbb{Z}^2} e^{inx} \hat{f}(n), \quad x \in \mathbb{T}^2 = \mathbb{R}^2/(2\pi \mathbb{Z})^2.
\]
Then on \( L^2(\mathbb{T}^2; \mathbb{C}^2) \), \( \mathcal{U}_V(-\Delta_v) \mathcal{U}_V^* \) is the operator of multiplication by
\[
H_0(x) = -\frac{1}{3} \begin{pmatrix} 1 & 0 \\ 1 + e^{-ix_1} + e^{-ix_2} & 1 + e^{ix_1} + e^{ix_2} \end{pmatrix}.
\]
The edge set \( \mathcal{E} \) consists of the segments \( e \) of length 1 with end points in \( \mathcal{V} \), endowed with arclength metric, as well as the identification with the interval \((0, 1) : e = \{(1 - z)e(0) + ze(1) : 0 \leq z \leq 1\}, \) where \( e(0), e(1) \in \mathcal{V} \). We put
\[
\mathcal{E}_v = \mathcal{E}_v(0) \cup \mathcal{E}_v(1), \quad \mathcal{E}_v(i) = \{e \in \mathcal{E} : e(i) = v\}, \quad i = 0, 1.
\]
For a function \( \tilde{f} \) on an edge \( e \in \mathcal{E}_v \), we define \( \tilde{f}'(v) \) to be the derivative at \( v \) along \( e \). A function \( \tilde{f} = \{\tilde{f}_e\}_{e \in \mathcal{E}} \) defined on \( \mathcal{E} \) is said to satisfy the Kirchhoff condition if \(\text{(K-1)} \) \( \hat{f} \) is continuous on \( \mathcal{E} \).
\(\text{(K-2)} \) \( \tilde{f}_e \in C^1([0, 1]) \) on each edge \( e \in \mathcal{E} \), and \( \sum_{e \in \mathcal{E}_v} \tilde{f}_e = 0 \) at any vertex \( v \in \mathcal{V} \).

### 2.2. Edge Laplacian

We consider 1-dimensional Schrödinger operators
\[
\begin{align*}
\hat{h}_e^{(0)} &= -d^2/dz^2, & \hat{h}_e &= \hat{h}_e^{(0)} + q_e(z)
\end{align*}
\]
on \( L^2(\mathbb{T}^2) \). We define the Hilbert space \( L^2(\mathcal{E}) \) of \( \mathbb{C} \)-valued \( L^2 \)-functions \( \tilde{f} = \{\tilde{f}_e\}_{e \in \mathcal{E}} \) on the edge set \( \mathcal{E} \) : \( L^2(\mathcal{E}) = \oplus_{e \in \mathcal{E}} L^2_0(\mathbb{T}^2) \) equipped with the inner product
\[
(\tilde{f}, \tilde{g})_{L^2(\mathcal{E})} = \sum_{e \in \mathcal{E}} (\tilde{f}_e, \tilde{g}_e)_{L^2(\mathbb{T}^2)}.
\]
Define the Hamiltonian
\[
\hat{H}_{\mathcal{E}} : \tilde{u} = \{\tilde{u}_e\}_{e \in \mathcal{E}} \to \{\hat{h}_e \tilde{u}_e\}_{e \in \mathcal{E}}
\]
with domain \( D(\hat{H}_{\mathcal{E}}) \) consisting of \( \tilde{u}_e \in H^2(\mathbb{T}^2) \)\(^3\) satisfying the Kirchhoff condition \(\text{(K-1)}, \text{(K-2)}\) and \( \sum_{e \in \mathcal{E}} \|h_e \tilde{u}_e\|_{L^2(\mathbb{T}^2)}^2 < \infty \). Then, \( \hat{H}_{\mathcal{E}} \) is self-adjoint in \( L^2(\mathcal{E}) \).
When \( q_e = 0 \), \( \hat{H}_{\mathcal{E}} \) is denoted by \( \hat{H}_{\mathcal{E}}^{(0)} \) or \( -\hat{\Delta}_{\mathcal{E}} \), i.e.
\[
( -\hat{\Delta}_{\mathcal{E}} \tilde{u})_e(z) = -\frac{d^2}{dz^2} \tilde{u}_e(z), \quad e \in \mathcal{E}.
\]
We call it edge Laplacian. Let \( q_e \) be the multiplication operator defined by
\[
(q_e \tilde{f}_e)(z) = q_e(z) \tilde{f}_e(z), \quad e \in \mathcal{E}.
\]
\(^2\)Note that the degree of each vertex in \( \mathcal{V} \) is 3.
\(^3\)This is the Sobolev space of order 2.
Then $\hat{H}_\varepsilon = \hat{H}_\varepsilon^{(0)} + q_\varepsilon$. We put
\begin{equation}
(2.5) \quad \hat{R}_\varepsilon^{(0)}(\lambda) = (\hat{H}_\varepsilon^{(0)} - \lambda)^{-1}, \quad \hat{R}_\varepsilon(\lambda) = (\hat{H}_\varepsilon - \lambda)^{-1}.
\end{equation}

Let $-(d^2/dz^2)_D$ be the Laplacian on $(0,1)$ with boundary condition $u(0) = u(1) = 0$. Let $\phi_{e0}(z, \lambda), \phi_{e1}(z, \lambda)$ be the solutions of
\begin{equation}
(2.6) \quad (- d^2/dz^2 + q_e(z) - \lambda)\phi = 0
\end{equation}
with initial data
\[
\begin{cases}
\phi_{e0}(0, \lambda) = 0, & \phi_{e1}(1, \lambda) = 0, \\
\phi'_{e0}(0, \lambda) = 1, & \phi'_{e1}(1, \lambda) = -1.
\end{cases}
\]
In the following, we assume that
\[
\lambda \notin \bigcup_{e \in \mathcal{E}} \sigma(-(d^2/dz^2)_D + q_e(z)),
\]
which guarantees that $\phi_{e0}(1, \lambda) \neq 0$ and $\phi_{e1}(0, \lambda) \neq 0$. If $w, v \in \mathcal{V}$ are two end points of an edge $e \in \mathcal{E}$, we define $\psi_{vw}(z, \lambda)$ by
\[
\psi_{vw}(z, \lambda) = \begin{cases}
\phi_{e0}(z, \lambda), & \text{if } e(0) = v, \\
\phi_{e1}(z, \lambda), & \text{if } e(0) = w.
\end{cases}
\]
Note that by the assumption (Q-3), we have $\phi_{e0}(z, \lambda) = \phi_{e1}(1-z, \lambda)$, hence
\[
\psi_{vw}(1, \lambda) = \psi_{vw}(1, \lambda).
\]

**Definition 2.1.** We define the reduced vertex Laplacian $\hat{\Delta}_{\mathcal{V}, \lambda}$ on $\mathcal{V}$ by
\begin{equation}
(2.7) \quad (\hat{\Delta}_{\mathcal{V}, \lambda} \hat{u})(v) = \frac{1}{3} \sum_{v \sim w \in \mathcal{V}} \frac{1}{\psi_{vw}(1, \lambda)} \hat{u}(w), \quad v \in \mathcal{V}
\end{equation}
for $\hat{u} \in L^2_{\text{loc}}(\mathcal{V})$, where $w \sim v$ means that there exists an edge $e \in \mathcal{E}$ such that $v, w$ are end points of $e$. We also define a scalar multiplication operator:
\[
(\hat{Q}_{\mathcal{V}, \lambda} \hat{u})(v) = \hat{Q}_{v, \lambda}(v) \hat{u}(v),
\]
where
\begin{equation}
(2.8) \quad \hat{Q}_{v, \lambda}(v) = \frac{1}{3} \sum_{w \in \mathcal{E}_v} \frac{\psi'_{vw}(1, \lambda)}{\psi_{vw}(1, \lambda)}.
\end{equation}

The resolvent $r_e(\lambda) = (- (d^2/dz^2)_D + q_e(z) - \lambda)^{-1}$ is written as
\[
(r_e(\lambda) \hat{f})(v) = \int_0^z \frac{\phi_{e1}(z, \lambda)\phi_{e0}(t, \lambda)}{\phi_{e0}(1, \lambda)} \hat{f}(t)dt + \int_z^1 \frac{\phi_{e0}(z, \lambda)\phi_{e1}(t, \lambda)}{\phi_{e1}(0, \lambda)} \hat{f}(t)dt.
\]
We put
\[
\Phi_{e0}(\lambda) \hat{f} = \frac{d}{dz} (r_e(\lambda) \hat{f}) \bigg|_{z=0} = \int_0^1 \frac{\phi_{e1}(t, \lambda)}{\phi_{e1}(0, \lambda)} \hat{f}(t)dt,
\]
\[
\Phi_{e1}(\lambda) \hat{f} = - \frac{d}{dz} (r_e(\lambda) \hat{f}) \bigg|_{z=1} = \int_0^1 \frac{\phi_{e0}(t, \lambda)}{\phi_{e0}(1, \lambda)} \hat{f}(t)dt,
\]
and define an operator $\hat{T}_{\mathcal{V}}(\lambda) : L^2_{\text{loc}}(\mathcal{E}) \to L^2_{\text{loc}}(\mathcal{V})$ by
\begin{equation}
(2.9) \quad (\hat{T}_{\mathcal{V}}(\lambda) \hat{f})(v) = \frac{1}{3} \left( \sum_{e \in \mathcal{E}_v(1)} \Phi_{e1}(\lambda) \hat{f}_e + \sum_{e \in \mathcal{E}_v(0)} \Phi_{e0}(\lambda) \hat{f}_e \right), \quad v \in \mathcal{V}.
\end{equation}
Let \( \hat{u} = \{ \hat{u}_e \}_{e \in \mathcal{E}} \) be a solution to the equation \((\hat{H}_\mathcal{E} - \lambda)\hat{u} = \hat{f} \). On each edge \( e \in \mathcal{E} \), it is written as
\[
\hat{u}_e(z, \lambda) = \Phi_{e_1}(\lambda)^*c_e(1, \lambda) + \Phi_{e_0}(\lambda)^*c_e(0, \lambda) + r_e(\lambda)\hat{f}_e
\]
with some constants \( c_e(0, \lambda), c_e(1, \lambda) \). Then, the condition (K-1) is satisfied if and only if for two edges \( e, e' \in \mathcal{E} \) and \( p, q = 0, 1 \), \( c_e(p, \lambda) = c_{e'}(q, \lambda) \) if \( e(p) = e'(q) \).

**Lemma 2.2.** Let \( \hat{u}|_\mathcal{V} \) be the restriction of \( \hat{u} \) on \( \mathcal{V} \). Then the condition (K-2) is rewritten as
\[
(\hat{\Delta}_{\mathcal{V}, \lambda} + \hat{Q}_{\mathcal{V}, \lambda}) \hat{u}|_\mathcal{V} = \hat{T}_\mathcal{V}(\lambda)\hat{f}.
\]
This lemma is well-known. In fact, (K-2) is rewritten as
\[
- \sum_{e \in \mathcal{E}, (0) \in E} \frac{1}{\phi_{e_0}(1, \lambda)} c_e(1, \lambda) - \sum_{e \in \mathcal{E}, (1) \in E} \frac{1}{\phi_{e_1}(0, \lambda)} c_e(0, \lambda)
- \sum_{e \in \mathcal{E}, (0) \in E} \frac{\phi'_{e_1}(0, \lambda)}{\phi_{e_0}(1, \lambda)} c_e(0, \lambda) + \sum_{e \in \mathcal{E}, (1) \in E} \frac{\phi'_{e_0}(1, \lambda)}{\phi_{e_1}(0, \lambda)} c_e(1, \lambda)
= \sum_{e \in \mathcal{E}, (1) \in E} \Phi_{e_1}(\lambda)\hat{f}_e + \sum_{e \in \mathcal{E}, (0) \in E} \Phi_{e_0}(\lambda)\hat{f}_e,
\]
which implies \((2.11)\). Therefore, \( \hat{u}|_\mathcal{V} \), should be written as
\[
(\hat{\Delta}_{\mathcal{V}, \lambda} + \hat{Q}_{\mathcal{V}, \lambda})^{-1} \hat{T}_\mathcal{V}(\lambda)\hat{f}.
\]
Here, we must be careful about the operator \((\hat{\Delta}_{\mathcal{V}, \lambda} + \hat{Q}_{\mathcal{V}, \lambda})^{-1} \). For \( \lambda \notin \mathbb{R} \), the operator \(\hat{\Delta}_{\mathcal{V}, \lambda} + \hat{Q}_{\mathcal{V}, \lambda} \) has complex coefficients, hence is not self-adjoint. Therefore, the existence of its inverse is not obvious. We discuss the validity of \((2.12)\) in Subsection 3.1. For the moment, we admit it as a formal formula.

Noting that \( \hat{T}_\mathcal{V}(\lambda)^* : L^2_{\text{loc}}(\mathcal{V}) \to L^2_{\text{loc}}(\mathcal{E}) \) is written as (see \((2.10)\))
\[
(\hat{T}_\mathcal{V}(\lambda)^*\hat{u})(e) = \Phi_{e_1}(\lambda)^*\hat{u}(e(1)) + \Phi_{e_0}(\lambda)^*\hat{u}(e(0)),
\]
we have the following lemma by \((2.11)\). Let \( r_\mathcal{E}(\lambda) \in \mathcal{B}(L^2(\mathcal{E})) \) be defined by
\[
r_\mathcal{E}(\lambda)\hat{f} = r_\mathcal{E}(\lambda)\hat{f}_e, \quad \text{on} \quad e.
\]

**Lemma 2.3.** The resolvent of \( \hat{H}_\mathcal{E} \) is written as
\[
\hat{R}_\mathcal{E}(\lambda) = \hat{T}_\mathcal{V}(\lambda)^* \left( -\hat{\Delta}_{\mathcal{V}, \lambda} + \hat{Q}_{\mathcal{V}, \lambda} \right)^{-1} \hat{T}_\mathcal{V}(\lambda) + r_\mathcal{E}(\lambda).
\]
For the unperturbed case \( \hat{q}_\mathcal{E} = 0 \), we put the superscript \((0)\) for every term. Then, we have
\[
\phi_{e_0}^{(0)}(z) = \frac{\sin \sqrt{\lambda} z}{\sqrt{\lambda}}, \quad \phi_{e_1}^{(0)}(z) = \frac{\sin \sqrt{\lambda}(1 - z)}{\sqrt{\lambda}}.
\]
Therefore by \((2.7)\) and \((2.8)\),
\[
\left( \hat{\Delta}_{\mathcal{V}, \lambda}^{(0)} \hat{u} \right)(v) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \frac{1}{3} \sum_{w \in \mathcal{E}_v} \hat{u}(w) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} (\hat{\Delta}_\mathcal{V} \hat{u})(v),
\]
Lemma 3.3 of [3] implies that
\[ (2.17) \quad \hat{R}_E^{(0)}(\lambda) = \hat{T}_V^{(0)}(\lambda) \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} (\lambda - \Delta_V + \cos \sqrt{\lambda})^{-1} \hat{T}_V^{(0)}(\lambda) + r_E^{(0)}(\lambda). \]

3. RESOLVENT ESTIMATES

3.1. Limiting absorption principle. In our previous work [3], we proved resolvent estimates of vertex Laplacian \(-\Delta_V\) in weighted \(L^2\) spaces or Besov spaces of \(C\)-valued functions. By virtue of the formulas (2.13) and (2.17), the resolvent estimates of edge Laplacian are derived from those of vertex Laplacian using the space of \(L^2(\mathcal{E})\)-valued functions. By virtue of the formulas (2.13) and (2.17), the resolvent estimates of edge Laplacian are derived from those of vertex Laplacian using the space of \(L^2(\mathcal{E})\)-valued functions on the edge set \(\mathcal{E}\) defined as follows.

For \(e \in \mathcal{E}\), we put
\[ c(e) = \frac{1}{2} (e(0) + e(1)). \]

Letting \(r_{j-1} = 0, r_j = 2^j (j \geq 0)\), we define
\[ \hat{B}(\mathcal{E}) \ni \hat{f} \iff \|\hat{f}\|_{\hat{B}(\mathcal{E})} = \sum_{j=0}^{\infty} r_j^{1/2} \left( \sum_{r_j-1 \leq |e| < r_j} \|\hat{f}_e\|_{L^2(0,1)}^2 \right)^{1/2} < \infty, \]
\[ \hat{B}^*(\mathcal{E}) \ni \hat{f} \iff \|\hat{f}\|_{\hat{B}^*(\mathcal{E})}^2 = \sup R > 1 \sum_{|e| < R} \|\hat{f}_e\|_{L^2(0,1)}^2 < \infty, \]
\[ \hat{B}_0^*(\mathcal{E}) \ni \hat{f} \iff \lim_{R \to \infty} \frac{1}{R} \sum_{|e| < R} \|\hat{f}_e\|_{L^2(0,1)}^2 = 0. \]
\[ \hat{L}^{2,s}(\mathcal{E}) \ni \hat{f} \iff \sum_{e \in \mathcal{E}} (1 + |e(0)|^2)^s \|\hat{f}_e\|_{L^2(0,1)}^2 < \infty, \quad s \in \mathbb{R}. \]

The function spaces \(\hat{B}(\mathcal{V})\) etc on the vertex set \(\mathcal{V}\) are defined similarly for \(C\)-valued functions with \(c(e)\) and \(\hat{f}_e\) replaced by \(v\) and \(\hat{f}(v)\), \(v \in \mathcal{V}\), respectively.

Taking account of (2.17), we define the characteristic surface of \(-\Delta_V^{(0)}\) by
\[ M_{\lambda} = \{ x \in \mathbb{T}^2 \mid \det(H_0(x) + \cos \sqrt{\lambda}) = 0 \}. \]

Lemma 3.3 of [3] implies that \(M_{\lambda}\) is smooth if \(\cos \sqrt{\lambda} \neq 0, \pm 1/2, \pm 1, \lambda \in \mathbb{R}\). Note that
\[ \sigma(-(d^2/dz^2)_D) = \{ (\pi n)^2 \mid n \in \mathbb{Z} \} = \{ \lambda \mid \cos \sqrt{\lambda} = \pm 1 \}. \]

We put
\[ \mathcal{T}^{(0)} = \{ \lambda \mid \cos \sqrt{\lambda} = 0, \pm 1/3, \pm 1 \}, \]
\[ \mathcal{T} = \mathcal{T}^{(0)} \cup (\bigcup_{e \in \mathcal{E}} \sigma(-(d^2/dz^2)_D + q_E(e))). \]

Let us return to the problem for \((-\Delta_{V,\lambda} + \hat{Q}_{V,\lambda})^{-1}\) we have encountered in \(\S 2\). First we consider the case \(q_E = 0\). For \(\lambda \in (0, \infty) \setminus \mathcal{T}^{(0)}\), arguing as in the proof of Theorem 7.7 in [3], one can prove the uniform boundedness of \((-\Delta_{V,\lambda} + \hat{Q}_{V,\lambda,i})^{-1}\) and the existence of strong limit in \(B(L^{2,s}(\mathcal{V}); L^{2,-s}(\mathcal{V}))\), \(s > 1/2\), and weak *-limit in \(B(B(\mathcal{V}); B^*(\mathcal{V}))\) of \((-\Delta_{V,\lambda} + \hat{Q}_{V,\lambda,i})^{-1}\). The arguments in \(\S 2\) are then justified if we consider all operators in \(B(\mathcal{E})\) or \(B^*(\mathcal{E})\). The limiting absorption principle is then extended to the edge Laplacian in the following way.
Theorem 3.1. (1) For any compact interval $I$ in $(0, \infty) \setminus \mathcal{T}$, there exists a constant $C > 0$ such that for any $\lambda \in I$ and $\epsilon > 0$
\[(3.2) \quad \|(\hat{H}_E - \lambda \mp i\epsilon)^{-1}\|_{\mathcal{B}(\hat{B}(\mathcal{E}); \hat{B}(\mathcal{E}))} \leq C.\]
(2) For any $\lambda \in (0, \infty) \setminus \mathcal{T}$ and $s > 1/2$, there exists a strong limit
\[(3.3) \quad s - \lim_{\epsilon \downarrow 0}(\hat{H}_E - \lambda \mp i\epsilon)^{-1} := (\hat{H}_E - \lambda \mp i0)^{-1} \in \mathcal{B}(\hat{L}^{2,s}(\mathcal{E}); \hat{L}^{2,s}(\mathcal{E})),\]
and for any $f \in \hat{L}^{2,s}(\mathcal{E})$, $(\hat{H}_E - \lambda \mp i0)^{-1} \hat{f}$ is an $\hat{L}^{2,s}(\mathcal{E})$-valued strongly continuous function of $\lambda$.
(3) For any $\hat{f}, \hat{g} \in \hat{B}(\mathcal{E})$ and $\lambda \in (0, \infty) \setminus \mathcal{T}$, there exists a limit
\[(3.4) \quad \lim_{\epsilon \downarrow 0}((\hat{H}_E - \lambda \mp i\epsilon)^{-1} \hat{f}, \hat{g}) := ((\hat{H}_E - \lambda \mp i0)^{-1} \hat{f}, \hat{g}),\]
and $((\hat{H}_E - \lambda \mp i0)^{-1} \hat{f}, \hat{g})$ is a continuous function of $\lambda$.

3.2. Analytic continuation of the resolvent. It is well-known that for the Schrödinger operator $-\Delta + V(x)$ in $\mathbb{R}^d$, where $V(x)$ has compact support, the boundary value of the resolvent $(-\Delta + V(x) - \lambda - i0)^{-1}$ has a meromorphic continuation into the lower half plane $\{\text{Re} \lambda > 0, \text{Im} \lambda < 0\}$ as an operator from the space of compactly supported $L^2(\mathbb{R}^d)$ functions to $L^2_{\text{loc}}(\mathbb{R}^d)$. This is proven by considering the free case, i.e. the operator
\[
\int_{\mathbb{R}^d} \frac{e^{ix\xi} \hat{f}(\xi)}{|\xi|^2 - \zeta} d\xi = \int_0^\infty \frac{\int_{S^{d-1}} e^{i\omega \cdot x} \hat{f}(\omega) d\omega}{\pi^d - \zeta} r^{d-1} dr
\]
($\hat{f}(\xi)$ being the Fourier transform of $f$) for $\text{Im} \zeta > 0$, deforming the path of integration into the lower half-plane, and then applying the perturbation theory. This method also works for the discrete case, and one can show that the resolvents of the vertex Hamiltonian and the edge Hamiltonian defined for $\{\text{Re} \lambda > 0, \text{Im} \lambda > 0\}$ can be continued meromorphically into the lower half-plane $\{\text{Re} \lambda > 0, \text{Im} \lambda < 0\}$ with possible branch points on $\mathcal{T}$, when the perturbation is compactly supported.

3.3. Spectral representation. We can then construct the spectral representation of the edge Laplacian. Letting $P_{V,j}(x)$ be the eigenprojection associated with the eigenvalue $\lambda_j(x)$ of $H_0(x)$, we put
\[(3.5) \quad D^{(0)}(\lambda \pm i0) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} U_V I_2(-\hat{\Delta}_V + \cos \sqrt{\lambda \pm i0})^{-1} I_2^\ast U_V^\ast
\]
where $\sigma(\lambda) = 1$ if $\lambda > 0$, $\sin \sqrt{\lambda} > 0$, $\sigma(\lambda) = -1$ if $\lambda > 0$, $\sin \sqrt{\lambda} < 0$. We also put
\[(3.6) \quad \Phi^{(0)}(\lambda) = U_V I_2 \hat{T}_V^{(0)}(\lambda).
\]
By (2.17), $\hat{R}_E^{(0)}(\lambda \pm i0)$ is rewritten as
\[(3.7) \quad \hat{R}_E^{(0)}(\lambda \pm i0) = \Phi^{(0)}(\lambda)^\ast D^{(0)}(\lambda \pm i0) \Phi^{(0)}(\lambda) + r_E^{(0)}(\lambda).
\]
We put
\[M_\lambda = \cup_{j=1}^2 M_{\lambda,j}, \quad M_{\lambda,j} = \{x \in T^d; \lambda_j(x) + \cos \sqrt{\lambda} = 0\},\]
where $dM_{\lambda,j}$ is the induced measure on $M_{\lambda,j}$. For $\hat{f} \in B(\mathcal{E})$, we define $\hat{\mathcal{F}}_j^{(0)}(\lambda)\hat{f}$ by

$$\hat{\mathcal{F}}_j^{(0)}(\lambda)\hat{f} = (P_{\nu,j}(x)\Phi(0)(\lambda)\hat{f})|_{M_{\lambda,j}},$$

i.e. the restriction of $P_{\nu,j}(x)\Phi(0)(\lambda)\hat{f}$ to $M_{\lambda,j}$, and

$$\hat{\mathcal{F}}^{(0)}(\lambda) = (\hat{\mathcal{F}}^{(0)}_1(\lambda), \hat{\mathcal{F}}^{(0)}_2(\lambda)), \quad \hat{h}_\lambda = L^2(M_{\lambda,j}; dS_j), \quad \mathbf{H} = L^2((0, \infty), \hat{h}_\lambda; d\lambda).$$

Noting that $\hat{\mathcal{F}}^{(0)}(\lambda) \in B(B(\mathcal{E}): \hat{h}_\lambda)$, the spectral representation associated with $\hat{H}_\mathcal{E}$ is constructed by the perturbation method. Define $\hat{\mathcal{F}}^{(\pm)}(\lambda)$ by

$$\hat{\mathcal{F}}^{(\pm)}(\lambda) = \hat{\mathcal{F}}^{(0)}(\lambda)\left(1 - qE\hat{\mathcal{E}}(\lambda \pm i0)\right) \in B(B(\mathcal{E}); \hat{h}_\lambda).$$

Then we have

$$\hat{\mathcal{F}}^{(\pm)}(\lambda) = \hat{\mathcal{F}}^{(0)}(\lambda)\left(1 - qE\hat{\mathcal{E}}(\lambda \pm i0)\right) \in B(B(\mathcal{E}); \hat{h}_\lambda).$$

We can prove (3.10) first for $\hat{H}_\mathcal{E}^{(0)}$ by (3.7), and then for $\hat{H}_\mathcal{E}$ by using the resolvent equation (see Lemma 7.8 in [3]).

**Theorem 3.2.** (1) The operator $\hat{\mathcal{F}}^{(\pm)}$ is uniquely extended to a partial isometry with initial set $\mathcal{H}_{ac}(\hat{H}_\mathcal{E})$ and final set $\mathbf{H}$ annihilating $\mathcal{H}_{p}(\hat{H}_\mathcal{E})$, the point spectral subspace for $\hat{H}_\mathcal{E}$.

(2) It diagonalizes $\hat{H}_\mathcal{E}$:

$$\langle \hat{\mathcal{F}}^{(\pm)}\hat{H}_\mathcal{E}\hat{f}\rangle(\lambda) = \lambda\langle \hat{\mathcal{F}}^{(\pm)}\hat{f}\rangle(\lambda), \quad \forall \hat{f} \in D(\hat{H}_\mathcal{E}).$$

(3) The adjoint operator $\hat{\mathcal{F}}^{(\pm)}(\lambda)^* \in B(\mathcal{H}_\lambda; B^*(\mathcal{E}))$ is an eigenoperator in the sense that

$$\langle \hat{H}_\mathcal{E} - \lambda \rangle \hat{\mathcal{F}}^{(\pm)}(\lambda)^* \phi = 0, \quad \forall \phi \in \mathcal{H}_\lambda.$$

(4) For $\hat{f} \in \mathcal{H}_{ac}(\hat{H}_\mathcal{E})$, the inversion formula holds:

$$\hat{f} = \int_0^\infty \hat{\mathcal{F}}^{(\pm)}(\lambda)^* \langle \hat{\mathcal{F}}^{(\pm)}\hat{f}\rangle(\lambda) d\lambda.$$

The crucial step for the inverse scattering procedure is Theorem 3.9 below, which can be proven by the same argument as in [3]. We do not repeat the whole procedure, but explain important intermediate steps. Let us prepare a lemma.

**Lemma 3.3.** For a solution $\hat{u}$ of the equation $(\hat{H}_\mathcal{E} - \lambda)\hat{u} = \hat{f}$ satisfying the Kirchhoff condition, we have the inequality

$$C_{\lambda}^{-1}\|\hat{u}\|_{B^*(\mathcal{E})} \leq \|\hat{u}\|_{\mathbf{V}} \leq C_{\lambda}\|\hat{u}\|_{B^*(\mathcal{E})},$$

and the equivalence

$$\hat{u} \in B_0^*(\mathcal{E}) \iff \hat{u}|_{\mathbf{V}} \in B_0^*(\mathbf{V}).$$
Proof. Note that \( \hat{u}_e(z) \) is written as in (2.10). Since \( \phi_{e_0}(t,\lambda) \) and \( \phi_{e_1}(t,\lambda) \) are linearly independent, there exists a constant \( C_\lambda > 0 \) independent of \( e \) such that
\[
C_\lambda^{-1} \parallel \hat{u}_e \parallel_{L^2} \leq |\phi_e(0)| + |\phi_e(1)| \leq C_\lambda \parallel \hat{u}_e \parallel_{L^2}.
\]
The lemma then follows from this inequality. \( \square \)

(I) Rellich type theorem. We define exterior and interior domains \( \mathcal{E}_{ext,R} \) and \( \mathcal{E}_{int,R} \) in \( \mathcal{E} \) by
\[
\mathcal{E}_{ext,R} \ni e \iff |c(e)| \geq R, \quad \mathcal{E}_{int,R} \ni e \iff |c(e)| < R.
\]

Theorem 3.4. Let \( \lambda \in (0,\infty) \setminus \mathcal{P}^{(0)}, \) and suppose \( \hat{u} \in \mathcal{B}_0^*(\mathcal{E}) \) satisfies \( \hat{H}_E^{(0)} \hat{u} = \lambda \hat{u} \) in \( \mathcal{E}_{ext,R}, \) and the Kirchhoff condition for some \( R > 0. \) Then \( \hat{u} = 0 \) on \( \mathcal{E}_{ext,R} \) for some \( R_1 > 0. \)

Proof. By Lemma 3.3, \( \hat{u} |_{\mathcal{V}} \in \mathcal{B}_0^*(\mathcal{V}). \) Since \( (-\Delta_\mathcal{V} + \cos \sqrt{\lambda}) \hat{u} |_{\mathcal{V}} = 0 \) near infinity, by Theorem 5.1 in [3], \( \hat{u} |_{\mathcal{V}} = 0 \) near infinity. This proves Theorem 3.4. \( \square \)

We say that the operator \( \hat{H}_E - \lambda \) has the unique continuation property on \( \mathcal{E} \) when the following assertion holds: If \( \hat{u} \) satisfies \( (\hat{H}_E - \lambda) \hat{u} = 0 \) on \( \mathcal{E} \) and \( \hat{u} = 0 \) on \( \mathcal{E}_{ext,R} \) for some \( R > 0, \) then \( \hat{u} = 0 \) on \( \mathcal{E}. \) The following lemma can be checked easily.

Lemma 3.5. For the hexagonal lattice in \( \mathbb{R}^2, \) the unique continuation property holds.

(II) Radiation condition. The radiation condition for the vertex Laplacian was introduced in [3] for the distinction between \( (-\Delta_\mathcal{V} - \lambda - i0)^{-1} \) and \( (-\Delta_\mathcal{V} - \lambda + i0)^{-1}. \) Hence it is extended to the edge Laplacian. Note that for the edge Laplacian, one must replace \( \lambda \) in the definition (6.2) of [3] by \( \cos \sqrt{\lambda}. \) See [6] for details.

Theorem 3.6. Let \( \lambda \in (0,\infty) \setminus \mathcal{P} \) and \( \hat{f} \in \mathcal{B}(\mathcal{E}). \)

(1) The solution \( \hat{u} \in \mathcal{B}_0^*(\mathcal{E}) \) of the equation \( (-\hat{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda) \hat{u} = \hat{f} \) satisfying the outgoing or incoming radiation condition is unique.

(2) \( (\hat{H}_E - \lambda - i0)^{-1} \hat{f} \) satisfies the outgoing radiation condition, and \( (\hat{H}_E - \lambda + i0)^{-1} \hat{f} \) satisfies the incoming radiation condition.

(III) Singularity expansion. Asymptotic behavior at infinity of the resolvent is closely related to the far-field behavior of the scattering waves. For the case of scattering on perturbed lattices, instead of observing the asymptotic expansion of \( (\hat{H}_E - \lambda \mp i0)^{-1} \) at infinity of the edge space \( \mathcal{E}, \) it is more convenient to consider the singularities of its Fourier transform in \( \mathcal{B}^*. \) For \( f, g \in \mathcal{B}^*(\mathcal{E}), \) we use the notation \( f \asymp g \) in the following sense:
\[
f \asymp g \iff f - g \in \mathcal{B}_0^*(\mathcal{E}).
\]

We use the same notation \( \asymp \) for \( \mathcal{B}^*(\mathcal{V}). \)

Since \( r_\mathcal{E}(\lambda) \) is bounded on \( L^2(\mathcal{E}), \) we have \( r_\mathcal{E}(\lambda) \hat{f} \asymp 0 \) for any \( \hat{f} \in L^2(\mathcal{E}). \) Then, by (2.10) and (2.12), the singularities of \( (\hat{H}_E - \lambda \mp i0)^{-1} \) appear from \( \left(-\hat{\Delta}_{\mathcal{V},\lambda} + \hat{Q}_{\mathcal{V},\lambda}\right)^{-1} \hat{T}_\mathcal{V}(\lambda) \hat{f}, \) which were studied in [3]. Therefore, in view of [3] Theorem 7.7, we have for \( f \in \mathcal{B}(\mathcal{V}) \)
\[
U_\mathcal{V} I_2 \left(-\hat{\Delta}_{\mathcal{V}} + \cos \sqrt{\lambda \mp i0}\right)^{-1} I_2 U_\mathcal{V} f
\approx \sum_{j=1}^2 \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda \mp i0}} \left(P_{\mathcal{V},j}(x)f\right)|_{M_{\lambda_j}}.
\]
We denote the right-hand side as
\[ (-\Delta_V + \cos \sqrt{\lambda} \pm i0)^{-1} f |_{M_{\lambda}}. \]

We can then prove the following theorem for \( \widehat{H}_{E}^{(0)} \) by using (3.11), and for \( \widehat{H}_{E} \) by the formula (3.9) and the resolvent equation.

**Theorem 3.7.** For any \( \lambda \in (0, \infty) \setminus \mathcal{T} \) and \( \widehat{f} \in \mathcal{B}(\mathcal{E}) \), we have
\[
\widehat{R}_{E}(\lambda \pm i0)\widehat{f} \simeq \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Phi^{(0)}(\lambda) (\widehat{H}_{E} - \lambda) \widehat{f} |_{M_{\lambda}}.
\]

### 3.4. Helmholtz equation and S-matrix.

Theorem 3.7 enables us to characterize the solution space to the Helmholtz equation.

**Lemma 3.8.** Let \( \lambda \in (0, \infty) \setminus \mathcal{T} \) and \( \widehat{f} \in \mathcal{B}(\mathcal{E}) \). Then
\[
\{ \widehat{u} \in \widehat{\mathcal{B}}^{*}(\mathcal{E}) \mid (\widehat{H}_{E} - \lambda) \widehat{u} = 0 \} = \widehat{\mathcal{F}}^{(-)}(\lambda)^{*} \mathbf{h}_{\lambda},
\]

**Theorem 3.9.** For any incoming data \( \phi^{\text{in}} \in L^{2}(M_{\lambda}) \), there exist a unique solution \( \widehat{u} \in \widehat{\mathcal{B}}^{*}(\mathcal{E}) \) of the following equation
\[
(\widehat{H}_{E} - \lambda) \widehat{u} = 0
\]

and an outgoing data \( \phi^{\text{out}} \in L^{2}(M_{\lambda}) \) satisfying
\[
\widehat{u} \simeq -\Phi^{(0)}(\lambda)^{*} \sum_{j=1}^{2} \frac{1}{\lambda_{j}(x) + \cos \sqrt{\lambda} \pm i0} \left( \langle \mathcal{P}_{V,j}(x) \phi^{\text{in}} \rangle |_{M_{\lambda,j}} \right)
\]
\[
+ \Phi^{(0)}(\lambda)^{*} \sum_{j=1}^{2} \frac{1}{\lambda_{j}(x) + \cos \sqrt{\lambda} \mp i0} \left( \langle \mathcal{P}_{V,j}(x) \phi^{\text{out}} \rangle |_{M_{\lambda,j}} \right).
\]

The mapping
\[ S(\lambda) : \phi^{\text{in}} \rightarrow \phi^{\text{out}} \]

is the S-matrix, which is unitary on \( \mathbf{h}_{\lambda} \).

We omit the proof of Lemma 3.8 and Theorem 3.9 since they are almost the same as that of Theorem 7.15 of [3].

As is proven in [31], using the wave operator
\[
\widehat{W}_{\pm} = s - \lim_{t \to \pm \infty} e^{it\widehat{H}_{E}} e^{-it\widehat{H}_{E}^{(0)}} \mathcal{P}_{\text{ac}}(\widehat{H}_{E}^{(0)}),
\]

where \( \mathcal{P}_{\text{ac}}(\widehat{H}_{E}^{(0)}) \) is the projection onto the absolutely continuous subspace of \( \widehat{H}_{E}^{(0)} \), one can define the scattering operator
\[ \widehat{S} = (\widehat{W}^{(+)})^{*} \widehat{W}^{(-)}, \]

which is unitary. Define \( S \) by
\[ S = \widehat{\mathcal{F}}^{(0)} \widehat{S}(\widehat{\mathcal{F}}^{(0)})^{*}. \]

The S-matrix \( S(\lambda) \) and the scattering amplitude \( A(\lambda) \) are defined by
\[ S(\lambda) = 1 - 2\pi i A(\lambda), \]
\[ A(\lambda) = \widehat{\mathcal{F}}^{(+)}(\lambda) q_{E} \widehat{\mathcal{F}}^{(-)}(\lambda). \]
Then $S(\lambda)$ is unitary on $\mathbf{h}_\lambda$, and for $\lambda \in (0, \infty) \setminus \mathcal{T}$

$$(Sf)(\lambda) = S(\lambda)f(\lambda), \quad f \in \mathbf{h}.$$  

Since the resolvent has a meromorphic extension into the lower half-plane $\{\Re \lambda > 0, \Im \lambda < 0\}$ with possible branch points on $\mathcal{T}$, the formula (3.14) implies that the $S$-matrix $S(\lambda)$ is also meromorphic in the same domain.

4. FROM $S$-MATRIX TO INTERIOR D-N MAP

4.1. Boundary value problem. For a subgraph $\Omega = \{V_\Omega, E_\Omega\} \subset \{V, E\}$ and $v \in V$, $v \sim \Omega$ means that there exist a vertex $w \in V_\Omega$ and an edge $e \in E$ such that $v \sim w$, $e(0) = v$ or $e(1) = v$. For a connected subgraph $\Omega \subset \{V, E\}$, we define a

subset $\partial \Omega = \{V_\partial \Omega, E_\partial \Omega\} \subset \{V, E\}$ by

$$V_\partial \Omega = \{v \not\in V_\Omega; v \sim \Omega\},$$

$$E_\partial \Omega = \{e \in E; e(0) \in V_\partial \Omega \text{ or } e(1) \in V_\partial \Omega\}.$$  

We then put $\Omega = \Omega \cup \partial \Omega$ and

$\circ V_\Omega = V_\Omega$, $\partial V_\Omega = V_\partial \Omega$, which are called the set of interior vertices and the set of boundary vertices of $\Omega$, respectively. We put

$$V_\Omega = \circ V_\Omega \cup \partial V_\Omega.$$  

As for the edges, we simply put

$$E_\Omega = E_\Omega \cup E_\partial \Omega.$$  

We then define the edge Dirichlet Laplacian $\hat{\Delta}_{E_\Omega}$ by

$$\hat{\Delta}_{E_\Omega}u_e(z) = \frac{d^2}{dz^2}u_e(z), \quad e \in E_\Omega$$  

whose domain $D(\hat{\Delta}_{E_\Omega})$ is the set of all $u = \{u_e\}_{e \in E_\Omega} \in H^2(E_\Omega)$ satisfying $u(v) = 0$ at any boundary vertex $v \in \partial V_\Omega$ and the Kirchhoff condition at any interior vertex $v \in V_\partial$. By the standard argument, $\hat{\Delta}_{E_\Omega}$ is self-adjoint.

The vertex Dirichlet Laplacian on $V_\Omega$ is defined in the same way as in (2.7):

$$\hat{\Delta}_{V_\Omega}(\vec{u})(v) = \frac{1}{\deg_{V_\Omega}(v)} \sum_{w \sim v, w \in V_\Omega} \frac{1}{\psi_{vw}(1, \lambda)} \vec{u}(w), \quad v \in V_\Omega.$$  

Recall that for a domain $W \subset V$, we define

$$\deg_{V,W}(v) = \begin{cases} z \{w \in W; w \sim v\}, & v \in W, \\ z \{w \not\in W; w \sim v\}, & v \in \partial W. \end{cases}$$  

(See (2.6) of [3]). We impose the Dirichlet boundary condition for the domain $D(\hat{\Delta}_{V_\Omega}, \lambda)$:

$$\vec{u} \in D(\hat{\Delta}_{V_\Omega}, \lambda) \iff \vec{u} \in L^2(V_\Omega) \cap \{\vec{u}; \vec{u}(v) = 0, \quad v \in \partial V_\Omega\}.$$  

As in §3, we first define the vertex Dirichlet Laplacian for the case without potential and then add the potential $\hat{Q}_{V, \lambda}$ as a perturbation. By modifying the inner product,
−\Delta_{V,\lambda} + \hat{Q}_{V,\lambda} \text{ is self-adjoint. The normal derivative at the boundary associated with } \hat{\Delta}_{V,\lambda} \text{ is defined by}
\begin{align}
(\partial_{\hat{\Delta}_{V,\lambda}} \hat{u})(v) &= -\frac{1}{\deg_{V}(v)} \sum_{w \sim v, w \in V} \frac{1}{\psi_{uv}(1, \lambda)} \hat{u}(w).
\end{align}
(c.f. (2.7) of [4]). Note that in the right-hand side, \(w\) is taken only from \(V_0\).

Let us give an example of interior and exterior domains as well as their boundaries for the case of hexagonal lattice. We identify \(\mathbb{R}^2\) with \(\mathbb{C}\) and put \(\omega = e^{2\pi i/6} = (1 + \sqrt{3}i)/2\). Let \(D\) be the hexagon with center at the origin and vertices \(\omega^n, 1 \leq n \leq 6\).

Recalling that the basis of the hexagonal lattice are \(2 - \omega\) and \(1 + \omega\), we put \(D_{k\ell} = D + k(2 - \omega) + \ell(1 + \omega)\), which denotes the translation of \(D\) by \(k(2 - \omega)\) and \(\ell(1 + \omega)\). For an integer \(L \geq 1\), let
\[D_L = \bigcup_{|k| \leq L, |\ell| \leq L} D_{k\ell}.
\]
As is illustrated in Figure 1, we take an interior domain \(\Omega_{\text{int}}\) in such a way that
\[\partial_{\text{int}} = V \cap D_L, \quad \partial_{\text{int}} = E \cap D_L.
\]
In Figure 1, \(\partial_{\Omega_{\text{int}}}\) is denoted by white dots.

**Figure 1.** Boundary of a domain in the hexagonal lattice

The exterior domain \(\Omega_{\text{ext}}\) is defined similarly. We then put
\[V_{\text{int}} = V_{\Omega_{\text{int}}}, \quad E_{\text{int}} = E_{\Omega_{\text{int}}},
\]
\[V_{\text{ext}} = V_{\Omega_{\text{ext}}}, \quad E_{\text{ext}} = E_{\Omega_{\text{ext}}},
\]
for the sake of simplicity. Note that
\[V = V_{\text{int}} \cup V_{\text{ext}}, \quad \partial V_{\text{int}} = \partial V_{\text{ext}},
\]
\[E = E_{\text{int}} \cup E_{\text{ext}}, \quad E_{\text{int}} \cap E_{\text{ext}} = \emptyset.
\]
We define the edge Dirichlet Laplacians on \(E_{\text{int}}, E_{\text{ext}}\), which are denoted by \(\hat{\Delta}_{\text{int},E}, \hat{\Delta}_{\text{ext},E}\):
\[\hat{\Delta}_{\text{int},E} = \hat{\Delta}_{E_{\text{int}}}, \quad \hat{\Delta}_{\text{ext},E} = \hat{\Delta}_{E_{\text{ext}}}.
\]
Let us note that
\[ \sigma_e(-\tilde{\Delta}_e) = \sigma_e(-\tilde{\Delta}_{ext,e}). \]

We assume that the support of the potential lies strictly inside of \( \mathcal{E}_{int} \). Namely, introducing a set:
\[ \tilde{\mathcal{E}}_{int} = \{ e \in \mathcal{E}_{int} : e(0) \not\in \partial\mathcal{V}_{int}, \ e(1) \not\in \partial\mathcal{V}_{int} \}, \]
we assume
\[ (4.2) \quad \text{supp} q_e \subset \tilde{\mathcal{E}}_{int}. \]

The formal formulas (2.13), (2.17) are also valid for boundary value problems of edge Laplacians. For the case of the exterior problem, the resolvent of \( -\tilde{\Delta}_{ext,e} \) is written by (2.17) with \( \hat{H}_e^{(0)} \) replaced by \( -\tilde{\Delta}_{ext,e} \). In our previous work [4], we studied the spectral properties of the vertex Laplacian in the exterior domain by reducing them to the whole space problem. Therefore, all the results for the edge Laplacian in the previous section also hold in the exterior domain. In particular, we have

- Rellich type theorem (Theorem 3.4),
- Limiting absorption principle (Theorem 3.1),
- Spectral representation (Theorem 3.2),
- Resolvent expansion (Theorem 3.7),
- Expansion of solutions to the Helmholtz equation (Theorem 3.9),
- S-matrix (Theorem 3.9)

in the exterior domain \( \mathcal{E}_{ext} \). In fact, Theorem 3.4 holds without any change. Using the formula (2.10) and the limiting absorption principle for \( \hat{\Delta}_{ext} \) proven in Theorem 7.7 in [3], one can extend Theorem 3.1 for the exterior domain. The radiation condition is also extended to the exterior domain. Then, the remaining theorems (Theorems 3.2, 3.9) are proven by the same argument.

4.2. Exterior and interior D-N maps. We consider the edge model for the exterior problem. Let \( \tilde{u}^{(\pm)} = \{ \tilde{u}_{e}^{(\pm)} \}_{e \in \mathcal{E}_{ext}} \) be the solution to the equation
\[ \begin{cases} \left( -\tilde{\Delta}_{ext,e} - \lambda \right) \tilde{u}^{\circ} = 0, & \text{in } \mathcal{E}_{ext}^{\circ}, \\ \tilde{u} = \tilde{f}, & \text{on } \partial \mathcal{E}_{ext}^{\circ}, \end{cases} \]
satisfying the radiation condition (outgoing for \( \tilde{u}^{(+)} \) and incoming for \( \tilde{u}^{(-)} \)). Then, the exterior D-N map \( \Lambda_{ext,e}^{(\pm)}(\lambda) \) is defined by
\[ \Lambda_{ext,e}^{(\pm)}(\lambda) \tilde{f}(v) = -\frac{d}{dz} \tilde{u}_{e}^{(\pm)}(v), \quad v \in \partial \mathcal{V}_{ext}, \]
where \( e \) is the edge having \( v \) as its end point. Here, to compute \( \frac{d}{dz} \tilde{u}_{e}^{(\pm)}(v) \), we neglect the original orientation of \( e \). Namely, we parametrize \( e \) by \( z \in [0,1] \) so that \( v \in \partial \mathcal{V} \) corresponds to \( z = 0 \), and define \( \frac{d}{dz} \tilde{u}_{e}^{(\pm)}(z) = \frac{d}{dz} \tilde{u}_{e}^{(\pm)}(z) \big|_{z=0} \).

For the case of the interior problem, the Dirichlet boundary value problem for the edge Laplacian
\[ \begin{cases} \left( -\tilde{\Delta}_{int,e} + q_e - \lambda \right) \tilde{u}^{\circ} = 0, & \text{in } \mathcal{E}_{int}^{\circ}, \\ \tilde{u} = \tilde{f}, & \text{on } \partial \mathcal{V}_{int}, \end{cases} \]
is formulated as above. Note that the spectrum of $-\hat{\Delta}_{\text{int},\varepsilon} + q_\varepsilon$ is discrete. In the following, we assume that

$$\lambda \notin \sigma(-\hat{\Delta}_{\text{int},\varepsilon} + q_\varepsilon).$$

The D-N map $\Lambda_{\text{int},\varepsilon}(\lambda)$ is defined by

$$\Lambda_{\text{int},\varepsilon}(\lambda) \hat{f}(v) = \frac{d}{dz} \hat{u}_e(v), \quad v \in \partial \mathcal{V}_{\text{int}},$$

where $e$ is the edge having $v$ as its end point and $\hat{u} = \{\hat{u}_e(\pm)\}_{e \in E_{\text{int}}}$ is the solution to the equation (4.5). The same remark as above is applied to $\frac{d}{dz} \hat{u}_e(v), v \in \partial \mathcal{V}_{\text{int}}$.

The D-N maps are also defined for vertex operators. Let us slightly change the notation. For a subset $V_D \subset V$ and $v \in V_D$, let

$$\hat{\Delta}_{V_D}^{(0)}(\lambda) \hat{u}(v) = \frac{1}{\deg V_D(v)} \sum_{w \sim v, w \in V_D} \hat{u}(w).$$

By this definition, we have (see (2.15))

$$\hat{\Delta}_{V_D}^{(0)} = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \hat{\Delta}_{V_D}^{(0)}.\,$$

For the exterior and interior domains $\Omega_{\text{ext}}$ and $\Omega_{\text{int}}$ defined in the previous section, $\hat{\Delta}_{V_D}^{(0)}$ is denoted by $\hat{\Delta}_{\text{ext},V}$ and $\hat{\Delta}_{\text{int},V}$, respectively:

$$\hat{\Delta}_{\text{ext},V} = \hat{\Delta}_{V_{\text{ext}}}^{(0)}, \quad \hat{\Delta}_{\text{int},V} = \hat{\Delta}_{V_{\text{int}}}^{(0)}.$$

Now, consider the exterior boundary value problem

$$\begin{cases} (-\hat{\Delta}_{V_{\lambda}} + \hat{Q}_{V_{\lambda}}) \hat{u} = 0, & \text{in } V_{\text{ext}}, \\ \hat{u} = \hat{f}, & \text{on } \partial V_{\text{ext}}. \end{cases}$$

Note that by (4.8) and (2.16) this is equivalent to

$$\begin{cases} (-\hat{\Delta}_{V_{\lambda}}^{(0)} + \cos \sqrt{\lambda}) \hat{u} = 0, & \text{in } V_{\text{ext}}, \\ \hat{u} = \hat{f}, & \text{on } \partial V_{\text{ext}}. \end{cases}$$

Let $\hat{u}_{\text{ext},V}^{(\pm)}$ be the solution of this equation satisfying the radiation condition. Then, taking account of (4.11) and (4.8), we define the exterior D-N map by

$$\hat{\Lambda}_{\text{ext},V}(\lambda) \hat{f} = \frac{1}{\deg V_{\text{ext}}(v)} \sum_{w \sim v, w \in V_{\text{ext}}} \hat{u}_{\text{ext},V}^{(\pm)}(w).$$

We also consider the interior boundary value problem

$$\begin{cases} (-\hat{\Delta}_{V_{\lambda}} + \hat{Q}_{V_{\lambda}}) \hat{u} = 0, & \text{in } V_{\text{int}}, \\ \hat{u} = \hat{f}, & \text{on } \partial V_{\text{int}}. \end{cases}$$
Taking account of (4.2), we define the interior D-N map by

\[
\tilde{\Lambda}_{\text{int, } V}(\lambda) \tilde{f}(v) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \partial_{\Delta_{\text{int, } V}}^{\nu} \tilde{u}_{\text{int, } V} = -\partial_{\Delta_{\text{int, } V}}^{\nu} \tilde{u}_{\text{int, } V} \\
- \frac{1}{\deg_v(\nu)} \sum_{w \sim v, w \in \mathcal{V}_{\text{int}}} \tilde{u}_{\text{int, } V}(w).
\]

(4.12)

Note that by virtue of Lemma 2.2, if \( \tilde{u} \) satisfies the edge Schrödinger equation

\[
(\hat{H}_E - \lambda)\tilde{u} = 0
\]

and the Kirchhoff condition, \( \tilde{u}|_{\mathcal{V}} \) satisfies the vertex Schrödinger equation

\[
(\hat{\Delta}_{\mathcal{V}} + \hat{Q}_{\mathcal{V}}) \tilde{u}|_{\mathcal{V}} = 0.
\]

Therefore, if the exterior boundary value problem (4.3) for the edge model is solvable, so is the exterior boundary value problem (4.9) for the vertex model. The same remark applies to the interior boundary value problem.

If \( \varphi(z) \) satisfies

\[
-\varphi''(z) - \lambda \varphi(z) = 0 \quad \text{in} \quad (0, 1),
\]

we have

\[
\varphi(1) = \varphi(0) \cos \sqrt{\lambda} + \varphi'(0) \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}}.
\]

Since the D-N map for the vertex model is computed by \( \tilde{u}|_{\mathcal{V}} \), where \( \tilde{u} \) is the solution to the edge Schrödinger equation, this implies, by (4.4), (4.7), (4.10) and (4.12), the following formulas between the D-N maps of edge-Laplacian and vertex Laplacian.

Lemma 4.1. The following equalities hold:

\[
\tilde{\Lambda}^{(\pm)}_{\text{ext, } E}(\lambda) = \cos \sqrt{\lambda} - \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Lambda^{(\pm)}_{\text{ext, } \mathcal{E}}(\lambda), \quad \lambda \in (0, \infty) \setminus \mathcal{T},
\]

\[
\tilde{\Lambda}_{\text{int, } V}(\lambda) = -\cos \sqrt{\lambda} - \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Lambda_{\text{int, } \mathcal{E}}(\lambda), \quad \lambda \in \mathbb{C} \setminus \sigma(-\hat{\Delta}_{\text{int, } \mathcal{E}} + q_{\mathcal{E}}).
\]

Therefore, the D-N map for the edge model and the D-N map for the vertex model determine each other.

4.3. Relations between S-matrices and D-N maps. We show that the S-matrices for the vertex Laplacian and the edge Laplacian coincide.

In [3], Theorem 7.15, we have proven the following theorem, which is the counterpart of Theorem 3.9 for the discrete Laplacian \( -\hat{\Delta}_{\mathcal{V}} \) at the energy \( -\cos \sqrt{\lambda} \): For any incoming data \( \varphi^{\text{in}} \in L^2(M_\lambda) \), there exist a unique solution \( \tilde{u}_{\mathcal{V}} \in \hat{\mathcal{B}}^*(\mathcal{V}) \) of the equation

\[
(-\hat{\Delta}_\mathcal{V} + \cos \sqrt{\lambda}) \tilde{u}_{\mathcal{V}} = 0
\]

and an outgoing data \( \tilde{\varphi}^{\text{out}} \in L^2(M_\lambda) \) satisfying

\[
I_2 \tilde{u}_{\mathcal{V}} \simeq -\sum_{j=1}^{\lambda_j(x) + \cos \sqrt{\lambda} + i0} \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda} + i0} \left( P_{\mathcal{V}, j} (x) \varphi^{\text{in}}_j \right) |_{M_\lambda,j} \\
+ \sum_{j=1}^{\lambda_j(x) + \cos \sqrt{\lambda} - i0} \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda} - i0} \left( P_{\mathcal{V}, j} (x) \varphi^{\text{out}}_j \right) |_{M_\lambda,j},
\]

(4.13)

in the sense that the difference of both sides is in \( \mathcal{B}_0^*(\mathcal{T}; \mathcal{C}^2) \). The mapping

\[
\tilde{S}(\lambda) : \varphi^{\text{in}} \rightarrow \tilde{\varphi}^{\text{out}}
\]

is the S-matrix of \( -\hat{\Delta}_\mathcal{V} \) at the energy \( -\cos \sqrt{\lambda} \), which is unitary on \( h_\lambda \).
By virtue of Lemma 3.3, we see that 
\[ \tilde{u}_E := \Phi^{(0)}(\lambda)^* \tilde{u}_V \]
has the properties in Theorem 3.9, hence by the uniqueness \( u = \tilde{u}_E \). Therefore, \( \tilde{\phi}(\text{out}) = \phi(\text{out}) \), which implies \( S(\lambda) = \tilde{S}(\lambda) \). We have thus proven the followin theorem.

**Theorem 4.2.** The S-matrix for the vertex Schrödinger operator at the energy 
\[ -\cos \sqrt{\lambda} \]
coincides with that of the edge Schrödinger operator at the energy \( \lambda \).

In [4], we have proven that for the vertex Laplacian the scattering matrix and 
the interior D-N map determine each other. By virtue of Theorems 4.1 and 4.2, we 
have the following theorem.

**Theorem 4.3.** For the edge Laplacian on the hexagonal lattice, the S-matrix and 
the D-N map in the interior domain determine each other.

## 5. Inverse Scattering

### 5.1. Hexagonal parallelogram

We are now in a position to consider the inverse scattering problem. Note here that although the choice of fundamental domain of the lattice \( \mathcal{L} \) is not unique, different choices give rise to unitarily equivalent Hamiltonians. In this section, we take \( v_1, v_2 \) and \( p^{(1)}, p^{(2)} \) as in (5.1) and (5.2) to make use of our previous results in [3], [4]. We identify \( \mathbb{R}^2 \) with \( \mathbb{C} \), and put 
\[ \omega = e^{\pi i/3}. \]

For \( n = n_1 + i n_2 \in \mathbb{Z}[i] = \mathbb{Z} + i\mathbb{Z} \), let 
\[ \mathcal{L}_0 = \{ v(n); n \in \mathbb{Z}[i] \}, \quad v(n) = n_1 v_1 + n_2 v_2, \]
(5.1) 
\[ v_1 = 1 + \omega, \quad v_2 = \sqrt{3}i, \]
(5.2) 
\[ p_1 = \omega^{-1} = \omega^5, \quad p_2 = 1, \]
and define the vertex set \( \mathcal{V}_0 \) by 
\[ \mathcal{V}_0 = \mathcal{V}_{01} \cup \mathcal{V}_{02}, \quad \mathcal{V}_{0i} = p_i + \mathcal{L}_0. \]

By virtue of Theorem 4.3 given an S-matrix and a bounded domain \( \mathcal{E}_{\text{int}} \), we can compute the D-N map associated with \( \mathcal{E}_{\text{int}} \). The problem is now reduced to the reconstruction of the potentials on the edges from the knowledge of the D-N map for the vertex Schrödinger operator defined on \( \mathcal{V}_{\text{int}} \), the set of the vertices in \( \mathcal{E}_{\text{int}} \).

As \( \mathcal{V}_{\text{int}} \), we use the following domain which is different from the one in Figure 1. Let \( \mathcal{D}_0 \) be the Wigner-Seitz cell of \( \mathcal{V}_0 \). It is a hexagon having 6 vertices \( \omega^k, 0 \leq k \leq 5 \), with center at the origin. Take \( \mathcal{D}_N = \{ n \in \mathbb{Z}[i]; 0 \leq n_1 \leq N, 0 \leq n_2 \leq N \} \), where \( N \) is chosen large enough, and put 
\[ \mathcal{D}_N = \bigcup_{n \in \mathcal{D}_N} \left( \mathcal{D}_0 + v(n) \right). \]

This is a parallelogram in the hexagonal lattice (see Figure 2). The interior angle of each vertex on the periphery of \( \mathcal{D}_N \) is \( 2\pi/3 \) or \( 4\pi/3 \). Let \( \mathcal{A} \) be the set of the former, and for each \( z \in \mathcal{A} \), we assign a new edge \( e_{z,\zeta} \), and a new vertex \( \zeta = t(e_{z,\zeta}) \) on its terminal point, hence \( \zeta \) is in the outside of \( \mathcal{D}_N \). Let 
\[ \Omega = \{ v \in \mathcal{V}_0; v \in \mathcal{D}_N \} \]
be the set of vertices in the inside of the resulting graph. The boundary $\partial \Omega = \{t(e,z) : z \in A\}$ is divided into 4 parts, called top, bottom, right, left sides, which are denoted by $(\partial \Omega)_T$, $(\partial \Omega)_B$, $(\partial \Omega)_R$, $(\partial \Omega)_L$, i.e.

$$(\partial \Omega)_T = \{\alpha_0, \cdots, \alpha_N\},$$

$$(\partial \Omega)_B = \{2\omega^5 + k(1 + \omega) ; 0 \leq k \leq N\},$$

$$(\partial \Omega)_R = \{2 + N(1 + \omega) + k\sqrt{3}i ; 1 \leq k \leq N\} \cup \{2 + N(1 + \omega) + N\sqrt{3}i + 2\omega^2\},$$

$$(\partial \Omega)_L = \{2\omega^4\} \cup \{\beta_0, \cdots, \beta_N\},$$

where $\alpha_k = \beta_N + 2\omega + k(1 + \omega)$ and $\beta_k = -2 + k\sqrt{3}i$ for $0 \leq k \leq N$.

5.2. Special solutions to the vertex Schrödinger equation. Taking $N$ large enough so that $\mathcal{D}_N$ contains all the supports of the potentials $q_e(z)$ in its interior, we consider the following Dirichlet problem for the vertex Schrödinger equation

\[
\begin{cases}
(\hat{-}\Delta_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u} = 0, & \text{in } \hat{\Omega}, \\
\hat{u} = \hat{f}, & \text{on } \partial\hat{\Omega}.
\end{cases}
\]

Let $\Lambda_{\hat{Q}}$ be the associated D-N map. The key to the inverse procedure is the following partial data problem.

**Lemma 5.1.** (1) Given a partial Dirichlet data $\hat{f}$ on $\partial\hat{\Omega} \setminus (\partial\Omega)_R$, and a partial Neumann data $\hat{g}$ on $(\partial\Omega)_L$, there is a unique solution $\hat{u}$ on $\hat{\Omega} \cup (\partial\hat{\Omega})_R$ to the equation

\[
\begin{cases}
(\hat{-}\Delta_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u} = 0, & \text{in } \hat{\Omega}, \\
\hat{u} = \hat{f}, & \text{on } \partial\hat{\Omega} \setminus (\partial\hat{\Omega})_R, \\
\hat{\partial}_N^{D-N}\hat{u} = \hat{g}, & \text{on } (\partial\hat{\Omega})_L.
\end{cases}
\]
Given the D-N map $\Lambda_{Q}$, a partial Dirichlet data $\hat{f}_{2}$ on $\partial\Omega \setminus (\partial\Omega)_{R}$ and a partial Neumann data $\hat{g}$ on $(\partial\Omega)_{L}$, there exists a unique $\hat{f}$ on $\partial\Omega$ such that $\hat{f} = \hat{f}_{2}$ on $\partial\Omega \setminus (\partial\Omega)_{R}$ and $\Lambda_{Q}\hat{f} = \hat{g}$ on $(\partial\Omega)_{L}$.

For the proof, see [4], Lemma 6.1.

Now, for $0 \leq k \leq N$, let us consider a diagonal line $A_{k}$ (see Figure 3):

$$A_{k} = \{x_{1} + ix_{2}; x_{1} + \sqrt{3}x_{2} = a_{k}\},$$

where $a_{k}$ is chosen so that $A_{k}$ passes through

$$\alpha_{k} = \alpha_{0} + k(1 + \omega) \in (\partial\Omega)_{T}.$$

The vertices on $A_{k} \cap \Omega$ are written as

$$\alpha_{k,\ell} = \alpha_{k} + \ell(1 + \omega^{5}), \quad \ell = 0, 1, 2, \ldots.$$

**Figure 3.** Line $A_{k}$

**Lemma 5.2.** Let $A_{k} \cap \partial\Omega = \{\alpha_{k,0}, \alpha_{k,m}\}$. Then, there exists a unique solution $\hat{u}$ to the equation

$$(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u} = 0 \quad \text{in} \quad \hat{\Omega},$$

with partial Dirichlet data $\hat{f}$ such that

$$\begin{cases} \hat{f}(\alpha_{k,0}) = 1, \\ \hat{f}(z) = 0 \quad \text{for} \quad z \in \partial\Omega \setminus (\partial\Omega)_{R} \cup \alpha_{k,0} \cup \alpha_{k,m} \end{cases}$$

and partial Neumann data $\hat{g} = 0$ on $(\partial\Omega)_{L}$. It satisfies

$$\hat{u}(x_{1} + ix_{2}) = 0 \quad \text{if} \quad x_{1} + \sqrt{3}x_{2} < a_{k}.$$

An important feature is that $\hat{u}$ vanishes below the line $A_{k}$. By using this property, we reconstructed the vertex potentials and defects of the hexagonal lattice in [4]. We make use of the same idea.
Let \( \hat{u} \) be a solution of the equation
\[
(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u} = 0, \quad \text{in} \quad \hat{\Omega},
\]
which vanishes in the region \( x_1 + \sqrt{3}x_2 < a_k \). Let \( a, b, b', c \in \mathcal{V} \) and \( e, e' \in \mathcal{E} \) be as in Figure 4.

\[\text{Figure 4. } \hat{u}(b) \text{ and } \hat{u}(b')\]

Then, evaluating the equation (5.11) at \( v = a \) and using (2.7), (2.8), we obtain
\[
(5.12) \quad \frac{1}{\psi_{ba}(1, \lambda)} \hat{u}(b) + \frac{1}{\psi_{b'a}(1, \lambda)} \hat{u}(b') = 0.
\]

Here, for any edge \( e \in \mathcal{E} \), we associate an edge \([e]\) without orientation and a function \( \phi_{[e]}(z, \lambda) \) satisfying
\[
\begin{cases}
-\frac{d^2}{dz^2} + q_e(z) - \lambda \phi_{[e]}(z, \lambda) = 0, & \text{for} \quad 0 < z < 1, \\
\phi_{[e]}(0, \lambda) = 0, & \phi_{[e]}'(0, \lambda) = 1.
\end{cases}
\]

By the assumption (Q-3), \( \phi_{[e]}(z, \lambda) \) is determined by \( e \) and independent of the orientation of \( e \). Then, the equation (5.12) is rewritten as
\[
(5.13) \quad \hat{u}(b) = -\frac{\phi_{[e]}(1, \lambda)}{\phi_{[e']}^{(1, \lambda)}} \hat{u}(b').
\]

Let \( e_{k,1}, e'_{k,1}, e_{k,2}, e'_{k,2}, \ldots \) be the series of edges just below \( A_k \) starting from the vertex \( \alpha_k \), and put
\[
(5.14) \quad f_{k,m}(\lambda) = -\frac{\phi_{[e_{k,m}]}(1, \lambda)}{\phi_{[e'_{k,m}]}(1, \lambda)}.
\]

Then, we obtain the following lemma.

**Lemma 5.3.** The solution \( \hat{u} \) in Lemma 5.2 satisfies
\[
\hat{u}(\alpha_{k,\ell}) = f_{k,1}(\lambda) \cdots f_{k,\ell}(\lambda).
\]

### 5.3. Reconstruction procedure

We now prove Theorem 1.1 by showing the reconstruction algorithm of the potential \( q_e(z) \).

**1st step.** We first take a sufficiently large hexagonal parallelogram \( \Omega \) as in Figure 2 which contains all the supports of the potential \( q_e(z) \).

**2nd step.** For an arbitrary \( k \), draw a line \( A_k \) as in Figure 3 and take the boundary data \( \hat{f} \) having the properties in Lemma 5.2.
3rd step. Compute the values of the associated solution \( \hat{u} \) to the boundary value problem in Lemma 5.2 at the points \( \alpha_{k,\ell} \), \( \ell = 0, 1, 2, \ldots \).

4th step. Look at Figure 2. Two edges \( e \) and \( e' \) between \( A_k \) and \( A_k' \) are said to be \( A_k' \)-adjacent if they have a vertex in common on \( A_k' \) (see Figure 4). Take two \( A_k' \)-adjacent edges \( e \) and \( e' \) between \( A_k \) and \( A_k' \), and use the formula (5.14) to compute the ratio of \( \phi_{[e]}(1, \lambda) \) and \( \phi_{[e']}(1, \lambda) \).

5th step. Rotate the whole system by the angle \( \pi \) and take a hexagonal parallelogram congruent to the previous one. Then, the roles of \( A_k \) and \( A_k' \) are exchanged. One can then compute the ratio of \( \phi_{[e]}(1, \lambda) \) and \( \phi_{[e']}(1, \lambda) \) for \( A_k' \)-adjacent pairs in the sense after the rotation, which are \( A_k \)-adjacent before the rotation.

After the 4th and 5th steps, for all pairs \( e \) and \( e' \) which are either \( A_k \)-adjacent or \( A_k' \)-adjacent, one has computed the ratio of \( \phi_{[e]}(1, \lambda) \) and \( \phi_{[e']}(1, \lambda) \).

6th step. Take a zigzag line on the hexagonal lattice (see Figure 5), and take any two edges \( e \) and \( e' \) on it. They are between \( A_k \) and \( A_k' \) for some \( k \). Then, using the 4th and 5th steps, one can compute the ratio of \( \phi_{[e]}(1, \lambda) \) and \( \phi_{[e']}(1, \lambda) \) by computing the ratio for two successive edges between \( e \) and \( e' \).

7th step. For a sufficiently remote edge \( e' \), one knows \( \phi_{[e']}(1, \lambda) \) since \( q_{e'}(z) = 0 \) on \( e' \). One can thus compute \( \phi_{[e]}(1, \lambda) \) for any edge \( e \). Then, by the analytic continuation, one can compute the zeros of \( \phi_{[e]}(1, \lambda) \) for any edge \( e \).

8th step. Note that the zeros of \( \phi_{[e]}(1, \lambda) \) are the Dirichlet eigenvalues for the operator \(-\frac{d^2}{dz^2} + q_e(z)\) on \((0, 1)\). Since the potential is symmetric, by Borg’s theorem (see e.g. [47], p. 117) these eigenvalues determine the potential \( q_e(z) \).

We have now completed the proof of Theorem 1.1.

Note that for the 1st step, we need a-priori knowledge of the size of the support of the potential \( q_e(z) \). The knowledge of the D-N map is used in the 2nd step (in the proof of Lemma 5.1). In the 3rd step, one uses the equation (5.8) and the fact that \( \hat{u} = 0 \) below \( A_k \).

The proof of Theorem 1.2 requires no essential change. Instead of \( \frac{\sin \sqrt{\lambda}z}{\sqrt{\lambda}} \) and \( \frac{\sin \sqrt{\lambda}(1-z)}{\sqrt{\lambda}} \), we have only to use the corresponding solutions to the Schrödinger equation \(-\frac{d^2}{dz^2} + q_0(z) - \lambda \varphi = 0\).
Acknowledgement
K. A. is supported by Grant-in-Aid for Scientific Reserch (C) 17K05303, Japan Society for the Promotion of Science (JSPS). H. I. is supported by Grant-in-Aid for Scientific Research (C) 20K03667, JSPS. E. K. is supported by the RFBR grant No. 19-01-00094. H. M. is supported by Grant-in-Aid for Young Scientists (B) 16K17630, JSPS. The authors express their gratitude to these supports.

References

[1] S. Agmon and L. Hörmander, *Asymptotic properties of solutions of differential equations with simple characteristics*, J. d’Anal. Math., 30 (1976), 1-38.
[2] K. Ando, *Inverse scattering theory for discrete Schrödinger operators on the hexagonal lattice*, Ann. Henri Poincaré 14 (2013), 347-383.
[3] K. Ando, H. Isozaki and H. Morioka, *Spectral properties of Schrödinger operators on perturbed lattices*, Ann. Henri Poincaré 17 (2016), 2103-2171.
[4] K. Ando, H. Isozaki and H. Morioka, *Inverse scattering for Schrödinger operators on perturbed lattices*, Ann. Henri Poincaré 19 (2018), 3397-3455.
[5] K. Ando, H. Isozaki and H. Morioka, *Correction to Inverse scattering for Schrödinger operators on perturbed lattices*, Ann. Henri Poincaré 20 (2019), 337-338.
[6] K. Ando, H. Isozaki, E. Korotyaev and H. Morioka, *Inverse scattering on the quantum graph — Edge model for graphene*, arXiv:1911.05233.
[7] S. Avdonin, B. P. Belinskiy, and J. V. Matthews, *Dynamical inverse problem on a metric tree*, Inverse Problems 27 (2011), 075011.
[8] M. I. Belishev, *Boundary spectral inverse problem on a class of graphs (trees) by the BC method*, Inverse Problems 20 (2004), 647-672.
[9] J. von Below, *A characteristic equation associated to an eigenvalue problem on c²-networks*, Linear Algebra Appl. 71 (1985), 309-325.
[10] G. Berkolaiko and P. Kuchment, *Introduction to Quantum Graphs*, Mathematical Surveys and Monographs 186, AMS (2013).
[11] N. Bondarenko and C. T. Shieh, *Partial inverse problem for Sturm-Liouville operators on trees*, Proceedings of the Royal Society of Edinburgh 147A (2017), 917-933.
[12] N. Bondarenko, *Spectral data characterization for the Sturm-Liouville operator on the star-shaped graph*, arXiv:2009.02522v1.
[13] G. Borg, *Eine Umkehrung der Sturm-Liouvilleschen Eigenwertaufgabe. Bestimmung der Differentialgleichung durch die Eigenwerte*, Acta Math. 78 (1946), 1-96.
[14] B. M. Brown and R. Weikard, *A Borg-Levinson theorem for trees*, Proc. Royal Soc. Lond. Ser. A Math. Phys. Eng. Sci. 461 2062 (2005), 3231-3243.
[15] J. Brüning, V. Geyley and K. Pankrashkin, *Spectra of self-adjoint extensions and applications to solvable Schrödinger operators*, Rev. Math. Phys. 20 (2008), 1-70.
[16] C. Cattaneo, *The spectrum of the continuous Laplacian on a graph*, Monatsh. Math. 124 (1997), 215-235.
[17] T. Chen, P. Exner and O. Turek, *Inverse scattering for quantum graph vertices*, Phys. Rev. A (2011), 86:062715.
[18] F. Chung, *Spectral Graph Theory*, AMS. Providence, Rhode Island (1997).
[19] Y. Colin de Verdière, *Spectre de graphes*, Cours spécialisés 4, S. M. F., Paris, (1998).
[20] E. B. Curtis and J. A. Morrow, *Inverse Problems for Electrical Networks*, On Applied Mathematics, World Scientific, (2000).
[21] D. Cvetkovic, M. Doob, I. Gutman and A. Torgasev, *A recent result in the theory of graph spectra*, Annals of Discrete Mathematics 36, North-Holland Publishing Co., Amsterdam (1988).
[22] D. Cvetkovic, M. Doob and H. Saks, *Spectra of graphs, Theory and applications*, 3rd edition, Johann Ambrosius Barth, Heidelberg (1995).
[23] P. Exner, A. Kostenko, M. Malamud and H. Neidhardt, *Spectral theory for infinite quantum graph*, Ann. Henri Poincaré 19 (2018), 3457-3510.
[24] M. S. Eskina, *The direct and the inverse scattering problem for a partial difference equation*, Soviet Math. Doklady, 7 (1966), 193-197.
[25] B. Gutkin and U. Smilansky, *Can one hear the shape of a graph?* J. Phys. A **34** (2001), 6061-6068.
[26] H. Isozaki and E. Korotyaev, *Inverse problems, trace formulae for discrete Schrödinger operators*, Ann. Henri Poincaré, **13** (2012), 751-788.
[27] H. Isozaki and H. Morioka, *Inverse scattering at a fixed energy for discrete Schrödinger operators on the square lattice*, Ann. l’Inst. Fourier **65** (2015), 1153-1200.
[28] E. Korotyaev and I. Lobanov, *Schrödinger operators on zigzag nanotubes*, Ann. Henri Poincaré **8** (2007), 1151-1076.
[29] E. Korotyaev and N. Saburova, *Schrödinger operators on periodic discrete graphs*, J. Math. Anal. Appl. **420** (2014), 576-611.
[30] E. Korotyaev and N. Saburova, *Spectral band localization for Schrödinger operators on periodic graphs*, Proc. Amer. Math. Soc. **143** (2015), 3951-3967.
[31] E. Korotyaev and N. Saburova, *Scattering on metric graphs*, arXiv:1507.06441v1 [math.SP] 23 Jul 2015.
[32] E. Korotyaev and N. Saburova, *Estimates of bands for Laplacians on periodic equilateral metric graphs*, Proc. Amer. Math. Soc. **114** (2016), 1605-1617.
[33] E. Korotyaev and N. Saburova, *Effective masses for Laplacians on periodic graphs*, J. Math. Anal. Appl. **436** (2016), 104-130.
[34] V. Kostrykin and R. Schrader, *Kirchhoff’s rule for quantum wires*, J. Phys. A **32** (1999), 595-630.
[35] P. Kuchment, *Quantum graph spectra of a graphyne structure*, NanoNMTA, **2** (2013), 107-123.
[36] P. Kuchment and O. Post, *On the spectra of carbon nano-structures*, Commun. Math. Phys. **256** (2005), 805-826.
[37] K. Pankraskin, *Spectra of Schrödinger operators on equilateral quantum graphs*, Lett. Math. Phys. **77** (2006), 139-154.
[38] D. Parra and S. Richard, *Spectral and scattering theory for Schrödinger operators on perturbed topological crystals*, Rev. Math. Phys. **30** (2018), Article No. 1850009, pp 1-39.
[39] V. Pivovarchik, *Inverse problem for the Sturm-Liouville equation on a simple graph*, SIAM J. Math. Anal. **32** (2000), 801-819.
[40] J. Pöschel and E. Trubowitz, *Inverse Spectral Theory*, Academic Press, Boston, (1987).
[41] Y. Tadano, *Long-range scattering for discrete Schrödinger operators*, Ann. Henri Poincaré **20** (2019), 1439-1499.
[42] F. Visco-Comandini, M. Mirrahimi, and M. Sorine, *Some inverse scattering problems on star-shaped graphs*, J. Math. Anal. Appl. **387** (2011), 343-358.
