INVERSE SCATTERING ON THE QUANTUM GRAPH
— EDGE MODEL FOR GRAPHEN

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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, we show that the S-matrix for all energies in any open set in the continuous spectrum determines the potentials.

1. Introduction

1.1. Assumptions and main results. In this article, we study the spectral and inverse scattering theory associated with quantum graph, which is by definition a graph endowed with metric on its edges and equipped with differential operators on them. The quantum graph was introduced in 1930s as a simple model for free electrons in organic molecules [41], and its role has been increasing in physics, chemistry and engineering with particular interest in material science. A physical example we have in mind in this paper is the graphen, for which there are two mathematical models, both being based on the periodic hexagonal lattice. One model considers the propagation of waves only on the vertices, and deals with the discrete Laplacian on the vertex set, while the other focuses on the propagation of waves generated by Schrödinger operators defined on each edge and scattered by vertices and potentials. This latter is the quantum graph, and the former is often called the discrete graph. In this paper, we call the former the vertex model and the latter the edge model.

The edge model thus deals with a family of one-dimensional Schrödinger operators

$$-rac{d^2}{dz^2} + q_e(z)$$

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 $z \in (0, 1)$.

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Under these assumptions, the Schrödinger operator
\[ \hat{H}_E = \left\{ -\frac{d^2}{dz^2} + q_e(z); \ e \in \mathcal{E} \right\} \]
is self-adjoint and its essential spectrum \( \sigma_e(\hat{H}_E) \) is equal to \([0, \infty)\). We are interested in the spectral properties of this operator from two-sided viewpoints, the forward and the inverse problems. We start from the forward problem. We show that there exists a discrete (but infinite) subset \( T \subset \mathbb{R} \) such that \( \sigma_e(\hat{H}_E) \setminus T \) is absolutely continuous. We construct a complete family of generalized eigenfunctions describing the continuous spectrum, and represent Heisenberg's S-matrix. Based on these results on the forward problem, we turn to the inverse problem. The following two theorems are our main aim.

**Theorem 1.1.** Assume (Q-1), (Q-2) and (Q-3). Then, given any open interval \( I \subset (0, \infty) \setminus T \), 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), the S-matrix is meromorphic in the complex domain \( \{ \text{Re} \lambda > 0 \} \) with possible branch points at \( T \). Therefore, the assumption of Theorem 1.1 is equivalent to the condition that we are given the S-matrix for all energies in the continuous spectrum except for the set of exceptional points \( T \).

One can also deal with a perturbation of periodic edge potentials.

**Theorem 1.2.** Assume (Q-1) and (Q-3). Assume that there exists a real \( q_0(z) \in L^2(0,1) \) satisfying \( q_0(z) = q_0(1 - z) \) and that \( q_e(z) = q_0(z) \) on \((0,1)\) except for a finite number of edges \( e \in \mathcal{E} \). Given an open interval \( I \subset \sigma_e(\hat{H}_E) \setminus T \) and the S-matrix \( S(\lambda) \) for all \( \lambda \in I \), one can uniquely reconstruct the potential \( q_e(z) \) for all edges \( e \in \mathcal{E} \).

Note that under the assumption of Theorem 1.2, \( \sigma_e(\hat{H}_E) \) is a union of intervals with possible gaps between them.

Our proof gives not only the identification but also the reconstruction procedure of the potential, although some parts are transcendental. Our results are not restricted to the hexagonal lattice. Theorems 1.1 and 1.2 also hold for the square lattice and the triangular lattice. In fact, the forward problem part, i.e. the study of the spectral structure of the quantum graph encompasses a larger class of quantum graphs. The method for solving the inverse problem, however, leans over geometric features of the graph, hence should be discussed individually for the graph in question.

**1.2. Basic strategy.** There is a close similarity between Schrödinger operators in the continuous model and those in the discrete model or in the quantum graph. Let us explain it by reviewing the basic strategy of the stationary scattering theory.

For the Schrödinger operator \(-\Delta + V(x)\) in \( \mathbb{R}^d \), where \( V(x) \) decays sufficiently rapidly at infinity, there exists a generalized eigenfunction \( \varphi(x,\xi), x, \xi \in \mathbb{R}^d \), satisfying the equation
\[ (-\Delta + V(x) - |\xi|^2)\varphi(x,\xi) = 0 \]
having the following behavior at infinity
\[ \varphi(x,\xi) = e^{ix \cdot \xi} + e^{ikr} \frac{1}{r^{(d-1)/2}} a(k,\theta,\omega) + o(r^{-(d-1)/2}), \quad r = |x| \to \infty, \]
where \( k = |\xi| \), \( \theta = x/r \), \( \omega = \xi/k \). This family of generalized eigenfunctions \( \{ \varphi(x, \xi); \xi \in \mathbb{R}^d \} \) defines a generalized Fourier transform
\[
(F f)(\xi) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} \varphi(x, \xi) f(x) dx,
\]
which is a unitary operator from the absolutely continuous subspace for \( -\Delta + V(x) \) to \( L^2(\mathbb{R}^d) \) diagonalizing \( -\Delta + V(x) \). Heisenberg’s S-matrix is defined to be \( S(k) = I + C_0(k)A(k) \), where \( C_0(k) \) is a suitable constant and \( A(k) \), called the scattering amplitude, is an integral operator with kernel \( a(k, \theta, \omega) \). This S-matrix is unitary on \( L^2(S^{d-1}) \) for each \( k > 0 \) and is believed to contain all the information of the physical system in question. Note that \( \omega, \theta \) in (1.1) correspond to the incoming and outgoing directions of scattered particles, and, by passing to the Fourier transformation, \( kS^{d-1} = \{ k\omega; \omega \in S^{d-1} \} \) is the characteristic surface of the unperturbed operator \( -\Delta - k^2 \). This surface should be called the manifold at infinity, since it parametrizes the vectors representing the incoming and outgoing scattering states.

One can draw the same picture for discrete Schrödinger operators (in the vertex model) on perturbed periodic lattices of rank \( d \). In this case, by the Floquet (or Floquet-Bloch) theory, the manifold at infinity is the characteristic surface of the discrete Laplacian (difference operator) and is called the Fermi surface, \( M_{V, \lambda} \), which is a submanifold of codimension 1 in the torus \( T^d \). As for the quantum graph (the edge model), the action of \( \mathbb{Z}^d \) transforms the vertex set \( V \) into the torus \( T^d \) as in the case of vertex model, and, in addition, the edge set into the fundamental graph \( E^* \), which is a graph on the torus \( T^d \):

\[
\mathbb{Z}^d : V \to T^d, \quad E \to E^*.
\]

Therefore, in the case of quantum graph, the underlying Hilbert space is unitarily equivalent to \( L^2(T^d \times E^*) \). The notion of the characteristic surface is not obvious for the case of the quantum graph. However, the Kirchhoff condition induces the Laplacian on the set of vertices, which is the source of the continuous spectrum of \( \hat{H}_E \), and the Laplacian \( -(d/dz)^2 + q_e(z) \) on each edge \( e \) gives rise to the eigenvalues embedded in the continuous spectrum. Observing the resolvent of the free Hamiltonian, i.e. the one for the case \( q_e = 0 \) for all \( e \in E \) (cf. Lemma 3.7 below), we see that the manifold at infinity for the Schrödinger operator on the quantum graph is \( M_{V, -\cos \sqrt{\lambda}} \), i.e. the Fermi surface of the vertex Laplacian. The key of our arguments lies in the fact that the continuous spectrum of the edge model is determined by that of the vertex model. The stationary scattering theory for the edge model is thus developed as in the case of the vertex model, which in turn can be discussed in a way parallel to the continuous model.

The procedure of the inverse scattering is as follows. Since the perturbation is compactly supported, the S-matrix for the quantum graph is shown to be equivalent to the Dirichlet-to-Neumann map (D-N map in short) for an interior boundary value problem in the lattice space. The inverse problem of scattering is then reduced to the inverse boundary value problem for vertex Schrödinger operator in a bounded domain. Applying ideas developed for the inverse boundary value problems for the continuous model as well as the discrete model, from the knowledge of the D-N map, one can recover the Dirichlet eigenvalues for Schrödinger operators on each edge. By the classical result of Borg [10] (see also [35]), which is the starting point of the 1-dimensional inverse spectral theory, one can recover the edge potentials from the knowledge of the S-matrix.
In the course of the proof, we also prove that the knowledge of the D-N map for the edge model is equivalent to the knowledge of the D-N map for the vertex model (Lemma 6.1). This is significant, because it enables us to study the lattice structure from the S-matrix of the edge model (see Theorem 6.8). Suppose we are given an edge model on the hexagonal lattice without perturbation. We deform its compact part arbitrarily as a planar graph, and add $L^2$ potentials on edges for this compact part. Take an interior domain which contains all the perturbations. One can then develop the spectral theory for this perturbed edge model in the same way as in this paper. In particular, the S-matrix of any fixed energy for the whole space determines the D-N map for the finite domain of the graph as a vertex model. One can then apply the results in [4] to this finite part, e.g.

- Reconstruction of the potential on vertices.
- Location of defects of the lattice.
- Reconstruction as a planar graph, if one knows all the S-matrices of the edge model near the 0-energy.

1.3. Related works. Because of its theoretical as well as practical importance, plenty of works have been presented for Schrödinger operators on the graph. The monographs [18], [19], [15], [13], [9] 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 [9] together with an abundance of references therein. We note, in particular, that the relation between the vertex model and the edge model is a key step to understand the spectral structure of the quantum graph and studied by [8], [13], [39], [12]. See also [25], [38] for more recent results. As for the inverse problem for the quantum graph, the issue has been centered around the compact graph, the tree and the scattering problem by the infinite edges (leads). See e.g. [8], [31], [42], [22], [7], [11], [48], [14], [6], [47], [36] and other interesting papers cited in the above books. We must also mention the works [16], [17] on the planar discrete graph, which solved the inverse problem by giving the characterization of the D-N map of the associated boundary value problem and the reconstruction procedure starting from the D-N map.

Let us mention recent developments in the study of inverse problems for perturbed periodic systems dealing with vertex models and edge models. In [25], stationary problems and the existence and completeness of wave operators for the edge model were proved. For more detailed spectral properties, see [29], [30]. The long-range scattering for the perturbed periodic lattice is discussed in [37], [46] and [40]. As for the inverse problem of the perturbed periodic lattices, [23] showed that for the square lattice, compactly supported potentials are determined by the S-matrix of all energies. The case of hexagonal lattice was proved by [2]. Inverse scattering at a fixed energy was studied by [24] for the square lattice case. Spectral properties and inverse problems for more general vertex models were studied in [3] and [4], where it is shown that the S-matrix of the vertex model with one fixed energy determines compactly supported potentials as well as the convex hull of defects of the lattice, in the case of hexagonal lattice. Also, for the general perturbation of the finite part of the graph, the knowledge of the S-matrix with energies near the end points of the spectrum determines the graph structure as a planar graph. In [4], to prove these facts, the works [16], [17] played an essential role. The
The present paper is based on the results in [3] and [4] as well as [28]. As regards the quantum graph, in the recent work [20], spectral properties of quantum graphs are pursued on the structure without assuming the equal length property on edges, in particular, allowing \( \inf_{\mathbf{e} \in \mathcal{E}} |\mathbf{e}| = 0 \). We restrict ourselves to the case of periodic lattices perturbed by edge potentials and pursue detailed spectral properties. In [28], the eigenvectors and the generalized eigenfunctions for the free Hamiltonian are computed explicitly. In this paper, we adopt a more operator theoretical approach. The quantum graph is now a rapidly growing area in mathematical physics and material science. However, compared to the case of trees for instance, not so much is known about the perturbed periodic lattice and the corresponding quantum graph, especially on the inverse scattering. Even restricted to the forward problem, the results in this paper are new.

### 1.4. Plan of the paper

Spectral properties of the metric graph can be studied in a rather general framework. In §2, we introduce the periodic graph and the associated vertex model and edge model as well as Laplacians on them. The fundamental graph \( \mathcal{G} \) is also introduced. The basic assumptions (\( P \)), (\( E \)), (\( A-1 \)) \( \sim \) (\( A-4 \)) are given there. The main ingredients are the Kirchhoff condition (\( K \)), the discrete Fourier transforms \( \mathcal{U}_V, \mathcal{U}_E \), function spaces \( \mathcal{B}, \mathcal{B}^* \), which are used throughout the subsequent arguments. In §3, we derive representations of the resolvent of the perturbed edge Hamiltonian and the spectral measure of the free edge Hamiltonian. The key formula is (3.26), which describes the resolvent of the edge Laplacian in terms of the resolvent of the vertex Laplacian. We are mainly concerned with the formal relation between the vertex Laplacian and the edge Laplacian in this section. We prove the detailed estimates in §4. We proceed to derive the spectral representation of the edge Hamiltonian and the S-matrix in §5. We discuss the exterior and interior boundary value problems for the edge Laplacian in §6, and show that the S-matrix for the whole space determines uniquely the Dirichlet-to-Neumann map for the interior domain. Although our arguments are restricted to the hexagonal lattice in this section, we can actually consider in the general framework for the forward scattering theory on the metric graph until the end of §6. In §7, we study the inverse scattering for the hexagonal lattice and prove the main theorems.

### 1.5. Notation

The notation used in this paper is standard. Let \( \mathbf{Z} \) be the set of all integers, and \( \mathbf{N} = \{1, 2, 3, \cdots \} \) the set of natural numbers. For Banach spaces \( X \) and \( Y \), \( \mathcal{B}(X;Y) \) denotes the set of all bounded operators from \( X \) to \( Y \). For an operator \( A \), \( D(A) \) denotes the domain of \( A \). For a self-adjoint operator \( A \), let \( \sigma(A), \sigma_d(A), \sigma_e(A), \sigma_p(A), \sigma_{ac}(A) \) and \( \rho(A) \) be the spectrum, discrete spectrum, essential spectrum, point spectrum, absolutely continuous spectrum and the resolvent set of \( A \), respectively. Moreover, \( \mathcal{H}_{ac}(A) \) and \( \mathcal{H}_{pp}(A) \) denote the absolutely continuous subspace for \( A \) and the closure of the linear hull of the eigenvectors of \( A \), respectively. For an interval \( I \subset \mathbb{R} \) and a Hilbert space \( \mathbf{h} \), let \( L^2(I, \mathbf{h}; \rho(\lambda)d\lambda) \) be the set of \( \mathbf{h} \)-valued \( L^2 \)-functions on \( I \) with respect to the measure \( \rho(\lambda)d\lambda \). For a vertex set \( \mathcal{V} \), let \( \ell^2(\mathcal{V}) \) be the set of all square summable sequences on \( \mathcal{V} \), and \( \ell^2_{loc}(\mathcal{V}) \) the set of all sequences on \( \mathcal{V} \). Likewise, for an edge set \( \mathcal{E} \), let \( L^2(\mathcal{E}) \) be the set of all square integrable functions on \( \mathcal{E} \), and \( L^2_{loc}(\mathcal{E}) \) the set of functions which are square summable on any finite subset in \( \mathcal{E} \). Sobolev spaces \( H^m(\mathcal{E}) \) and \( H^m_{loc}(\mathcal{E}) \) are defined similarly. We often call a function defined on edges as an \textit{edge function}
and the one defined on vertices as vertex function. Similar expressions are also used when we contrast the vertex model and the edge model.

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2. Basic theory for the quantum graph

2.1. Periodic graph. We consider a periodic graph \( \Gamma = \{ V, E \} \) in \( \mathbb{R}^d \), where \( d \geq 2 \) is an integer, and \( V, E \) are a vertex set and an edge set defined as follows. Let \( L \) be a lattice of rank \( d \) in \( \mathbb{R}^d \) with basis \( v_j, j = 1, \cdots, d \), i.e.

\[
L = \{ v(n) ; n \in \mathbb{Z}^d \}, \quad v(n) = \sum_{j=1}^d n_j v_j, \quad n = (n_1, \cdots, n_d) \in \mathbb{Z}^d,
\]

and put

\[
\Gamma_* = \{ v(x) ; x \in [0, 1)^d \}, \quad v(x) = \sum_{j=1}^d x_j v_j.
\]

Given the points \( p^{(j)}, j = 1, \cdots, s \), satisfying

(P) \( p^{(j)} \in \Gamma_*, \quad p^{(i)} - p^{(j)} \notin L, \quad \text{if} \quad i \neq j, \)

we define the vertex set \( V \) by

\[
V = \bigcup_{j=1}^s (p^{(j)} + L).
\]

If \( s = 1 \), we assume that \( p^{(1)} = 0 \). There exists a bijection \( \mathcal{V} \ni v \to (j(v), n(v)) \in \{1, \cdots, s\} \times \mathbb{Z}^d \) such that

\[
v = v^{(j(v))} + v(n(v)).
\]

The group \( \mathbb{Z}^d \) acts on \( \mathcal{V} \) as follows:

\[
\mathbb{Z}^d \times \mathcal{V} \ni (m, v) \to m \cdot v := p^{(j(v))} + v(m + n(v)) \in \mathcal{V}.
\]

For \( v, w \in \mathcal{V} \), \( v \sim w \) means that they are the mutually opposite end points of a same edge. They are assumed to satisfy

\[
v \sim w \implies m \cdot v \sim m \cdot w, \quad \forall m \in \mathbb{Z}^d.
\]

For \( v \in \mathcal{V} \), the degree of \( v \) is the number of edges whose one end point is \( v \), and is denoted by \( \deg(v) \). Then \( \deg(p^{(j)} + v(n)) \) depends only on \( j \), and is denoted by \( \deg(j) \). In this paper, we deal with the case in which \( \deg(j) \) is independent of \( j \).

This is for the notational simplicity, and is not an essential restriction. In what follows, \( \deg(v) \) and \( \deg(j) \) are the same constant which we denote by \( d_g \):

\[
\deg(v) = \deg(j) = d_g.
\]

Let \( \Gamma = \{ \mathcal{V}, \mathcal{E} \} \) be as above. We identify each edge \( e \in \mathcal{E} \) with the interval \([0, 1]\), which introduces an orientation on the edge set \( \mathcal{E} \). Our argument below, in particular the spectrum of edge Laplacian, does not depend on this orientation. We assume that the \( \mathbb{Z}^d \)-action \( \text{(2.5)} \) preserves this orientation. Thus each edge
\( e \in \mathcal{E} \) is identified with an oriented pair \((e(0), e(1)) \in \mathcal{V} \times \mathcal{V}\), and is written as \( e = (e(0), e(1)) \). We call \( e(0) \) the initial vertex of \( e \), and \( e(1) \) the terminal vertex of \( e \). For a vertex \( v \in \mathcal{V}\), we put
\[
\mathcal{E}_v(0) = \{ e \in \mathcal{E} ; e(0) = v \}, \quad \mathcal{E}_v(1) = \{ e \in \mathcal{E} ; e(1) = v \},
\]
\[
\mathcal{E}_v = \mathcal{E}_v(0) \cup \mathcal{E}_v(1).
\]
If \( e \in \mathcal{E}_v \), we say that the edge \( e \in \mathcal{E} \) is associated with the vertex \( v \in \mathcal{V} \).

Finally, although not essential, we assume that our periodic graph is connected.

2.2. **Edge basis.** For an edge \( e \) and \( n \in \mathbb{Z}^d \), we define its translation \( e + [n] \) by
\[
e + [n] = (e(0) + v(n), e(1) + v(n)).
\]
By this \( \mathbb{Z}^d \)-action, \( \mathbb{Z}^d \times \mathcal{E} \ni (n, e) \mapsto e + [n] \in \mathcal{E} \), \( \mathcal{E} \) is decomposed into the orbits, i.e. there exist \( e_1, \ldots, e_{\nu} \in \mathcal{E} \) such that
\[
\mathcal{E} = \bigcup_{\ell=1}^{\nu} \mathcal{E}_\ell, \quad \mathcal{E}_\ell = \{ e_\ell + [n] ; n \in \mathbb{Z}^d \}.
\]
We call the set
\[
[\mathcal{E}] = \{ e_1, \ldots, e_{\nu} \}
\]
the edge basis. Note that the edge basis is not defined uniquely. Later, we will fix it in applying the Floquet theory on \( \Gamma \).

2.3. **Index.** Decompose the end points of an edge \( e \) into
\[
e(0) = e_\ast(0) + v(m^{(0)}), \quad e(1) = e_\ast(1) + v(m^{(1)}),
\]
where \( e_\ast(0), e_\ast(1), m^{(0)}, m^{(1)} \) are determined uniquely by the condition
\[
e_\ast(0), e_\ast(1) \in \Gamma_\ast, \quad m^{(0)}, m^{(1)} \in \mathbb{Z}^d.
\]
The index of \( e \) is introduced by [26] and defined as
\[
\text{Ind} \ (e) = m^{(1)} - m^{(0)}.
\]
Its meaning is as follows. For \( m = (m_1, \ldots, m_d) \in \mathbb{Z}^d \), let
\[
\Gamma_m = \{ v(x) ; x \in [m_1, m_1 + 1] \times \cdots \times [m_d, m_d + 1] \}.
\]
Then, there exist \( m^{(0)}, m^{(1)} \in \mathbb{Z}^d \) such that \( e(0) \in \Gamma_{m^{(0)}}, e(1) \in \Gamma_{m^{(1)}} \). Let \( e'(0) = e(0) + v(m^{(1)} - m^{(0)}) \in \Gamma_{m^{(1)}} \). Then, in \( \mathbb{R}^d \), the edge \( e = (e(0), e(1)) \) is homotopic to a curve from \( e(0) \) to \( e'(0) \) plus \( \{ e'(0), e(1) \} \), which is a curve in \( \Gamma_{m^{(1)}} \). Therefore, its projection to \( \Gamma_\ast \) is homotopic to a curve
\[
(e_\ast(0), e_\ast(1)) + n_1[C_1] + \cdots + n_d[C_d],
\]
where \( e_\ast(0), e_\ast(1) \) are projections of \( e(0), e(1) \) to \( \Gamma_\ast \), and \( \{ [C_1], \ldots, [C_d] \} \) is a standard basis of the homotopy group \( \pi_1(\mathbb{T}^d) \). Then, \( n = (n_1, \ldots, n_d) \) in (2.10) is the index of \( e \).
2.4. **Fundamental graph.** We impose the following assumption.

(E) The edge basis $[\mathcal{E}]$ defined by (2.9) forms a tree in $\Gamma$, i.e. a connected subgraph in $\Gamma$ without cycles. Moreover, every edge $e \in [\mathcal{E}]$ is given by $e = (v, w + \text{Ind}(e))$ where $v, w \in \Gamma_{s} \cap \mathcal{V}$.

Let $e_\ell$ be one of the edge basis. The projection of $e_\ell$ to $\Gamma_{s}$ is naturally identified with an edge on $T^d$, which is denoted by $e_\ell^*$. The assumption (E) implies that $\{e_1^*, \cdots, e_{\nu}^*\}$ forms a connected graph on $T^d$, whose edge set is denoted by $\mathcal{E}_*$:

$$\mathcal{E}_* = \{e_1^*, \cdots, e_{\nu}^*\}.$$  

**Definition 2.1.** We call $\mathcal{E}_*$ the fundamental graph of $\Gamma$.

For the connected periodic graph in $\mathbb{R}^d$, the fundamental graph contains at least $d$ cycles. The edge set $[\mathcal{E}]$ has no cycle, however, the fundamental graph $\mathcal{E}_*$ may contain cycles. The following lemma is a consequence of the assumption (P).

**Lemma 2.2.** Let $e_\ell^*(0), e_\ell^*(1)$ be the projections of $e_\ell(0), e_\ell(1)$ onto $\Gamma_{s}$, and put

$$V_* = \{e_\ell^*(0), e_\ell^*(1) : \ell = 1, \cdots, \nu\}.$$  

Then

$$V_* = \Gamma_{s} \cap \mathcal{V} = \{p^{(1)}, \cdots, p^{(s)}\}.$$  

Note that in Lemma 2.2, $\nu$ and $s$ are the number of edges and vertices of the fundamental graph. It says that any $p^{(i)}$ is an end point of some $e_\ell^*$, hence $\nu \geq s$. In fact, we have $\nu \geq s + d - 1$ for connected periodic graphs ([27]). The end points of $e_\ell^*$ may coincide, however, the edge $e_\ell^*$ is not reduced to a point. The fundamental graph is thus a graph on $T^d$ with the vertex set $V_*$ and the edge set $\mathcal{E}_*$.

**Figure 1.** Square lattice
2.5. Example (1) - \(d\)-dimensional Square lattice. Let \(s = 1, p^{(1)} = 0, \) and
\[n_1 = (1, 0, \cdots, 0), \cdots, n_d = (0, \cdots, 0, 1)\]
be the standard basis of \(\mathbb{R}^d\). Then, letting \(v_i = n_i\), we have

\[\mathcal{V} = \mathbb{Z}^d, \quad \Gamma_* = \{0, 1\}^d, \quad \mathcal{V}_* = \{0\},\]

\[|\mathcal{E}| = \{e_1, \cdots, e_d\}, \quad \mathcal{E}_* = \{e_{1*}, \cdots, e_{d*}\}, \quad e_{\ell*}(0) = e_{\ell*}(1) = 0, \quad \text{Ind}(e_{\ell*}) = n_\ell.\]

2.6. Example (2) - Hexagonal lattice. Let \(d = s = 2, \) and

\[
\begin{align*}
   v_1 &= \left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right), \quad v_2 = \left(\frac{3}{2}, \frac{\sqrt{3}}{2}\right), \\
   p^{(1)} &= (1, 0), \quad p^{(2)} = (2, 0), \\
   \mathcal{V} &= \bigcup_{j=1}^2 \left(p^{(j)} + \mathcal{L}\right), \quad \mathcal{L} = \{v(n); n \in \mathbb{Z}^2\}.
\end{align*}
\]

Then, we have

\[\Gamma_* = \left\{(x_1, x_2); -\frac{x_1}{\sqrt{3}} \leq x_2 \leq \frac{x_1}{\sqrt{3}}, -\sqrt{3} + \frac{x_1}{\sqrt{3}} < x_2 < \sqrt{3} - \frac{x_1}{\sqrt{3}} \right\},\]

which is the shaded region in Figure 3 and

\[\mathcal{V}_* = \{p^{(1)}, p^{(2)}\}, \quad |\mathcal{E}| = \{e_1, e_2, e_3\}, \quad \mathcal{E}_* = \{e_{1*}, e_{2*}, e_{3*}\}, \quad e_1 = \left(p^{(2)}, \left(\frac{5}{2}, \frac{\sqrt{3}}{2}\right)\right), \quad e_2 = \left(p^{(1)}, p^{(2)}\right), \quad e_3 = \left(p^{(1)}, \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)\right),\]

\[e_{1*}(0) = p^{(2)}, \quad e_{1*}(1) = p^{(1)}, \quad \text{Ind}(e_1) = (0, 1), \quad e_{2*}(0) = p^{(1)}, \quad e_{2*}(1) = p^{(2)}, \quad \text{Ind}(e_2) = (0, 0), \quad e_{3*}(0) = p^{(1)}, \quad e_{3*}(1) = p^{(2)}, \quad \text{Ind}(e_3) = (-1, 0).\]

In Figure 3 the edges \(e_1\) and \((e_1), e_3\) and \((e_3)\) are identified in \(\Gamma_*\).

Let us recall here the definition of fundamental domain. Given a lattice \(\mathbf{L}\) generated by a discrete group \(G\) acting on \(\mathbb{R}^d\), a set \(F \subset \mathbb{R}^d\) is said to be a fundamental domain of \(\mathbf{L}\) (or \(G\)) if it has the property

\[\mathbb{R}^d = \bigcup_{g \in G} g(F), \quad g(F) \cap g'(F) = \emptyset \quad \text{if} \quad g \neq g'.\]
The fundamental domain is not defined uniquely. An often used choice is
\[
\bigcap_{v \in L \setminus \{0\}} \left\{ x \in \mathbb{R}^d \mid x \cdot \frac{v}{|v|} \leq \frac{|v|}{2} \right\},
\]
the physical terminology of which is the Wigner-Seitz cell.

![Hexagonal lattice](image1)

**Figure 3. Hexagonal lattice**

![Fundamental graph](image2)

**Figure 4. Fundamental graph for the hexagonal lattice**

Let \( \mathcal{L} \) be the lattice in \( \mathbb{R}^2 \) generated by \( [2.12] \). Then \( \Gamma_* \) is a fundamental domain of \( \mathcal{L} \). Letting \( p^{(1)}, p^{(2)} \) be as in \( [2.13] \), put \( \mathcal{V} \) as in \( [2.14] \), which we regard as lattice. By the choice of \( p^{(1)}, p^{(2)} \), the neighboring points of any \( v \in \mathcal{V} \) have the same distance from \( v \). To fix the idea, we have defined the fundamental domain.
of $\mathcal{L}$ of (2.1) by (2.2). However, any rotation and translation of $\Gamma_*$ is again a fundamental domain of $\mathcal{L}$. In [3], we chose $v_1, v_2$ and $p^{(1)}, p^{(2)}$ to be

$$(2.15) \quad v_1 = (\frac{3}{2}, \frac{\sqrt{3}}{2}), \quad v_2 = (0, \sqrt{3}), \quad p^{(1)} = (\frac{1}{2}, -\frac{\sqrt{3}}{2}), \quad p^{(2)} = (1, 0),$$

which are obtained from $v_1, v_2$ of (2.12), and $p^{(1)}, p^{(2)}$ of (2.13) by rotation of angle $\pi/3$ followed by the translation $x \rightarrow x + (0, -\sqrt{3})$.

Taking the dual basis of $v_1, v_2$, $(v_i^* \cdot v_j = 2\pi \delta_{ij})$, we define the dual lattice of $V$. The Wigner-Seitz cell of this dual lattice is called the Brioullin zone. As is seen in Figure 3, the Wigner-Seitz cell for the hexagonal lattice is a hexagon centered at the origin.

2.7. Fourier series. Let $\ell^2(\mathcal{V})$ be the set of $C$-valued functions $\hat{f} = \{\hat{f}(v)\}_{v \in \mathcal{V}}$ on $\mathcal{V}$ satisfying

$$\|\hat{f}\|_2 := \sum_{v \in \mathcal{V}} |\hat{f}(v)|^2 d_g < \infty,$$

$d_g$ being defined by (2.6), which is a Hilbert space equipped with the inner product

$$(2.16) \quad (\hat{f}, \hat{g}) = \sum_{v \in \mathcal{V}} \hat{f}(v) \overline{\hat{g}(v)} d_g.$$

Recalling that the vertex set $\mathcal{V}$ is written as a disjoint union $\mathcal{V} = \bigcup_{j=1}^{s} (p^{(j)} + \mathcal{L})$, for any $C$-valued function $\hat{f}(v)$ on $\mathcal{V}$, we associate a function on $\mathbf{Z}^d$ by

$$\hat{f}(p^{(j)} + v(n)) = \hat{f}_j(n), \quad n \in \mathbf{Z}^d.$$ 

Using the correspondence

$$(2.17) \quad \hat{f}(v) \longleftrightarrow (\hat{f}_1(n), \cdots, \hat{f}_s(n)),$$

we identify $\hat{f}(v)$ with $(\hat{f}_1(n), \cdots, \hat{f}_s(n))$, and write

$$\hat{f}(n) = (\hat{f}_1(n), \cdots, \hat{f}_s(n)).$$

This induces a natural identification:

$$\ell^2(\mathcal{V}) = (\ell^2(\mathbf{Z}^d))^s.$$

We then define a unitary operator $U_{\mathcal{V}} : \ell^2(\mathcal{V}) \rightarrow L^2(\mathbf{T}^d)^s$ by

$$(2.18) \quad (U_{\mathcal{V}} \hat{f})(x) = (2\pi)^{-d/2} \sqrt{d_g} \sum_{n \in \mathbf{Z}^d} \hat{f}(n) e^{i n \cdot x},$$

where $L^2(\mathbf{T}^d)^s$ is equipped with the inner product

$$(2.19) \quad (f, g)_{L^2(\mathbf{T}^d)^s} = \sum_{j=1}^{s} \int_{\mathbf{T}^d} f_j(x) \overline{g_j(x)} dx.$$
2.8. **Vertex Laplacian.** The vertex Laplacian \( \hat{\Delta}_V \) on \( V \) is defined by the following formula

\[
(\hat{\Delta}_V \hat{f})(n) = (\hat{g}_1(n), \cdots, \hat{g}_s(n)),
\]

\[
\hat{g}_i(n) = \frac{1}{d_g} \sum_{b \sim p^{(i)} + v(n)} \hat{f}_{j(b)}(n(b)), \quad b = p^{(j(b))} + v(n(b)).
\]

Passing to the Fourier series, we rewrite it into the following form :

\[
(U_V(-\hat{\Delta}_V)U_V^{-1} f)(x) = H_0(x) f(x), \quad f \in L^2(T^d)^s,
\]

where \( H_0(x) \) is an \( s \times s \) Hermitian matrix whose entries are trigonometric functions.

Let \( D \) be the \( s \times s \) diagonal matrix whose \((j,j)\) entry is \( \sqrt{\text{deg}(j)} \). Then

\[
H_0(x) = DH_0^0(x)D^{-1}, \quad H_0^0(x) = U_V(-\hat{\Delta}_V)U_V^{-1}.
\]

Let \( \lambda_j(x), j = 1, \cdots, s \), be the eigenvalues of \( H_0(x) \):

\[
\lambda_1(x) \leq \lambda_2(x) \leq \cdots \leq \lambda_s(x).
\]

Then, we have

\[
\sigma(-\hat{\Delta}_V) = \bigcup_{j=1}^s \lambda_j(T^d).
\]

In the following examples, the sum in (2.20) is ranging over all nearest neighboring vertices of \( p^{(i)} + v(n) \).

**Example (1) - \( d \)-dimensional Square lattice.** Here, \( \hat{u}(n) \) is a \( \mathbb{C} \)-valued function on \( \mathbb{Z}^d \) and the Laplacian is

\[
(\hat{\Delta}_V \hat{u})(n) = \frac{1}{2d} \sum_{|n' - n|_1 = 1} \hat{u}(n').
\]

Hence

\[
H_0(x) = -\frac{1}{d} (\cos x_1 + \cdots + \cos x_d).
\]

**Example (2) - Hexagonal lattice.** Here, \( \hat{u}(n) \) has two components \( \hat{u}(n) = (\hat{u}_1(n), \hat{u}_2(n)) \), and the Laplacian is defined by

\[
(\hat{\Delta}_V \hat{u})(n) = (\hat{w}_1(n), \hat{w}_2(n)),
\]

\[
\hat{w}_1(n) = \frac{1}{3} \sum_{|v(n') - v(n)|_1 = 1} \hat{u}_2(n'),
\]

\[
\hat{w}_2(n) = \frac{1}{3} \sum_{|v(n') - v(n)|_1 = 1} \hat{u}_1(n').
\]

Hence

\[
H_0(x) = -\frac{1}{3} \begin{pmatrix} 0 & 1 + e^{-ix_1} + e^{-ix_2} \\ 1 + e^{ix_1} + e^{ix_2} & 0 + e^{-ix_1} + e^{-ix_2} \end{pmatrix}.
\]
2.9. **Kirchhoff condition.** As is noted above, we employ the identification:

\[ \mathcal{E} \ni (\mathbf{e}(0), \mathbf{e}(1)) \leftrightarrow (0, 1) \subset \mathbb{R}. \]

Therefore, given \( \mathbf{e} \in \mathcal{E} \), we use the abbreviation

\[ (2.22) \quad \hat{u}_e(z) = \hat{u}_e((1 - z)e(0) + ze(1)). \]

Hence on each edge \( \mathbf{e} \in \mathcal{E} \), we consider the Hilbert space \( L^2_e = L^2(0, 1) \), and define the Hilbert space \( L^2(\mathcal{E}) \) of \( L^2 \)-functions

\[ \hat{f} = \{ \hat{f}_e \}_{e \in \mathcal{E}} \]

on the edge set \( \mathcal{E} \) equipped with the inner product

\[ (2.23) \quad (\hat{f}, \hat{g})_{L^2(\mathcal{E})} = \sum_{e \in \mathcal{E}} (\hat{f}_e, \hat{g}_e)_{L^2(0, 1)}. \]

**Definition 2.3.** A function \( \hat{u} = \{ \hat{u}_e \}_{e \in \mathcal{E}} \) defined on \( \mathcal{E} \) is said to satisfy the Kirchhoff condition if

\( (K-1) \) \( \hat{u} \) is continuous on \( \mathcal{E} \),

\( (K-2) \) \( \hat{u}_e \in C^1([0, 1]) \) on each edge \( \mathbf{e} \in \mathcal{E} \), and

\[ \sum_{e \in \mathcal{E}_+(1)} \hat{u}_e'(1) - \sum_{e \in \mathcal{E}_+(0)} \hat{u}_e'(0) = 0. \]

In (K-1), we regard \( \mathcal{E} \) as a closed subset of \( \mathbb{R}^d \) by the induced topology. Therefore, \( \hat{u}_e(e(p)) = \hat{u}_{e'}(e'(q)) \) if \( e(p) = e'(q) \) for \( p, q = 0 \) or 1.

2.10. **Edge Laplacian.** On \( L^2_e = L^2(0, 1) \), we consider the 1-dimensional Schrödinger operator

\[ h^{(0)}_e = -d^2/dz^2, \quad h_e = h^{(0)}_e + q_e(z). \]

Assume that \( q_e \) satisfies (Q-1) and (Q-2). Define the Hamiltonian

\[ (2.24) \quad \hat{H}_e : \hat{u} = \{ \hat{u}_e \}_{e \in \mathcal{E}} \rightarrow \{ h_e \hat{u}_e \}_{e \in \mathcal{E}} \]

with domain \( D(\hat{H}_e) \) consisting of \( \hat{u}_e \in H^2(0, 1) \) satisfying the Kirchhoff condition (K-1), (K-2) and \( \sum_{e \in \mathcal{E}} \| -d^2\hat{u}_e/dz^2 + q_e \hat{u}_e \|_{L^2(0,1)}^2 < \infty \). By integration by parts, one can show that \( \hat{H}_e \) is self-adjoint in \( L^2(\mathcal{E}) \).

When \( q_e = 0 \), \( \hat{H}_e \) is denoted by \( \hat{H}_e^{(0)} \) or \( -\hat{\Delta}_e \), i.e.

\[ ( -\hat{\Delta}_e \hat{u} )_e(z) = -\frac{d^2}{dz^2} \hat{u}_e(z), \quad e \in \mathcal{E}. \]

We call it the **edge Laplacian.** Let \( q_e \) be the multiplication operator defined by

\[ (q_e \hat{f})_e(z) = q_e(z) \hat{f}_e(z), \quad e \in \mathcal{E}. \]

Then

\[ \hat{H}_e = \hat{H}_e^{(0)} + q_e. \]
2.11. Floquet theory. The Floquet (or Floquet-Bloch) theory transforms operators periodic on $\mathbb{Z}^d$ into the one on $\mathbb{T}^d \times M$, where $M$ is a suitable manifold. Recall that, by fixing a set of edge basis $\{e_1, \ldots, e_\nu\}$ satisfying the assumption (E), any $e \in \mathcal{E}$ is uniquely written as
\[
e = e_\ell + [n], \quad 1 \leq \ell \leq \nu, \quad n \in \mathbb{Z}^d.
\]
Using the action of $\mathbb{Z}^d$ on $\mathcal{E}$: $n \to e + [n]$, (see (2.27)), we define a unitary operator $U_\mathcal{E} : L^2(\mathbb{T}^d \times (0, 1)) \to (L^2(\mathbb{T}^d \times (0, 1)))^\nu$ by
\[
U_\mathcal{E} = (U_{\mathcal{E}, 1}, \ldots, U_{\mathcal{E}, \nu}),
\]
(2.25)
\[
(U_{\mathcal{E}, \ell}\hat{f})(x, z) = (2\pi)^{-d/2} \sum_{n \in \mathbb{Z}^d} e^{i n \cdot x} \hat{f}_{e_\ell + [n]}(z), \quad (x, z) \in \mathbb{T}^d \times [0, 1].
\]
The adjoint operator of $U_{\mathcal{E}, \ell}$ is
\[
(U_{\mathcal{E}, \ell}^* g)(n, z) = (2\pi)^{-d/2} \int_{\mathbb{T}^d} e^{-i n \cdot x} g(x, z) dx.
\]
(2.26)
The Fourier series gives rise to a unitary operator from $\ell^2(\mathbb{Z}^d; L^2(0, 1))$, the set of the $L^2(0, 1)$-valued $\ell^2$-functions on $\mathbb{Z}^d$, to $L^2(\mathbb{T}^d \times (0, 1))$. By Definition 2.1 and the above formulas (2.26) and (2.27), $U_\mathcal{E}$ is unitary:
\[
U_\mathcal{E} : L^2(\mathcal{E}) \to L^2(\mathbb{T}^d \times \mathcal{E}_*).
\]
The following Lemma 2.4 is proved in [28], Theorem 1.1.

**Lemma 2.4.** Let $\hat{f} \in H^2(\mathcal{E})$. Then, $\hat{f}$ satisfies the Kirchhoff condition if and only if $f = (f_1, \ldots, f_\nu) = U_\mathcal{E} \hat{f}$ satisfies
\[
e^{i \delta_\ell(v) \text{Ind}(e_k)} f_\ell(x, \delta_k(v)) = e^{i \delta_\ell(v) \text{Ind}(e_k)} f_\ell(x, \delta_k(v)),
\]
provided $v \in \partial_\mathcal{E}(e_k) \cap \partial_\mathcal{E}(e_k)$, and for $v \in \mathcal{V}_*$
\[
\sum_{\ell \in L_+(v)} (-1)^{\delta_\ell(v)} e^{i \delta_\ell(v) \text{Ind}(e_k)} f'_\ell(x, \delta_k(v)) = 0,
\]
where $f'_\ell(x, z) = \frac{\partial}{\partial z} f_\ell(x, z)$. 

Let $\mathcal{V}_*$ be as in (2.11), and for $v \in \mathcal{V}_*$, put
\[
L_+(v) = \{\ell; e_\ell(0) = v \text{ or } e_\ell(1) = v\},
\]
and for $\ell \in L_+(v)$
\[
\delta_\ell(v) = \begin{cases} 
1 & \text{if } v = e_\ell(1), \\
0 & \text{if } v = e_\ell(0).
\end{cases}
\]
(2.28)
The Floquet operator $-\Delta_{\mathcal{E}_s}(x)$ is a differential operator on $L^2(\mathcal{E}_s)$ with parameter $x \in \mathbb{T}^d$ defined by
\[
(-\Delta_{\mathcal{E}_s}(x)u)_{\mathcal{E}_s}(x,z) = -u''_{\mathcal{E}_s}(x,z), \quad u'' = \frac{\partial^2}{\partial x^2},
\]
where $u_{\mathcal{E}_s}(x, \cdot) \in H^2(0,1)$ for each $x \in \mathbb{T}^d$ and satisfies the following quasi-periodic condition at any $v \in \mathcal{V}_s$
\[
e^{i\delta_k(v)\text{Ind}(e_k')x}u_{\mathcal{E}_s}(x, \delta_k(v)) = e^{i\delta_{\ell}(v)\text{Ind}(e_{\ell})x}u_{\mathcal{E}_s}(x, \delta_{\ell}(v)),
\]
where $e_{k}, e_{\ell}$ satisfy $v \in \partial_s(e_k) \cap \partial_s(e_{\ell})$, and
\[
\sum_{\ell \in L_s(v)}(-1)^{\delta_k(v)\text{Ind}(e_{\ell})}u'_{\mathcal{E}_s}(x, \delta_{\ell}(v)) = 0.
\]
For $U^2 \in D(-\tilde{\Delta}_{\mathcal{E}})
\[
- (U^2 \tilde{\Delta}_{\mathcal{E}} U^2 u)(x,z) = -\Delta_{\mathcal{E}_s}(x)u(x,z)
\]
holds, and $-\Delta_{\mathcal{E}_s}(x)$ is self-adjoint in $L^2(\mathcal{E}_s)$.

2.12. Fermi surface. Spectral properties of the vertex Laplacian depend on its characteristic surface, i.e. the Fermi surface. To describe it, we use the following notations.

Let $\lambda_1(x) \leq \lambda_2(x) \leq \cdots \leq \lambda_s(x)$ be the eigenvalues of $H_0(x)$, and
\begin{equation}
M_{V,\lambda,j} = \{x \in \mathbb{T}^d : \lambda_j(x) = \lambda\},
\end{equation}
\begin{equation}
p(x, \lambda) = \det(H_0(x) - \lambda) = \prod_{j=1}^{s}(\lambda_j(x) - \lambda),
\end{equation}
\begin{equation}
M_{V,\lambda} = \{x \in \mathbb{T}^d : p(x, \lambda) = 0\} = \bigcup_{j=1}^{s} M_{V,\lambda,j},
\end{equation}
\[
\mathbb{T}^d_C = \mathbb{C}^d/(2\pi \mathbb{Z})^d, \quad M_{V,\lambda}^C = \{z \in \mathbb{T}^d_C : p(z, \lambda) = 0\},
\]
\[
M_{V,\lambda,\text{reg}}^C = \{z \in M_{V,\lambda}^C : \nabla z p(z, \lambda) \neq 0\},
\]
\[
M_{V,\lambda,\text{reg}}^C = \{z \in M_{V,\lambda}^C : \nabla z p(z, \lambda) = 0\}.
\]

Let $H_0$ be the self-adjoint operator of multiplication by $H_0(x)$ on $\mathbb{T}^d$. As in [3], we impose the following assumptions on the free system.

(A-1) There exists a subset $\mathcal{T}_1 \subset \sigma(H_0)$ such that for $\lambda \in \sigma(H_0) \setminus \mathcal{T}_1$,

(A-1-1) $M_{V,\lambda,\text{reg}}^C$ is discrete.

(A-1-2) Each connected component of $M_{V,\lambda,\text{reg}}^C$ intersects with $\mathbb{T}^d$ and the intersection is a $(d-1)$-dimensional real analytic submanifold of $\mathbb{T}^d$.

(A-2) There exists a finite set $\mathcal{T}_0 \subset \sigma(H_0)$ such that

\[M_{V,\lambda,i} \cap M_{V,\lambda,j} = \emptyset, \quad \text{if} \quad i \neq j, \quad \lambda \in \sigma(H_0) \setminus \mathcal{T}_0.\]

(A-3) $\nabla z p(x, \lambda) \neq 0$, on $M_{V,\lambda}$, $\lambda \in \sigma(H_0) \setminus \mathcal{T}_0$.

(A-4) The unique continuation property holds for $-\Delta_V$ in $\mathcal{V}$, i.e., if there exist $\tilde{u}$ and a constant $\lambda$ such that $(-\Delta_V - \lambda)\tilde{u} = 0$ holds on $\mathcal{V}$, and $\tilde{u} = 0$ except for a finite number of vertices, then $\tilde{u} = 0$ on $\mathcal{V}$.

\[^1\text{This assumption is incorrectly stated in [4]. Here, we give a correct assumption. See [5].}\]
We put
(2.34) \( T = \mathcal{T}_0 \cup \mathcal{T}_1 \cup \sigma_p(-\Delta_V). \)

For the square, triangular, hexagonal, Kagome, diamond lattices and the subdivision of square lattice, \( \mathcal{T}_1 \) is a finite set. However, for the ladder and graphite, \( \mathcal{T}_1 \) fills closed intervals. See \( [3], \S 5. \)

2.13. Function spaces. We use the following function spaces on the edge set \( \mathcal{E} \):

\[
\hat{L}^{2,\sigma}(\mathcal{E}) \ni \hat{f} \iff \sum_{\ell=1}^{\nu} \sum_{n \in \mathbb{Z}^d} (1 + |n|^2)^{\sigma/2} \| \hat{\mathcal{F}}_{\ell}[\hat{f}(n)] \|_{L^2(0,1)}^2 < \infty,
\]

where \( \sigma \in \mathbb{R} \) is a parameter,

\[
\hat{B}(\mathcal{E}) \ni \hat{f} \iff \| \hat{f} \|_{\hat{B}(\mathcal{E})} = \sup_{R > 1} \frac{1}{R} \sum_{J \subseteq \mathbb{Z}^d} \sum_{|n| < R} \| \hat{\mathcal{F}}_{\ell}[\hat{f}(n)] \|_{L^2(0,1)}^2 < \infty,
\]

where \( r_{-1} = 0, r_j = 2^j (j \geq 0), \)

\[
\hat{B}^*(\mathcal{E}) \ni \hat{f} \iff \lim_{R \to \infty} \frac{1}{R} \sum_{\ell=1}^{\nu} \sum_{|n| < R} \| \hat{\mathcal{F}}_{\ell}[\hat{f}(n)] \|_{L^2(0,1)}^2 = 0.
\]

Their counter parts on the vertex set \( \mathcal{V} \) are:

\[
\hat{L}^{2,\sigma}(\mathcal{V}) \ni \hat{f} \iff \sum_{n \in \mathbb{Z}^d} (1 + |n|^2)^{\sigma/2} \| \hat{\mathcal{F}}(n) \|_{L^2(0,1)}^2 < \infty,
\]

\[
\hat{B}(\mathcal{V}) \ni \hat{f} \iff \| \hat{f} \|_{\hat{B}(\mathcal{V})} = \sum_{J \subseteq \mathbb{Z}^d} \sum_{|n| < r_{-1}} \| \hat{\mathcal{F}}(n) \|_{L^2(0,1)}^2 < \infty,
\]

\[
\hat{B}^*(\mathcal{V}) \ni \hat{f} \iff \lim_{R \to \infty} \frac{1}{R} \sum_{|n| < R} \| \hat{\mathcal{F}}(n) \|_{L^2(0,1)}^2 = 0.
\]

We also introduce their counter parts on the torus: Letting \( f = U \hat{f}, \)

\[
H^\sigma(\mathbb{T}^d \times \mathcal{E}_*) \ni f \iff \hat{f} \in \hat{L}^{2,\sigma}(\mathcal{E}),
\]

\[
\hat{B}(\mathbb{T}^d \times \mathcal{E}_*) \ni f \iff \hat{f} \in \hat{B}(\mathcal{E}),
\]

\[
\hat{B}^*(\mathbb{T}^d \times \mathcal{E}_*) \ni f \iff \hat{f} \in \hat{B}^*(\mathcal{E}),
\]

\[
\hat{B}_0^*(\mathbb{T}^d \times \mathcal{E}_*) \ni f \iff \hat{f} \in \hat{B}_0^*(\mathcal{E}).
\]

Their counter parts for the vertex set \( \mathcal{V} \) are:

\[
H^\sigma(\mathbb{T}^d) \ni f \iff \hat{f} \in \hat{L}^{2,\sigma}(\mathcal{V}),
\]

\[
\hat{B}(\mathbb{T}^d) \ni f \iff \hat{f} \in \hat{B}(\mathcal{V}),
\]

\[
\hat{B}^*(\mathbb{T}^d) \ni f \iff \hat{f} \in \hat{B}^*(\mathcal{V}),
\]

\[
\hat{B}_0^*(\mathbb{T}^d) \ni f \iff \hat{f} \in \hat{B}_0^*(\mathcal{V}).
\]
Here, the discrete Fourier transform \( \hat{f} \rightarrow f \) is the usual Fourier series defined on the vertex set \( \mathcal{V} \).

Note that letting \( H^{s}(\mathbb{T}^d) \), \( B_{1/2}(\mathbb{T}^d) \) and \( B_{-1/2}(\mathbb{T}^d) \) be the Sobolev and Besov spaces on \( \mathbb{T}^d \) (see [1]), we have
\[
H^{s}(\mathbb{T}^d \times \mathcal{E}_*) = H^{s}(\mathbb{T}^d) \otimes L^2(\mathcal{E}_*),
\]
\[
B(\mathbb{T}^d \times \mathcal{E}_*) = B_{1/2}(\mathbb{T}^d) \otimes L^2(\mathcal{E}_*),
\]
\[
B^{*}(\mathbb{T}^d \times \mathcal{E}_*) = B_{-1/2}(\mathbb{T}^d) \otimes L^2(\mathcal{E}_*).
\]

**Definition 2.5.** For \( f, g \in B^{*}(\mathbb{T}^d \times \mathcal{E}_*) \), we use the notation \( f \simeq g \) in the following sense:
\[
f \simeq g \iff f - g \in E_0(\mathbb{T}^d \times \mathcal{E}_*).
\]

We use the same notation \( \simeq \) for \( \hat{B}^{*}(\mathcal{E}_1) \), \( \hat{B}^{*}(\mathcal{V}) \) and \( \hat{B}^{*}(\mathbb{T}^d) \).

### 3. Resolvent Formulae

The purpose of this section is to represent the resolvents of the Schrödinger operators
\[
(3.1) \quad \hat{R}_{\mathcal{E}}^{(0)}(\lambda) = (\hat{H}_{\mathcal{E}}^{(0)} - \lambda)^{-1}, \quad \hat{R}_{\mathcal{E}}(\lambda) = (\hat{H}_{\mathcal{E}} - \lambda)^{-1}
\]
in terms of those of the vertex Laplacian and the 1-dimensional Schrödinger operator on each edge. We give a formal derivation here, and justify them in the next section.

#### 3.1. Green operator on the edge

Let \( -(d^2/dz^2)_D \) be the Laplacian on \((0,1)\) with boundary condition \( u(0) = u(1) = 0 \). By the assumption (Q-1), the operator \( -(d^2/dz^2)_D + q_{e}(z) \) equipped with domain \( H^2(0,1) \cap H^1_0(0,1) \) is self-adjoint. Let \( r_{e}(\lambda) \) be the resolvent:
\[
r_{e}(\lambda) = \left( - (d^2/dz^2)_D + q_{e}(z) - \lambda \right)^{-1}.
\]
Let \( \phi_{e0}(z, \lambda), \phi_{e1}(z, \lambda) \) be the solutions of
\[
( -d^2/dz^2 + q_{e}(z) - \lambda) \phi = 0
\]
with initial data
\[
\begin{align*}
\phi_{e0}(0, \lambda) &= 0, & \phi_{e1}(1, \lambda) &= 0, \\
\phi'_{e0}(0, \lambda) &= 1, & \phi'_{e1}(1, \lambda) &= -1.
\end{align*}
\]
Note that \( \phi_{e0}(1, \lambda) = 0 \) or \( \phi_{e1}(0, \lambda) = 0 \) if and only if \( \lambda \) is an eigenvalue of \( -(d^2/dz^2)_D + q_{e}(z) \). In the following, we assume that
\[
\lambda \notin \bigcup_{e \in \mathcal{E}} \sigma \left( -(d^2/dz^2)_D + q_{e}(z) \right).
\]

The resolvent \( r_{e}(\lambda) \) is then written as
\[
(3.2) \quad (r_{e}(\lambda) \hat{f})(z) = \frac{1}{C(\lambda)} \int_0^\infty \phi_{e1}(z, \lambda) \phi_{e0}(t, \lambda) \hat{f}(t) \, dt + \frac{1}{C(\lambda)} \int_z^1 \phi_{e0}(z, \lambda) \phi_{e1}(t, \lambda) \hat{f}(t) \, dt,
\]
\[
C(\lambda) = \phi_{e0}(1, \lambda) = \phi_{e1}(0, \lambda),
\]
the last line of which is proven by computing the Wronskian. Then, we have

$$\frac{d}{dz}r_e(\lambda)\tilde{f}(z)_{|z=0} = \frac{1}{C(\lambda)} \int_0^1 \phi_{e1}(t, \lambda)\tilde{f}(t)dt,$$

$$\frac{d}{dz}r_e(\lambda)\tilde{f}(z)_{|z=1} = -\frac{1}{C(\lambda)} \int_0^1 \phi_{e0}(t, \lambda)\tilde{f}(t)dt.$$ 

We define operators $\Phi_{e0}(\lambda), \Phi_{e1}(\lambda) : L^2(0, 1) \to C$ by

$$(3.4) \quad \Phi_{e1}(\lambda)\tilde{f} = \int_0^1 \frac{\phi_{e0}(t, \lambda)}{\phi_{e0}(1, \lambda)}\tilde{f}(t)dt, \quad \Phi_{e0}(\lambda)\tilde{f} = \int_0^1 \frac{\phi_{e1}(t, \lambda)}{\phi_{e1}(0, \lambda)}\tilde{f}(t)dt.$$ 

Their adjoints : $C \to L^2(0, 1)$ are defined for $c \in C$ by

$$\Phi_{e1}(\lambda)^*c = c\frac{\phi_{e0}(z, \lambda)}{\phi_{e0}(1, \lambda)}, \quad \Phi_{e0}(\lambda)^*c = c\frac{\phi_{e1}(z, \lambda)}{\phi_{e1}(0, \lambda)}.$$ 

3.2. Kirchhoff condition and vertex Laplacian. We put

$$(3.5) \quad \tilde{u}_e(z, \lambda) = \Phi_{e1}(\lambda)^*c_e(1, \lambda) + \Phi_{e0}(\lambda)^*c_e(0, \lambda) + r_e(\lambda)\tilde{f}_e,$$

where $c_e(0, \lambda), c_e(1, \lambda)$ are to be specified later. It satisfies

$$\begin{cases} 
- \frac{d^2}{dz^2} + q_e - \lambda \tilde{u}_e = \tilde{f}_e, & \text{on} \ (0, 1), \\
\tilde{u}_e(0, \lambda) = c_e(0, \lambda), & \tilde{u}_e(1, \lambda) = c_e(1, \lambda).
\end{cases}$$

Here we have used (2.22). The following lemma reduces the edge Laplacian to the vertex Laplacian.

**Lemma 3.1.** (1) For $\tilde{u}_e(z, \lambda)$ defined by (3.5), the Kirchhoff condition (K-1) is fulfilled if and only if for two edges $e, e' \in \mathcal{E}$ and $p = 0, 1, q = 0, 1,$

$$e(p) = e'(q) \implies c_e(p, \lambda) = c_e(q, \lambda).$$

(2) The condition (K-2) is satisfied if and only if

$$-\sum_{e \in \mathcal{E}_v(0)} \frac{1}{\phi_{e0}(1, \lambda)}c_e(1, \lambda) - \sum_{e \in \mathcal{E}_v(1)} \frac{1}{\phi_{e0}(0, \lambda)}c_e(0, \lambda)$$

$$-\sum_{e \in \mathcal{E}_v(0)} \frac{\phi'_{e1}(0, \lambda)}{\phi_{e1}(0, \lambda)}c_e(0, \lambda) + \sum_{e \in \mathcal{E}_v(1)} \frac{\phi'_{e0}(1, \lambda)}{\phi_{e0}(1, \lambda)}c_e(1, \lambda)$$

$$= \sum_{e \in \mathcal{E}_v(1)} \Phi_{e1}(\lambda)\tilde{f}_e + \sum_{e \in \mathcal{E}_v(0)} \Phi_{e0}(\lambda)\tilde{f}_e$$

holds at any $v \in \mathcal{V}.$

Proof. Take $v \in \mathcal{V}$ and $e \in \mathcal{E}_v$. Then $e(p) = v$ for $p = 0$ or $1$ and $\tilde{u}_e(e(p), \lambda) = c_e(p, \lambda).$ The condition (K-1) means that the value of $\tilde{u} = \{\tilde{u}_e\}_{e \in \mathcal{E}}$ at $v$ depends only on $v$ and is independent of the edge $e$. This proves (1).

By (3.5), for $p = 0, 1,$

$$\tilde{u}'_e(p, \lambda) = c_e(1, \lambda)\frac{\phi'_{e0}(p, \lambda)}{\phi_{e0}(1, \lambda)} + c_e(0, \lambda)\frac{\phi'_{e1}(p, \lambda)}{\phi_{e1}(0, \lambda)} + \frac{d}{dz}r_e(\lambda)\tilde{f}_e_{|z=p},$$

where $' = d/dz.$ In (K-2), we replace $\tilde{u}_e$ and $\tilde{u}'_e$ by (3.5) and (3.7). Using (3.3) and (3.4), we obtain (3.6). \qed

We rewrite (3.6). If $\hat{u}_e(z, \lambda)$ satisfies the Kirchhoff condition, by virtue of Lemma 3.1 (1), $c_e(p, \lambda)$ depends only on the end point $e(p)$ and is independent of the edge $e$. Therefore, we denote $c_e(p, \lambda) = c(v, \lambda)$ if $e(p) = v$.

For $v, w \in V$ such that $v \sim w$, there is a unique $e \in E$ whose end points are $v$ and $w$. We define a new edge $e_{vw}$ by

$$e_{vw} = \begin{cases} e & \text{if } e(0) = v, \\ e^{-1} & \text{if } e(0) = w, \end{cases}$$

where $e^{-1}$ means $e$ with reverse direction. Therefore, $e_{vw}$ is a directed edge with initial vertex $v$ and terminal vertex $w$. We also define a function $\psi_{vw}(z, \lambda)$ on the edge $e_{vw}$ by

$$\psi_{vw}(z, \lambda) = \begin{cases} \phi_{e0}(z, \lambda) & \text{if } e(0) = v, \\ \phi_{e1}(1 - z, \lambda) & \text{if } e(1) = v. \end{cases}$$

This means that $\psi_{vw}(z) = \phi_{e0}(z, \lambda)$ if $e$ and $e_{vw}$ have the same direction, and $\psi_{vw}(z) = \phi_{e1}(1 - z, \lambda)$ if $e$ and $e_{vw}$ have the opposite direction.

Now, the assumption (Q-3) plays an important role. We put $q_{vw}(z, \lambda) = q_e(z, \lambda)$, which is well-defined by virtue of (Q-3). Moreover, $\psi_{vw}(z, \lambda)$ satisfies

$$\begin{cases} (\frac{d^2}{dz^2} + q_{vw}(z) - \lambda)\psi_{vw}(z, \lambda) = 0, & 0 < z < 1, \\ \psi_{vw}(0, \lambda) = 0, & \psi'_{vw}(0, \lambda) = 1. \end{cases}$$

The equality $\phi_{e0}(z, \lambda) = \phi_{e1}(1 - z, \lambda)$ implies

$$\phi_{e0}(1, \lambda) = \phi_{e1}(0, \lambda), \quad \phi'_{e0}(1, \lambda) = -\phi'_{e1}(0, \lambda).$$

Therefore, by (3.8), we have

$$\psi_{vw}(1, \lambda) = \begin{cases} \phi_{e0}(1, \lambda) & \text{if } e(0) = v, \\ \phi_{e1}(0, \lambda) & \text{if } e(1) = v, \end{cases}$$

$$\psi'_{vw}(1, \lambda) = \begin{cases} -\phi'_{e1}(0, \lambda) & \text{if } e(0) = v, \\ \phi'_{e0}(1, \lambda) & \text{if } e(1) = v. \end{cases}$$

**Definition 3.2.** We define the perturbed vertex Laplacian on $V$ by

$$\hat{\Delta}_{V, \lambda} \hat{u}(v) = \frac{1}{d_g} \sum_{w \sim v} \frac{1}{\psi_{vw}(1, \lambda)} \hat{u}(w), \quad v \in V$$

for $\hat{u} \in \ell^2_{loc}(V)$.

What we have defined in (3.11) is the so-called normalized discrete Laplacian. It is not the standard discrete Laplacian. By (3.9), the first and the second terms of the left-hand side of (3.6) divided by $d_g$ are summarized into $-\hat{\Delta}_{V, \lambda} \hat{u}(v)$. By (3.10), the third and the 4th terms are summarized into a scalar multiplication operator:

$$\hat{Q}_{V, \lambda} \hat{u}(v) = \hat{Q}_{v, \lambda}(v) \hat{u}(v),$$

where

$$\hat{Q}_{v, \lambda}(v) = \frac{1}{d_g} \sum_{w \sim v} \frac{\psi'_{vw}(1, \lambda)}{\psi_{vw}(1, \lambda)}.$$
Lemma 3.3. For $\hat{u}$ defined by (3.1.3), let $\hat{u}|_{V}$ be the restriction of $\hat{u}$ on $V$. Then the condition (3.6) is rewritten as

$$(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u}|_{V} = \hat{T}_{V}(\lambda)\hat{f}. \tag{3.14}$$

Therefore, $\hat{u}|_{V}$ should be written as

$$\hat{u}| _{V} = \left(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}\right)^{-1}\hat{T}_{V}(\lambda)\hat{f}. \tag{3.15}$$

Here, we must be careful about the operator $(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda})^{-1}$. For $\lambda \notin \mathbb{R}$, the operator $-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}$ has complex coefficients, hence is not self-adjoint. Therefore, the existence of its inverse is not obvious. We discuss the validity of this formula in Subsection 4.3. For the moment, we admit (3.15) as a formal formula.

We define an operator $\hat{T}_{E}(\lambda) : L_{loc}^{2}(E) \to L_{loc}^{2}(E)$ by

$$\hat{T}_{E}(\lambda)\hat{u}(z)_{e}(z) = \Phi_{e1}(\lambda)^{*}\hat{u}(e(1)) + \Phi_{e0}(\lambda)^{*}\hat{u}(e(0)). \tag{3.16}$$

We also define $r_{E}(\lambda) : L_{loc}^{2}(E) \to L_{loc}^{2}(E)$ by

$$r_{E}(\lambda)\hat{f}_{e} = r_{e}(\lambda)\hat{f}_{e}, \quad e \in E. \tag{3.17}$$

Lemma 3.3 and (3.5) yield the following lemma.

Lemma 3.4. The resolvent of $\hat{H}_{E}$ is written as

$$\hat{R}_{E}(\lambda) = \hat{T}_{E}(\lambda)\left(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}\right)^{-1}\hat{T}_{V}(\lambda) + r_{E}(\lambda). \tag{3.18}$$

In other words, $\hat{u} = \hat{R}_{E}(\lambda)\hat{f}$ is given by $\hat{u} = \{\hat{u}_{e}\}_{e \in E}$ with $\hat{u}_{e}(z, \lambda)$ defined by (3.5), and

$$c_{e}(p, \lambda) = \left(\hat{R}_{V}(\lambda)\hat{T}_{V}(\lambda)\hat{f}\right)(e(p)), \quad p = 0, 1, \tag{3.19}$$

$$\hat{R}_{V}(\lambda) = \left(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}\right)^{-1}. \tag{3.20}$$

We also have a symmetric form:

$$\hat{R}_{E}(\lambda) = \hat{T}_{V}(\lambda)^{*}\left(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}\right)^{-1}\hat{T}_{V}(\lambda) + r_{E}(\lambda). \tag{3.21}$$

The formula (3.21) follows from the following lemma.

Lemma 3.5.

$$\hat{T}_{V}(\lambda)^{*} = \hat{T}_{E}(\lambda).$$
Proof. Suppose \( \hat{f} \in L^2_{loc}(\mathcal{E}) \) and \( \hat{u} \in L^2_{loc}(\mathcal{V}) \) are compactly supported. Then, recalling that the inner product of \( \ell^2(\mathcal{V}) \) contains \( d_g \) (see (2.16)),

\[
(\hat{T}_V(\lambda)\hat{f},\hat{u}) = \frac{1}{d_g} \sum_{v \in V} \left( \sum_{e \in \mathcal{E}_v(1)} (\Phi_{e_1}(\lambda) \hat{f}_e \hat{u}(e(1)) \right) + \sum_{e \in \mathcal{E}_v(0)} (\Phi_{e_0}(\lambda) \hat{f}_e \hat{u}(e(0))))d_g
\]

\[
= \sum_{e \in \mathcal{E}} \int_0^1 \hat{f}_e(\lambda,z) \left( \Phi_{e_1}(\lambda)^* \hat{u}(e(1)) + \Phi_{e_0}(\lambda)^* \hat{u}(e(0)) \right)(z)dz
\]

\[
= (\hat{f},\hat{T}_E(\lambda)\hat{u}),
\]

which proves the lemma. \( \square \)

3.3. Unperturbed resolvent. We rewrite the above formula for the unperturbed resolvent \( \hat{R}_V^{(0)}(\lambda) \) to make it more explicit. We put the superscript \( (0) \) for every term. For \( \lambda = r e^{i\theta} \in \mathbb{C} \) with \( 0 \leq \theta < 2\pi \), we define

\[
\sqrt{\lambda} = \sqrt{re^{i\theta/2}}
\]

so that \( \text{Im} \sqrt{\lambda} \geq 0 \) and \( \sqrt{r \pm i0} = \pm \sqrt{r} \) for \( r > 0 \). When \( q_e = 0 \), we have

\[
(3.22) \quad \phi_{e_0}^{(0)}(z) = \frac{\sin \sqrt{\lambda}z}{\sqrt{\lambda}}, \quad \phi_{e_1}^{(0)}(z) = \frac{\sin \sqrt{\lambda}(1-z)}{\sqrt{\lambda}}, \quad \phi_{c_0}^{(0)}(\lambda) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}}.
\]

Then, in view of (3.11), we have

\[
(3.23) \quad \left( \hat{\Delta}_{V,\lambda}^{(0)} \hat{u} \right)(v) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \frac{1}{d_g} \sum_{w \sim v} \hat{u}(w) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( \hat{\Delta}_V \hat{u} \right)(v).
\]

\[
(3.24) \quad \hat{Q}_{c_0,\lambda}^{(0)} = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \cos \sqrt{\lambda},
\]

We can then factor out the term \( \sqrt{\lambda}/\sin \sqrt{\lambda} \) in the formula for \( \hat{R}_V^{(0)}(\lambda) \):

\[
(3.25) \quad \hat{R}_V^{(0)}(\lambda) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \left( -\hat{\Delta}_V + \cos \sqrt{\lambda} \right)^{-1},
\]

which gives a definite meaning to \( \hat{R}_V^{(0)}(\lambda) \) since \( \cos \sqrt{\lambda} \notin \mathbb{R} \) for \( \lambda \notin \mathbb{R} \). By virtue of (3.2), the Green operator of \( -(d^2/dz^2)_D \) is written as

\[
(3.26) \quad (r_{c_0}^{(0)}(\lambda) \hat{f}_e)(z) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( \int_0^z \frac{\sin \sqrt{\lambda}(1-z)}{\sqrt{\lambda}} \frac{\sin \sqrt{\lambda}w}{\sqrt{\lambda}} \hat{f}_e(w)dw \right.
\]

\[
+ \left. \int_z^1 \frac{\sin \sqrt{\lambda}z}{\sqrt{\lambda}} \frac{\sin \sqrt{\lambda}(1-w)}{\sqrt{\lambda}} \hat{f}_e(w)dw \right).
\]
This implies, by (3.4) and (3.13),
\[
\Phi^{(0)}_{el}(\lambda)f = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \int_0^1 \sin \sqrt{\lambda} f(z)dz,
\]
\[
\Phi^{(0)}_{el}(\lambda)f = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \int_0^1 \sin \sqrt{\lambda}(1-z) f(z)dz,
\]
\[
(\hat{T}_V^{(0)}(\lambda)\hat{f})(v) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( \sum_{e \in E_{(1)}} \int_0^1 \sin \sqrt{\lambda} \hat{f}_e(z)dz, 
+ \sum_{e \in E_{(0)}} \int_0^1 \sin \sqrt{\lambda}(1-z) \hat{f}_e(z)dz \right).
\]

In view of Lemmas 3.3, 3.5 and (3.16), we have proven the following lemma.

**Lemma 3.6.** For \( \lambda \not \in \mathbb{R} \), the resolvent of \( \hat{R}_e^{(0)} \) is represented as
\[
\hat{R}_e^{(0)}(\lambda) = \hat{T}_V^{(0)}(\lambda)(-\widehat{\Delta}_V + \widehat{\Phi}_{V,(0)}^{(0)})^{-1}\hat{T}_V^{(0)}(\lambda) + r_e^{(0)}(\lambda)
\]
(3.26)

More explicitly, \( \hat{u}_e^{(0)} = (\hat{H}_e^{(0)} - \lambda)^{-1}\hat{f} = \hat{R}_e^{(0)}(\lambda)\hat{f} \) is written as
\[
\hat{u}_e^{(0)}(z, \lambda) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( \tau_e^{(0)}(1, \lambda) \sin \sqrt{\lambda}z \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} + c_e^{(0)}(0, \lambda) \sin \sqrt{\lambda}(1-z) \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \right) + r_e^{(0)}(\lambda)\hat{f}_e,
\]
(3.28)

Recall that \( T \) is defined by (2.34). We put
\[
\sigma_T^{(0)} = \left\{ \lambda \in \text{Int}(\sigma_e(\hat{H}_e^{(0)})); -\cos \sqrt{\lambda} \in T \right\},
\]
(3.29)
\[
\sigma_V^{(0)} = \{ (\pi j)^2; j = 1, 2, \cdots \},
\]
(3.30)
\[
\sigma_e^{(0)} = \{ \lambda; -\cos \sqrt{\lambda} \in \sigma(-\widehat{\Delta}_V) \}.
\]
(3.31)

As will be proven in the next section, for \( \lambda \in (\text{Int} \sigma_e(\hat{H}_e)) \setminus (\sigma_T^{(0)} \cup \sigma_V^{(0)}) \), there exists a limit \( (-\widehat{\Delta}_V + \cos \sqrt{\lambda} \pm i0)^{-1} = \lim_{\epsilon \downarrow 0} (-\widehat{\Delta}_V + \cos \sqrt{\lambda} \pm i\epsilon)^{-1} \) in a suitable topology. Here, for a subset \( A \subset \mathbb{R} \), \( \text{Int} A \) means its interior. Hence, we have the following expression for \( \hat{R}_e^{(0)}(\lambda \pm i0) \).

**Lemma 3.7.** For \( \lambda \in (\text{Int} \sigma_e(\hat{H}_e)) \setminus (\sigma_T^{(0)} \cup \sigma_V^{(0)}) \), the following formula holds
\[
\hat{R}_e^{(0)}(\lambda \pm i0) = \hat{T}_V^{(0)}(\lambda)^* \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} (-\widehat{\Delta}_V + \cos \sqrt{\lambda} \pm i0)^{-1}\hat{T}_V^{(0)}(\lambda) + r_e^{(0)}(\lambda).
\]

We put for \( \lambda > 0 \)
\[
\sigma(\lambda) = \text{sgn}(\sin \sqrt{\lambda}) = \begin{cases} 1 & \text{if } \sin \sqrt{\lambda} > 0, \\ -1 & \text{if } \sin \sqrt{\lambda} < 0, \end{cases}
\]
(3.32)
holds, where $E$ is any compact interval in $\sigma(E)$ and $\lambda$ is any interval in $\{\operatorname{Int} \sigma_e(\hat{H}_\mathcal{E})\} \setminus \{\sigma^0_T \cup \sigma^0_V\}$ and $J$ is the image of $I$ by the mapping $\lambda \rightarrow k$.

Here, we define $\sqrt{\lambda} = \arccos(-k)$ to be first the principal branch and next its analytic continuation. The multi-valuedness of the mapping $k \rightarrow \lambda$ then gives rise to the band structure of the spectrum of $\hat{H}^{(0)}_\mathcal{E}$, which has already been studied by many authors.

3.4. Spectra. Let $\{\lambda_j(x)\}_{j=1}^s$ be the eigenvalues of $H_0(x)$. We arrange them in such a way that there exists $1 \leq s_0 \leq s$ such that $\lambda_j(x)$ is non-constant for $1 \leq j \leq s_0$, but constant for $s_0 + 1 \leq j \leq s$. Put

$$E^{(0)}_{j,k} = \begin{cases} \arccos(-\lambda_j) + \pi k, & \text{when } k \text{ is even,} \\ - \arccos(-\lambda_j) + \pi (k + 1), & \text{when } k \text{ is odd,} \end{cases}$$

for $s_0 \leq j \leq s$, where $\arccos$ is the principal value, i.e. $\arccos(\lambda) \in [0, \pi]$ for $-1 \leq \lambda \leq 1$. We put

$$\sigma_{fb}(\hat{H}^{(0)}_\mathcal{E}) = \sigma^{(0)}_V \cup \{E^{(0)}_{j,k}; s_0 + 1 \leq j \leq s, \ k = 0, 1, 2, \cdots \},$$

and call it the flat band of the spectrum of $\hat{H}^{(0)}_\mathcal{E}$. The following theorem is proved in [28].
Theorem 3.9.\hfill (3.36)\hfill 
\[ \sigma(\hat{H}_E^{(0)}) = \sigma_V^{(0)} \cup \sigma_E^{(0)}. \]
\hfill (3.37)\hfill 
\[ \sigma_p(\hat{H}_E^{(0)}) = \sigma_{fb}(\hat{H}_E^{(0)}). \]
Moreover, \( \sigma_{fb}(\hat{H}_E^{(0)}) \) consists of the eigenvalues of \( \hat{H}_E^{(0)} \) with infinite multiplicities.

In the sequel, we consider the case in which \( s_0 = s \) for the sake of simplicity (mainly for the simplicity of notation). The results below are also extended to the case where \( s_0 < s \).

4. Resolvent estimates

We give a definite meaning to the expressions of the resolvents \( \{ \lambda \} \).

4.1. Rellich type theorem. We put
\hfill (4.1)\hfill 
\[ \sigma(qE) = \bigcup_{e \in E} \sigma(-(d^2/dz^2)D + q_E). \]

Note that by (Q-1) and (Q-2), \( \sigma(qE) \) is a discrete subset of \( \mathbb{R} \), furthermore \( \sigma_V^{(0)} \subset \sigma(qE) \). For \( R > 0 \), the exterior domain \( E_{ext,R} \) and the interior domain \( E_{int,R} \) are defined to be the set of edges such that
\hfill (4.2)\hfill 
\[ E_{ext,R} \ni e \iff |e(0)| \geq R \quad \text{and} \quad |e(1)| \geq R, \]
\hfill (4.3)\hfill 
\[ E_{int,R} \ni e \iff |e(0)| < R \quad \text{or} \quad |e(1)| < R. \]

Theorem 4.1. Let \( \lambda \in (\text{Int} \sigma_{e}(\hat{H}_E^{(0)})) \setminus (\sigma_V^{(0)} \cup \sigma_T^{(0)}) \), and suppose \( \hat{u} \in \hat{B}_0(E) \)

\[ E^{(0)} \hat{u} = \lambda \hat{u} \quad \text{in} \quad E_{ext,R}, \]

and the Kirchhoff condition for some \( R > 0 \). Then \( \hat{u} = 0 \) on \( E_{ext,R} \) for some \( R_1 > 0 \).

Proof. We can assume that \( \hat{u} \) is real-valued. Take \( R > 0 \) large enough so that \( \text{supp} q_E \subset E_{int,R} \). On \( e \in E_{ext,R} \), \( \hat{u} \) is written as
\hfill \( \hat{u}(z) = c_e(1) \frac{\sin \sqrt{\lambda} z}{\sin \sqrt{\lambda}} + c_e(0) \frac{\sin \sqrt{\lambda}(1 - z)}{\sin \sqrt{\lambda}}. \)

Then, we have
\hfill \( \int_0^1 |\hat{u}(z)|^2 dz = \frac{1}{2 \sin^2 \sqrt{\lambda}} \left( 1 - \frac{\sin \sqrt{\lambda} \cos \sqrt{\lambda}}{\sqrt{\lambda}} \right) \left( c_e(0)^2 + c_e(1)^2 \right) \)
\hfill \( + \frac{1}{\sin^2 \sqrt{\lambda}} \left( \sin \sqrt{\lambda} - \cos \sqrt{\lambda} \right) c_e(0)c_e(1). \)

Note that \( \sin \sqrt{\lambda} < \sqrt{\lambda} \) and \( |\cos \sqrt{\lambda}| < 1 \) for \( \lambda > 0 \) and \( \sqrt{\lambda}/\pi \notin \mathbb{Z} \). Also \( |a - b| < 1 - ab \) for \( |a| < 1 \) and \( |b| < 1 \). Then, letting \( a = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \) and \( b = \cos \sqrt{\lambda}, \) we have
\hfill \( |\frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} - \cos \sqrt{\lambda}| < 1 - \frac{\sin \sqrt{\lambda} \cos \sqrt{\lambda}}{\sqrt{\lambda}}. \)

Hence there exists a constant \( C(\lambda) > 0 \) such that
\hfill (4.4)\hfill 
\[ C(\lambda)^{-1} (|c_e(0)| + |c_e(1)|) \leq ||\hat{u}_e||_{L^2} \leq C(\lambda) (|c_e(0)| + |c_e(1)|). \]
for all \( e \in \mathcal{E}_{\text{ext,R}} \). For \( v \in \mathcal{V} \), we put \( \hat{w}(v) = \tilde{u}(v) \). Then, taking account of Lemma 3.3, we have

\[
\frac{\partial}{\partial v} + \cos \sqrt{\lambda} \tilde{u} = 0, \quad \text{on} \quad \mathcal{E}_{\text{ext,R}}.
\]

Since \( \tilde{u} \in \mathcal{B}_\delta(G) \), the inequality (4.4) implies that \( \tilde{u} \in \mathcal{B}_\delta(V) \). By the Rellich type theorem for lattice Schrödinger operators (see Theorem 5.1 in [3]), \( \tilde{w} \) vanishes for \( |v| > R' > 0 \). This proves the theorem. \( \Box \)

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

We introduce a new assumption.

\[ (UC) \quad \text{For any} \quad \lambda \in \text{Int}\sigma_e(\hat{H}_E(0)) \setminus \sigma_T(0), \quad \hat{H}_E - \lambda \text{ has the unique continuation property on} \quad \mathcal{E}. \]

**Theorem 4.2.** Assume (UC). Then,

\[
\sigma_p(\hat{H}_E) \cap \sigma_e(\hat{H}_E) \subset \sigma_T(0) \cup \sigma_T(0).
\]

Proof. Let \( \lambda \in \sigma_p(\hat{H}_E) \cap \sigma_e(\hat{H}_E) \), and \( \tilde{u} \) be the associated eigenfunction. If \( \lambda \notin \sigma_T(0) \cup \sigma_T(0) \), \( \tilde{u} \) is compactly supported by Theorem 4.1. By the unique continuation property, \( \tilde{u} \) vanishes identically. This is a contradiction. \( \Box \)

Let us check that the square lattice and the hexagonal lattice satisfy (UC).

**Lemma 4.3.** For the square lattice in \( \mathbb{R}^d \) with \( d \geq 2 \), (UC) holds.

Proof. Suppose \( (\hat{H}_E - \lambda)\tilde{u} = 0 \) on \( \mathcal{E} \), and \( \tilde{u} = 0 \) on any edge in the region \( \{x_n > k\} \), where \( k \) is an integer. Then, \( \tilde{u} = 0 \) on any vertex on the plane \( \{x_n = k\} \). Since \( \lambda \) is not a Dirichlet eigenvalue on any edge, \( \tilde{u} = 0 \) on any edge in the plane \( \{x_n = k\} \). Due to the Kirchhoff condition, this implies that \( \tilde{u}'(z) = 0 \) on any vertex on the plane \( \{x_n = k\} \). By the uniqueness of the initial value problem for \( -\Delta u + \gamma \Delta^2 u = 0 \), we have seen that \( \tilde{u} = 0 \) on \( \mathcal{E} \).

**Lemma 4.4.** For the hexagonal lattice in \( \mathbb{R}^2 \), (UC) holds.

Proof. Instead of the region \( \{x_n > k\} \), consider the region \( \{x_2 > k\sqrt{3}/2\} \) and argue as above. \( \Box \)

4.2. Radiation condition. Let \( \lambda_j(x), j = 1, 2, \ldots, s \), be the eigenvalues of \( H_0(x) \) and \( P_j(x) \) the associated eigenprojections. Let \( H_0 \) be the operator of multiplication by \( H_0(x) \) on \( (L^2(\mathbb{T}^d))^s \). In [3], Lemma 4.7, we have proven that if \( \rho \notin \text{Int}\sigma(H_0) \) \( \setminus \mathcal{T} \), the operator

\[
f \mapsto \frac{f(x)}{\lambda_j(x) - \rho + i0}
\]

is bounded from \( \mathcal{B}(\mathbb{T}^d) \) to \( \mathcal{B}(\mathbb{T}^d) \).

For a distribution \( u \in \mathcal{D}'(\mathbb{T}^d) \), its wave front set \( WF(u) \) is defined as follows: For \( (x_0, \omega) \in \mathbb{R}^d \times \mathbb{S}^{d-1}, (x_0, \omega) \notin WF(u) \) if and only if there exist \( 0 < \delta < 1 \) and \( \chi(x) \in C_0^\infty(\mathbb{R}^d) \) such that \( \chi(x_0) = 1 \) and

\[
\lim_{R \to \infty} \frac{1}{R} \int_{|\xi| < R} |C_{\omega, \delta}(\xi)(\hat{\chi}\tilde{u})(\xi)|^2 d\xi = 0,
\]

(4.5)
where $\tilde{\chi}u$ is the Fourier transform of $\chi u$ and $C_{\omega,\delta}(\xi)$ is the characteristic function of the cone $\{\xi \in \mathbb{R}^d : \omega \cdot \xi > \delta|\xi|\}$.  

In [3], Theorem 6.1, we have shown that for any $f \in \mathcal{B}(\mathbb{T}^d)$, $1 \leq j \leq s$ and $\rho \in \sigma(H_0) \setminus \tau$, it holds that

$$(RC)_+ : \quad WF^*(\frac{P_j f}{\lambda_j(x) - \rho - i0}) \subset \{(x, \omega_x) : x \in M_{\rho,j}\},$$

$$(RC)_- : \quad WF^*(\frac{P_j f}{\lambda_j(x) - \rho + i0}) \subset \{(x, -\omega_x) : x \in M_{\rho,j}\},$$

where $\omega_x \in S^{d-1} \cap T_x(M_{\rho,j})$, $\omega(x) \cdot \nabla \lambda_j(x) < 0$. Moreover, for $f \in \mathcal{B}(\mathbb{T}^d)$, $u = (H_0(x) - \lambda + i0)^{-1}f \in \mathcal{B}^*(\mathbb{T}^d)$ is a unique solution to the equation $(H_0(x) - \rho)u = f$ satisfying $(RC)_+$ or $(RC)_-$. 

These facts are also extended to the case with compactly supported perturbations.

In the following, if we say that $\tilde{u} \in \mathcal{B}^*(\mathcal{E})$ is a solution to the equation $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = \tilde{f}$, $\tilde{u}$ is assumed to satisfy the Kirchhoff condition. Taking account of (3.33), we define the radiation condition as follows.

**Definition 4.5.** Let $\lambda > 0$. We say that a solution $\tilde{u} \in \mathcal{B}^*(\mathcal{E})$ of the equation $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = \tilde{f}$ satisfies the outgoing radiation condition if either (i) or (ii) holds:

1. $\sin \sqrt{\lambda} > 0$, and $u = U_\mathcal{E} \tilde{u}$ satisfies $(RC)_+$ with $\rho = -\cos \sqrt{\lambda}$
2. $\sin \sqrt{\lambda} < 0$, and $u = U_\mathcal{E} \tilde{u}$ satisfies $(RC)_-$ with $\rho = -\cos \sqrt{\lambda}$.

Similarly, we say that a solution $\tilde{u} \in \mathcal{B}^*(\mathcal{E})$ of the equation $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = \tilde{f}$ satisfies the incoming radiation condition if either (i) or (ii) holds:

1. $\sin \sqrt{\lambda} > 0$, and $u = U_\mathcal{E} \tilde{u}$ satisfies $(RC)_-$ with $\rho = -\cos \sqrt{\lambda}$
2. $\sin \sqrt{\lambda} < 0$, and $u = U_\mathcal{E} \tilde{u}$ satisfies $(RC)_+$ with $\rho = -\cos \sqrt{\lambda}$.

If $\tilde{u}$ satisfies the outgoing or incoming radiation condition, we say that $\tilde{u}$ satisfies the radiation condition.

**Lemma 4.6.** Let $\lambda \in (\text{Int } \sigma_e(\tilde{H}_\mathcal{E})) \setminus (\sigma_{V,0}^1 \cup \sigma_{V,0}^2)$. Then, the solution $\tilde{u} \in \mathcal{B}^*(\mathcal{E})$ of the equation $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = \tilde{f}$ satisfying the radiation condition is unique.

Proof. We show that if $\tilde{u} \in \mathcal{B}^*(\mathcal{E})$ satisfies $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = 0$ and the radiation condition, then $\tilde{u} = 0$. On each edge $e$, $\tilde{u}(z)$ is rewritten as (see (3.5))

$$\tilde{u}_e(z) = c_e(1)\frac{\phi_{e0}(z, \lambda)}{\phi_{e0}(1, \lambda)} + c_e(0)\frac{\phi_{e1}(z, \lambda)}{\phi_{e1}(1, \lambda)}$$

Then, letting $\tilde{w}(v) = c_e(1)$ or $c_e(0)$, if $e(0) = v$ or $e'(1) = v$, we see that $(-\tilde{\Delta}_{V,\lambda} + \tilde{Q}_{V,\lambda})\tilde{w} = 0$ (see (3.14)) and $\tilde{w}$ satisfies the radiation condition. This implies $\tilde{w} = 0$ by Lemma 7.6 in [3].

In our previous work [3], the radiation condition was also introduced for the vertex Laplacian (see Lemmas 4.8 and 6.2 in [3]). Let $\tilde{f} \in \mathcal{B}(\mathcal{E})$. For a solution $\tilde{u}$ of the edge Schrödinger equation $(-\tilde{\Delta}_\mathcal{E} + q_\mathcal{E} - \lambda)\tilde{u} = \tilde{f}$, let $\tilde{u}|_V$ be its restriction on $\mathcal{V}$. Then $\tilde{u}|_V$ satisfies the vertex Schrödinger equation

$$(-\tilde{\Delta}_V + \cos \sqrt{\lambda})\tilde{u}|_V = \tilde{g},$$
where \( \hat{g} \in \mathcal{B}(\mathcal{V}) \). Comparing these two definitions of radiation condition, one can show the following lemma.

Lemma 4.7. A solution \( \hat{u} \) of the edge Schrödinger equation satisfies the radiation condition if and only if the solution \( \hat{u}(\mathcal{V}) \) of the vertex Schrödinger equation satisfies the radiation condition.

4.3. Limiting absorption principle.

Theorem 4.8. Let \( I \) be a compact interval in \((\text{Int} \sigma_{\epsilon}(\mathcal{H}_E)) \setminus (\sigma^{(0)}_V \cup \sigma^{(0)}_T)\).

1. There exists a constant \( C > 0 \) such that

\[
\|((\mathcal{H}_E - \lambda \mp i\epsilon)^{-1} \|_{\mathcal{B}(\mathcal{B}(\mathcal{E}); \mathcal{B}^*(\mathcal{E}))} \leq C
\]

for any \( \lambda \in I \) and \( \epsilon > 0 \).

2. For any \( \lambda \in I \) and \( \sigma > 1/2 \), there exists a strong limit

\[
\frac{\epsilon}{\epsilon^0} \lim_{\epsilon \to 0} (\mathcal{H}_E - \lambda \mp i\epsilon)^{-1} := (\mathcal{H}_E - \lambda \mp i0)^{-1} \in \mathcal{B}(E^{2-\sigma}(\mathcal{E}); E^{2-\sigma}(\mathcal{E})).
\]

3. For any \( \hat{f} \in \mathcal{E} \), \((\mathcal{H}_E - \lambda \mp i0)^{-1} \hat{f} \) is an \( \mathcal{E} \)-valued continuously continuous function of \( \lambda \in I \).

4. For any \( \hat{f}, \hat{g} \in \mathcal{B}(\mathcal{E}) \), there exists a limit

\[
\lim_{\epsilon \to 0} (\mathcal{H}_E - \lambda \mp i\epsilon)^{-1} \frac{\hat{f}}{\hat{g}} := ((\mathcal{H}_E - \lambda \mp i0)^{-1} \frac{\hat{f}}{\hat{g}}),
\]

and \((\mathcal{H}_E - \lambda \mp i0)^{-1} \hat{f} \) is a continuous function of \( \lambda \in I \).

5. For any \( \hat{f} \in \mathcal{B}(\mathcal{E}) \), \((\mathcal{H}_E - \lambda + i0)^{-1} \hat{f} \) satisfies the outgoing radiation condition, and \((\mathcal{H}_E - \lambda + i0)^{-1} \hat{f} \) satisfies the incoming radiation condition.

Proof. The limiting absorption principle for \((-\hat{\Delta}_V + \cos \sqrt{\lambda} \pm i0)^{-1}\) is proved in [3], Theorem 6.1. Taking account of this fact and the formula (3.26), one can prove this theorem for the case of \(\mathcal{H}_E^{(0)}\). Using the fact that the multiplication operator \(q_e\) is relatively compact, one can prove the theorem for the case of \(\mathcal{H}_E\) utilizing Lemmas 4.6 and 4.7 by the perturbation argument. Since the similar argument is already given in the proof of Theorem 7.7 in [3], we do not repeat it.

Let us return to the problem of \((-\hat{\Delta}_V,\lambda + \hat{Q}_V,\lambda)^{-1}\) we have encountered in §3. First we consider the case \(q_e = 0\). If \( \lambda \in \mathbb{R} \), \(-\hat{\Delta}_V,\lambda + \hat{Q}_V,\lambda\) is self-adjoint by modifying the inner product. Arguing as in the proof of Theorem 4.3, one can prove the existence of \((-\hat{\Delta}_V,\lambda + \hat{Q}_V,\lambda,\pm,\pm,\mp,\pm)\)^{-1} as a bounded operator in \(\mathcal{B}(\mathcal{B}(\mathcal{V}); \mathcal{B}^*(\mathcal{V}))\). Using this fact, one can see that when \( \epsilon \to 0 \), \((-\hat{\Delta}_V,\lambda,\pm,\epsilon + \hat{Q}_V,\lambda,\pm,\pm,\pm,\pm)\)^{-1} is uniformly bounded as an operator from \(\mathcal{B}(\mathcal{V})\) to \(\mathcal{B}^*(\mathcal{V})\). The same fact holds true if we add \(q_e\) and use the resolvent equation. Moreover, the existence of the limit \(\lim_{\epsilon \to 0} (\hat{\Delta}_V,\lambda,\pm,\epsilon + \hat{Q}_V,\lambda,\pm,\pm,\pm,\pm)^{-1}\) is guaranteed. The arguments in §3 are then justified if we consider all operators in \(\mathcal{B}(\mathcal{V})\) or \(\mathcal{B}^*(\mathcal{V})\).

4.4. Analytic continuation of the resolvent. It is well-known that for the continuous model, the resolvent of the Schrödinger operator \(-\Delta + V(x)\), 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 $L^2(\mathbb{R}^n)$ functions to $L^2_\text{loc}(\mathbb{R}^n)$. This is proven by considering the free case, i.e. the operator

$$
\int_{\mathbb{R}^n} \frac{e^{ix \cdot \xi} \tilde{f}(\xi)}{|\xi|^2 - \zeta} \, d\xi = \int_0^\infty \frac{\int_{S^{n-1}} e^{ir \omega \cdot x} \tilde{f}(r \omega) \, dr}{r^2 - \zeta} \, r^{n-1} \, d\zeta
$$

($\tilde{f}(\xi)$ 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 idea also works for the discrete model, and one can show that the boundary value of the resolvent of the vertex Hamiltonian and the edge Hamiltonian 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.

5. Spectral representation and S-matrix

The spectral representation, also called the generalized Fourier transformation, was introduced by K. O. Friedrichs. Given a selfadjoint operator $A$ with absolutely continuous spectrum $I \subset \mathbb{R}$, one prepares an auxiliary Hilbert space $\mathfrak{h}$ and a unitary operator $\mathcal{F}$ from $\mathcal{H}_{ac}(A)$ to $L^2(I, \mathfrak{h}; d\lambda)$ so that $(\mathcal{F}Au)(\lambda) = \lambda(\mathcal{F}u)(\lambda)$ holds for any $\lambda \in I$ and $u \in D(A)$. We apply this framework to scattering theory, where $A$ is a differential operator or a discrete operator, $\mathfrak{h}$ is the $L^2$-space over the characteristic set of $A$, and $\mathcal{F}$ is constructed by observing the behavior at infinity of the resolvent of $A$. The boundary values of the resolvent $(A - \lambda \mp i0)^{-1}$ give rise to two spectral representations, and their difference is described by the S-matrix, which is a unitary integral operator on the characteristic set. This is the operator theoretical background of the scattering experiment, which is originally a time-dependent phenomenon. Below, we elucidate this picture for the case of the edge model.

5.1. Spectral representation. We need to introduce a little more notation. Letting $P_{V,j}(x)$ be the projection associated with the eigenvalue $\lambda_j(x)$ of $H_0(x)$, we put

$$
D^{(0)}(\lambda \pm i0) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \sum_{j=1}^s \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda} \mp i0} P_{V,j}(x).
$$

Note that by (2.21)

$$
D^{(0)}(\lambda \pm i0) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \mathcal{U}_V (\Delta_V + \cos \sqrt{\lambda} \pm i0)^{-1} \mathcal{U}_V^*,
$$

where $\mathcal{U}_V$ is the discrete Fourier transformation defined by (2.18).

Recall that the multiple lattice structure comes from (2.3), to which, by passing to the Fourier series, one associates the function space $(L^2(\mathbb{T}^d))^s$ on the torus. Noting that by Lemma 2.2 the mapping

$$
\{1, \cdots, \nu\} \ni i \mapsto k \in \{1, \cdots, s\}
$$

defined by

$$
\nu_\ast = \{\mathbf{e}_{\ell \ast}(0), \mathbf{e}_{\ell \ast}(1) : 1 \leq \ell \leq \nu\} \ni \mathbf{e}_{\ell \ast}(i) \mapsto p^{(\ell)} \in \{p^{(1)}, \cdots, p^{(s)}\},
$$

where $\mathbf{e}_{\ell \ast}(i) = p^{(\ell)}$, is surjective. We define a projection $P_{\ell, \ast}(i)$ by

$$
P_{\ell, \ast}(i) : (L^2(\mathbb{T}^d))^s \ni (f_1(x), \cdots, f_\nu(x)) \mapsto f_k(x).
$$
We then define the operators \( \Pi_\ell(\lambda) \) and \( \Pi(\lambda) \) by
\[
\Pi_\ell(\lambda) = \frac{1}{\sqrt{d_y}} \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( e^{-i\text{ind}(e_\ell)x} \frac{\sin \sqrt{\lambda z}}{\sqrt{\lambda}} P_{e_\ell,1}^\lambda + \frac{\sin \sqrt{\lambda(1-z)}}{\sqrt{\lambda}} P_{e_\ell,0}^\lambda \right),
\]
\[
\Pi(\lambda) = (\Pi_1(\lambda), \cdots, \Pi_\nu(\lambda)) : (L^2(T^d))^\ast \to L^2(T^d \times \mathcal{E}_*),
\]
which is naturally extended to spaces of distributions \( \Pi(\lambda) : (D'(T^d))^\ast \to D'(T^d \times \mathcal{E}_*) \).

In view of (3.16), we have
\[
(5.4) \quad (\hat{T}^{(0)}_{\mathcal{E}}(\lambda) \hat{u})_e(z) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( \frac{\sin \sqrt{\lambda z}}{\sqrt{\lambda}} \hat{u}(e(1)) + \frac{\sin \sqrt{\lambda(1-z)}}{\sqrt{\lambda}} \hat{u}(e(0)) \right).
\]

Lemma 5.1. For \( \lambda \in (\text{Int } \sigma_\mathcal{E}(\hat{H}^{(0)}_{\mathcal{E}})) \setminus (\sigma_T^{(0)} \cup \sigma_\mathcal{V}^{(0)}) \),
\[
\mathcal{U}_\mathcal{E} \hat{T}^{(0)}_{\mathcal{E}}(\lambda) = \Pi(\lambda) \mathcal{U}_\mathcal{V}
\]
Proof. Recall that each edge \( e \) is written as \( e = e_\ell + [n] \), where
\[
e(0) = e_\ell(0) + v(n), \quad e(1) = e_\ell(1) + v(\text{Ind } (e_\ell) + n).
\]
By the definition (2.26) and (5.4), we compute
\[
\mathcal{U}_\mathcal{E} \hat{T}^{(0)}_{\mathcal{E}}(\lambda) f(x, z)
\]
\[
= (2\pi)^{-d/2} \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \sum_{n \in \mathbb{Z}^d} e^{i n \cdot x} \hat{f}(e_\ell(1) + v(\text{Ind } (e_\ell) + n)) \frac{\sin \sqrt{\lambda z}}{\sqrt{\lambda}}
\]
\[
+ (2\pi)^{-d/2} \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \sum_{n \in \mathbb{Z}^d} e^{i n \cdot x} \hat{f}(e_\ell(0) + v(n)) \frac{\sin \sqrt{\lambda(1-z)}}{\sqrt{\lambda}}
\]
\[
= (2\pi)^{-d/2} \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \sum_{n \in \mathbb{Z}^d} e^{i n \cdot x e^{-i\text{ind}(e_\ell)x}} \hat{f}(e_\ell(1) + v(n)) \frac{\sin \sqrt{\lambda z}}{\sqrt{\lambda}}
\]
\[
+ (2\pi)^{-d/2} \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \sum_{n \in \mathbb{Z}^d} e^{i n \cdot x} \hat{f}(e_\ell(0) + v(n)) \frac{\sin \sqrt{\lambda(1-z)}}{\sqrt{\lambda}}.
\]
The lemma then follows from this. \( \square \)

Using the identification (2.17), we put
\[
(5.5) \quad \Phi^{(0)}(\lambda) = \mathcal{U}_\mathcal{V} \hat{T}^{(0)}_{\mathcal{E}}(\lambda) = \mathcal{U}_\mathcal{V} \hat{T}^{(0)}_{\mathcal{V}}(\lambda).
\]

Lemma 5.2. The resolvent \( \hat{R}^{(0)}_{\mathcal{E}}(\lambda \pm i0) \) has the following expressions:
\[
(5.6) \quad \hat{R}^{(0)}_{\mathcal{E}}(\lambda \pm i0) = \Phi^{(0)}(\lambda) * D^{(0)}(\lambda \pm i0) \Phi^{(0)}(\lambda) + r^{(0)}_{\mathcal{E}}(\lambda)
\]
\[
(5.7) \quad = \mathcal{U}_\mathcal{E} * \Pi(\lambda) D^{(0)}(\lambda \pm i0) \Phi^{(0)}(\lambda) + r^{(0)}_{\mathcal{E}}(\lambda).
\]
Proof. The formula (5.6) follows from Lemma 3.7 and (5.2). By Lemma 3.5 we have \( \hat{T}^{(0)}_{\mathcal{E}} = \hat{T}^{(0)}_{\mathcal{E}}(\lambda) \). Therefore by (5.5), \( \Phi^{(0)}(\lambda)^* = \mathcal{U}_\mathcal{E} \Pi(\lambda) \), which proves (5.7). \( \square \)

Using these formulas, we can construct a spectral representation of the absolutely continuous part of \( \hat{H}^{(0)}_{\mathcal{E}} \). We put
\[
M_{\mathcal{E}, \lambda, j} = \{ x \in T^d : \lambda_j(x) + \cos \sqrt{\lambda} = 0 \},
\]
\[(\varphi, \psi)_{\lambda,j} = \int_{M_{E,\lambda,j}} \varphi(x)\overline{\psi(x)} dS_j,\]
\[dS_j = \frac{|\sin \sqrt{\lambda}|}{\sqrt{\lambda}} dM_{E,\lambda,j},\]

Then, by virtue of (5.6), for \(\lambda \in (\int \sigma_\varepsilon(\hat{H}_E^{(0)})) \setminus (\sigma_T^{(0)} \cup \sigma_V^{(0)} \cup \sigma_p(\hat{H}_E^{(0)}))\),

\[\frac{1}{2\pi i} \left( \hat{R}_E^{(0)}(\lambda + i0) - \hat{R}_E^{(0)}(\lambda - i0) \right) \hat{f}, \hat{g} \]
\[(5.8) \]
\[= \sum_{j=1}^s \left( P_{V,j} \Phi^{(0)}(\lambda) \hat{f}, P_{V,j} \Phi^{(0)}(\lambda) \hat{g} \right)_{\lambda,j},\]

where we have used
\[(\hat{R}_E^{(0)}(-\cos \sqrt{\lambda + i0}) - \hat{R}_E^{(0)}(-\cos \sqrt{\lambda - i0}) \hat{f}, \hat{g}) \]
\[= 2\pi i \sum_j \int_{M_{E,\lambda,j}} P_{V,j} \hat{f}, P_{V,j} \hat{g} \frac{dM_{E,\lambda,j}}{|\nabla \lambda_j(x)|},\]

(cf. (6.7) of [3]). Let \(u_j(x)\) be a normalized eigenvector of \(H_0(x)\) associated with the eigenvalue \(\lambda_j(x)\): \(H_0(x)u_j(x) = \lambda_j(x)u_j(x)\).

We put
\[(5.9) \hat{f}_j^{(0)}(\lambda) \hat{f} = (u_j(x) \cdot \Phi^{(0)}(\lambda) \hat{f})u_j(x),\]
\[\hat{F}^{(0)}(\lambda) = (\hat{f}_1^{(0)}(\lambda), \ldots, \hat{f}_s^{(0)}(\lambda)),\]
\[h_\lambda = \sum_{j=1}^s L^2(M_{\lambda,j}; dS_j),\]
\[H = L^2([0, \infty), h_\lambda; d\lambda).\]

By (5.8)
\[\frac{1}{2\pi i} \left( \hat{R}_E^{(0)}(\lambda + i0) - \hat{R}_E^{(0)}(\lambda - i0) \right) \hat{f}, \hat{g} \]
\[= (\hat{F}^{(0)}(\lambda) \hat{f}, \hat{F}^{(0)}(\lambda) \hat{g})_{h_\lambda}.\]

Letting \(E^{(0)}(\lambda)\) be the spectral measure for \(\hat{H}_E^{(0)}\) and integrating this equality, we have
\[(E^{(0)}(I) \hat{f}, \hat{g}) = \int_I (\hat{F}^{(0)}(\lambda) \hat{f}, \hat{F}^{(0)}(\lambda) \hat{g})_{h_\lambda} d\lambda\]
for any interval \(I \subset (\int \sigma_\varepsilon(\hat{H}_E^{(0)})) \setminus (\sigma_T^{(0)} \cup \sigma_V^{(0)} \cup \sigma_p(\hat{H}_E^{(0)})).\) Therefore, \(\hat{F}^{(0)}\) is uniquely extended to an isometry from \(H_{ac}(\hat{H}_E^{(0)})\) to \(H).\ We define
\[\hat{F}^{(0)} = 0, \ \text{on} \ H_p(\hat{H}_E^{(0)}).\]

The generalized Fourier transform for \(\hat{H}_E\) is constructed by the perturbation method. Define \(\hat{F}^{(\pm)}(\lambda)\) by
\[(5.10) \hat{F}^{(\pm)}(\lambda) = \hat{F}^{(0)}(\lambda) \left( 1 - q \hat{R}_E(\lambda \pm i0) \right) \in B(\mathcal{B}(\mathcal{E}); h_\lambda).\]

By using the resolvent equation (see Lemma 7. 8 in [3]), we have
\[\frac{1}{2\pi i} \left( \hat{R}_E(\lambda + i0) - \hat{R}_E(\lambda - i0) \right) \hat{f}, \hat{g} \]
\[= (\hat{F}^{(\pm)}(\lambda) \hat{f}, \hat{F}^{(\pm)}(\lambda) \hat{g})_{h_\lambda}.\]
We define the operator $\hat{\mathcal{F}}^{(\pm)}$ by $(\hat{\mathcal{F}}^{(\pm)} \hat{f})(\lambda) = \hat{\mathcal{F}}^{(\pm)}(\lambda) \hat{f}$. We define also
\[
\hat{\mathcal{F}}^{(\pm)} = 0, \quad \text{on} \quad \mathcal{H}_p(\hat{H}_E).
\]

Then, it gives a spectral representation for $\hat{H}_E$ in the following sense.

**Theorem 5.3.** (1) The operator $\hat{\mathcal{F}}^{(\pm)}$ is uniquely extended to a unitary operator from $\mathcal{H}_{ac}(\hat{H}_E)$ to $\mathbf{H}$ annihilating $\mathcal{H}_p(\hat{H}_E)$.
(2) It diagonalizes $\hat{H}_E$:
\[
(\hat{\mathcal{F}}^{(\pm)} \hat{H}_E \hat{f})(\lambda) = \lambda (\hat{\mathcal{F}}^{(\pm)} \hat{f})(\lambda), \quad \forall \hat{f} \in D(\hat{H}_E).
\]
(3) The adjoint operator $\hat{\mathcal{F}}^{(\pm)}(\lambda)^* \in \mathcal{B}(\mathfrak{h}_\lambda; \mathcal{B}^*(\mathcal{E}))$ is an eigenoperator in the sense that
\[
(\hat{H}_E - \lambda) \hat{\mathcal{F}}^{(\pm)}(\lambda)^* \phi = 0, \quad \forall \phi \in \mathfrak{h}_\lambda.
\]
(4) For $\hat{f} \in \mathcal{H}_{ac}(\hat{H}_E)$, the inversion formula holds:
\[
\hat{f} = \int_{\sigma_{ac}(\hat{H}_E)} \hat{\mathcal{F}}^{(\pm)}(\lambda)^* (\hat{\mathcal{F}}^{(\pm)} \hat{f})(\lambda) d\lambda.
\]

The proof is almost the same as that for Theorem 7.11 in [3], hence is omitted.

Note that the generalized eigenfunctions for the unperturbed operator $\hat{H}_E^{(0)}$ are constructed in [28]. Using this result, it is not difficult to construct a complete family of generalized eigenfunctions for the perturbed operator $\hat{H}_E$, which turns out to be the integral kernel of the above generalized Fourier transformation $\hat{\mathcal{F}}^{(\pm)}$.

**5.2. Resolvent expansion.** We observe the behavior at infinity of $\hat{R}_E(\lambda \pm i0) \hat{f}$ in the sense of $\mathcal{B}^*(\mathcal{E})$, which is equivalent to observing its singularities in the sense of $\mathcal{B}^*(\mathcal{E})$.

**Lemma 5.4.** For any compact interval $I \subset \left( \text{Int} \sigma_{ac}(\hat{H}_E^{(0)}) \right) \setminus \left( \sigma_T^{(0)} \cup \sigma_V^{(0)} \cup \sigma_p(\hat{H}_E^{(0)}) \right)$, there exists a constant $C > 0$ such that
\[
\| \{ r_0^{(0)}(\lambda) \hat{f}_e \}_{\hat{f}_e \in \mathcal{E}} \|_{\ell^2(\mathcal{E})} \leq C \| \hat{f} \|_{\ell^2(\mathcal{E})}
\]
holds for all $\lambda \in I$ and $\hat{f} \in \mathcal{E}$.

Proof. Since $I$ is in the resolvent set of $-(d/dz)^2 + q_e$, the lemma follows. □

Therefore, taking account of (3.26) and Lemma 5.4 we obtain the following asymptotic expansion. For $\hat{f}, \hat{g} \in \mathcal{B}^*(\mathcal{E})$, we use the following notation
\[
\hat{f} \sim \hat{g} \iff \hat{f} - \hat{g} \in \mathcal{B}_0^*(\mathcal{E}).
\]

**Theorem 5.5.** For any $\lambda \in \left( \text{Int} \sigma_{ac}(\hat{H}_E^{(0)}) \right) \setminus \left( \sigma_T^{(0)} \cup \sigma_V^{(0)} \cup \sigma_p(\hat{H}_E^{(0)}) \right)$ and $\hat{f} \in \mathcal{B}(\mathcal{E})$, we have
\[
\mathcal{U}_E \hat{\mathcal{R}}_E^{(0)}(\lambda \pm i0) \hat{f} \sim \Pi(\lambda) D^{(0)}(\lambda \pm i0) \hat{\mathcal{F}}_0(\lambda) \hat{f}.
\]

Proof. Use 5.7 and Lemma 5.4. □

By using the resolvent equation
\[
\hat{R}_E(\lambda \pm i0) = \hat{R}_E^{(0)}(\lambda \pm i0) (1 - q_E \hat{R}_E(\lambda \pm i0)),
\]
and (5.10), one can extend Theorem 5.5 to the perturbed case.
Theorem 5.6. For any $\lambda \in \left( \text{Int} \sigma_e(\hat{H}_E) \right) \setminus \left( \sigma_T(0) \cup \sigma_p(\hat{H}_E) \right)$ and $\hat{f} \in \mathcal{B}(\mathcal{E})$, we have

$$U_{E} \hat{R}_E (\lambda \pm i0) \hat{f} \simeq \Pi(\lambda) D(0)(\lambda \pm i0) \hat{F}^{(\pm)}(\lambda) \hat{f}. $$

This theorem shows that the spectral representation for the edge model arises from that of the vertex model, and that the theory developed for the vertex model in [3] works for the edge model as well. In fact, the only difference is that the latter contains the injection operator term $\Pi(\lambda)$.

5.3. Helmholtz equation and S-matrix. Theorem 5.6 enables us to characterize the solution space to the Helmholtz equation.

Lemma 5.7. Let $\lambda \in \left( \text{Int} \sigma_e(\hat{H}_E) \right) \setminus \left( \sigma_T(0) \cup \sigma_p(\hat{H}_E) \right)$ and $\hat{f} \in \mathcal{B}(E)$. Then

$$(5.11) \quad \{ \hat{u} \in \hat{B}^*(\mathcal{E}) : (\hat{H}_E - \lambda) \hat{u} = 0 \} = \hat{F}^{(\pm)}(\lambda)^* h_\lambda.$$ 

One can then obtain the asymptotic expansion of solutions to the Helmholtz equation and derive the S-matrix.

Theorem 5.8. For any incoming data $\phi^{in} \in L^2(M_{-\cos \sqrt{\lambda}})$, there exist a unique solution $\hat{u} \in \hat{B}^*(\mathcal{E})$ of the equation

$$(\hat{H}_E - \lambda) \hat{u} = 0$$

and an outgoing data $\phi^{out} \in L^2(M_{-\cos \sqrt{\lambda}})$ satisfying

$$U_{E} \hat{u} \simeq -\Pi(\lambda) \sum_{j=1}^{s} \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda} + i\sigma(\lambda)} P_{V,j}(x) \phi^{in} + \Pi(\lambda) \sum_{j=1}^{s} \frac{1}{\lambda_j(x) + \cos \sqrt{\lambda} - i\sigma(\lambda)} P_{V,j}(x) \phi^{out}. $$

The mapping

$$S(\lambda) : \phi^{in} \rightarrow \phi^{out}$$

is the S-matrix, which is unitary on $h_\lambda$.

We omit the proof of Lemma 5.7 and Theorem 5.8 since they are almost the same as that of Theorem 7. 15 of [3] by the reasoning given above.

As is proven in [29], the wave operator

$$\hat{W}_\pm = s - \lim_{t \rightarrow \pm \infty} e^{it\hat{H}_E} e^{-it\hat{H}_E(0)} \hat{P}_{ac}(\hat{H}_E(0)),$$

where $\hat{P}_{ac}(\hat{H}_E(0))$ is the projection onto the absolutely continuous subspace of $\hat{H}_E(0)$, exists and is complete, i.e. $\text{Ran} \hat{W}_\pm = \mathcal{H}_{ac}(\hat{H}_E)$. One can then follow the general scheme of scattering theory. The scattering operator

$$\hat{S} = (\hat{W}^{(\pm)})*\hat{W}^{(\mp)}$$

is unitary. Define $S$ by

$$S = \hat{F}^{(0)} \hat{S}^{(0)}(\hat{F}^{(0)})^*.$$ 

The S-matrix $S(\lambda)$ and the scattering amplitude $A(\lambda)$ are defined by

$$S(\lambda) = 1 - 2\pi i A(\lambda),$$

(5.12) $A(\lambda) = \hat{F}^{(\pm)}(\lambda) q_e \hat{F}^{(0)}(\lambda).$
Then $S(\lambda)$ is unitary on $h_\lambda$, and for $\lambda \in (\text{Int} \sigma_e(\tilde{H}_E)) \setminus (\sigma^{(0)}_T \cup \sigma^{(0)}_V \cup \sigma_p(\tilde{H}_E))$

$$(Sf)(\lambda) = S(\lambda)f(\lambda), \quad f \in H.$$  

Since the resolvent has a meromorphic extension into the lower half-plane $\{\text{Re} \lambda > 0, \text{Im} \lambda < 0\}$ with possible branch points on $\mathcal{T}$, the formula $\boxed{5.12}$ implies that the S-matrix $S(\lambda)$ is also meromorphic in the same domain.

6. FROM S-MATRIX TO INTERIOR D-N MAP

We first recall the framework of boundary value problems for both of the edge model and the vertex model. We then show that the S-matrix and the D-N map for the edge model determine each other.

6.1. 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

$$V_{\partial \Omega} = \{v \notin V_\Omega; v \sim \Omega\},$$

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

We then put $\overline{\Omega} = \Omega \cup \partial \Omega$ and

$$V_{\overline{\Omega}} = V_\Omega, \quad \partial V_{\overline{\Omega}} = V_{\partial \Omega},$$

which are called the set of interior vertices and the set of boundary vertices of $\overline{\Omega}$, respectively. We put

$$V_{\overline{\Omega}} = V_{\overline{\Omega}}^{\circ} \cup \partial V_{\overline{\Omega}}.$$

As for the edges, we simply put

$$E_{\overline{\Omega}} = E_{\partial \Omega}.$$

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

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

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

The vertex Dirichlet Laplacian on $V_{\overline{\Omega}}$ is defined in the same way as in $[3.11]$

$$(\tilde{\Delta}_{V_{\overline{\Omega}},\lambda}\hat{u})(v) = \frac{1}{\text{deg}_{V_{\overline{\Omega}}}(v)} \sum_{w \sim v, w \in V_{\overline{\Omega}}} \frac{1}{\psi_{wv}(1,\lambda)} \hat{u}(w), \quad v \in V_{\overline{\Omega}}.$$

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

$$\text{deg}_{\mathcal{W}}(v) = \begin{cases} \sharp \{w \in \mathcal{W}; w \sim v\}, & v \in \mathcal{W}, \\ \sharp \{w \in \mathcal{W}; w \sim v\}, & v \in \partial \mathcal{W}. \end{cases}$$

(See (2.6) of $[4]$). We impose the Dirichlet boundary condition for the domain $D(\tilde{\Delta}_{V_{\overline{\Omega}},\lambda})$

$$\hat{u} \in D(\tilde{\Delta}_{V_{\overline{\Omega}},\lambda}) \iff \hat{u} \in L^2(V_{\overline{\Omega}}) \cap \{\hat{u}; \hat{u}(v) = 0, \ v \in \partial V_{\overline{\Omega}}\}.$$
As in §3, we first define the vertex Dirichlet Laplacian for the case without potential and then add the potential $\tilde{Q}_{V,\lambda}$ as a perturbation. By modifying the inner product, $-\tilde{\Delta}_{V,\lambda} + \tilde{Q}_{V,\lambda}$ is self-adjoint. The normal derivative at the boundary associated with $\tilde{\Delta}_{V,\lambda}$ is defined by

$$\left( \partial^\nu \tilde{\Delta}_{V,\lambda} \tilde{u} \right)(v) = -\frac{1}{\deg_{V,\lambda}(v)} \sum_{w \sim v, w \in \mathcal{V}_{V,\lambda}} \frac{1}{\psi_{wv}(1, \lambda)} \tilde{u}(w).$$

(c.f. (2.7) of [4]). Note that in the right-hand side, $w$ is taken only from $\mathcal{V}_{V,\lambda}$.

![Boundary of a domain in the hexagonal lattice](image)

**Figure 5.** Boundary of a domain in the hexagonal lattice

Let us give examples of interior and exterior domains as well as their boundaries for the case of hexagonal lattice. In the sequel, all of our arguments are centered around these examples, although formulations and definitions are given for the general case.

We identify $\mathbb{R}^2$ with $\mathbb{C}$ and put $\omega = e^{2\pi i/6} = (1 + \sqrt{3}i)/2$. Let $\mathcal{D}$ 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

$$\mathcal{D}_{kl} = \mathcal{D} + k(2 - \omega) + \ell(1 + \omega),$$

which denotes the translation of $\mathcal{D}$ by $k(2 - \omega)$ and $\ell(1 + \omega)$. For an integer $L \geq 1$, let

$$\mathcal{D}_L = \bigcup_{|k| \leq L, |\ell| \leq L} \mathcal{D}_{kl}.$$

As is illustrated in Figure 5, we take an interior domain $\Omega_{int}$ in such a way that

$$\mathcal{V}_{\Omega_{int}}^\circ = \mathcal{V} \cap \mathcal{D}_L, \quad \mathcal{E}_{\Omega_{int}}^\circ = \mathcal{E} \cap \mathcal{D}_L.$$
In Figure 5, $\partial \mathcal{V}_{int}$ is denoted by white dots. The exterior domain $\Omega_{ext}$ is defined similarly. We then put
\[
\mathcal{V}_{int} = \mathcal{V}_{1int}, \quad \mathcal{E}_{int} = \mathcal{E}_{1int}, \\
\mathcal{V}_{ext} = \mathcal{V}_{1ext}, \quad \mathcal{E}_{ext} = \mathcal{E}_{1ext},
\]
for the sake of simplicity. Note that $\mathcal{V} = \mathcal{V}_{int} \cup \mathcal{V}_{ext}$, $\partial \mathcal{V}_{int} = \partial \mathcal{V}_{ext}$, $\mathcal{E} = \mathcal{E}_{int} \cup \mathcal{E}_{ext}$, $\mathcal{E}_{int} \cap \mathcal{E}_{ext} = \emptyset$.

We define the edge Dirichlet Laplacians on $\mathcal{E}_{int}$, $\mathcal{E}_{ext}$, which are denoted by $\hat{\Delta}_{int}$, $\hat{\Delta}_{ext}$:
\[
\hat{\Delta}_{int} = \hat{\Delta}_{E_{int}}, \quad \hat{\Delta}_{ext} = \hat{\Delta}_{E_{ext}}.
\]
We assume that the support of the potential lies strictly inside of $\mathcal{E}_{int}$. Namely introducing a set:
\[
\tilde{\mathcal{E}}_{int} = \{ e \in \mathcal{E}_{int} : e(0) \notin \partial \mathcal{V}_{int}, \quad e(1) \notin \partial \mathcal{V}_{int} \},
\]
we assume
\[
\text{supp} q \mathcal{E} \subset \tilde{\mathcal{E}}_{int}.
\]

The formal formulas (3.18), (3.26) are also valid for boundary value problems of edge Laplacians. For the case of the exterior problem, the resolvent of $-\hat{\Delta}_{ext}$ is written by (3.26) with $\hat{H}_E^{(0)}$ replaced by $-\hat{\Delta}_{ext}$. 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 4.1),
- Limiting absorption principle (Theorem 4.8),
- Spectral representation (Theorem 5.3),
- Resolvent expansion (Theorem 5.5),
- Expansion of solutions to the Helmholtz equation (Theorem 5.8),
- S-matrix (Theorem 5.8)
in the exterior domain $\mathcal{E}_{ext}$. In fact, Theorem 4.1 holds without any change. Using the formula (3.5) and the limiting absorption principle for $-\hat{\Delta}_{ext}$ proven in Theorem 7.7 in [3], one can extend Theorem 4.8 for the exterior domain. The radiation condition is also extended to the exterior domain. Then, the remaining theorems (Theorems 5.3, 5.5, 5.8) are proven by the same argument.

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

For the case of the interior problem, the Dirichlet boundary value problem for the edge Laplacian

\[
\begin{align*}
(-\hat{\Delta}_{\text{int},e} + q_e - \lambda)\hat{u} &= 0, \quad \text{in } \mathcal{E}_{\text{int}}, \\
\hat{u} &= \hat{f}, \quad \text{on } \partial V_{\text{int}}
\end{align*}
\]

(6.5)

is formulated as above. Note that the spectrum of \(-\hat{\Delta}_{\text{int},e} + q_e\) is discrete. In the following, we assume that

\[
\lambda \notin \sigma(-\hat{\Delta}_{\text{int},e} + q_e).
\]

(6.6)

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

\[
\Lambda_{\text{int},e}(\lambda)\hat{f}(v) = \frac{d}{dz}\hat{u}_e(v), \quad v \in \partial V_{\text{int}},
\]

(6.7)

where \( e \) is the edge having \( v \) as its end point and \( \hat{u} = \{\hat{u}_e^{(\pm)}\}_{e \in \mathcal{E}_{\text{int}}} \) is the solution to the equation (6.5). The same remark as above is applied to \( \frac{d}{dz}\hat{u}_e(v) \), \( v \in \partial V_{\text{int}} \).

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

\[
(\hat{\Delta}^{(0)}_{V_D})\hat{u}(v) = \frac{1}{d_{V_D}(v)} \sum_{w \sim v, w \in V_D} \hat{u}(w).
\]

By this definition, we have (see (3.23))

\[
(\hat{\Delta}^{(0)}_{V_D})\hat{u}(v) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} (\hat{\Delta}^{(0)}_{V_D}).
\]

(6.8)

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

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

Now, consider the exterior boundary value problem

\[
\begin{align*}
(-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda})\hat{u} &= 0, \quad \text{in } V_{\text{ext}}^0, \\
\hat{u} &= \hat{f}, \quad \text{on } \partial V_{\text{ext}}.
\end{align*}
\]

(6.9)

Note that by (6.8) and (3.24) this is equivalent to

\[
\begin{align*}
(-\hat{\Delta}^{(0)}_{V} + \cos \sqrt{\lambda})\hat{u} &= 0, \quad \text{in } V_{\text{ext}}^0, \\
\hat{u} &= \hat{f}, \quad \text{on } \partial V_{\text{ext}}.
\end{align*}
\]
Let $\hat{u}^{(\pm)}_{ext, V}$ be the solution of this equation satisfying the radiation condition. Then, taking account of (6.1) and (6.8), we define the exterior D-N map by

$$\hat{\Lambda}^{(\pm)}_{ext, V}(\lambda) \hat{f} = -\frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \partial_{\hat{\Delta}_{ext, \lambda}} \hat{u}^{(\pm)}_{ext, V} = \frac{1}{\deg_{\hat{\Delta}_{ext, \lambda}}(v)} \sum_{w \sim v, w \in V_{ext}} \hat{u}^{(\pm)}_{ext, V}(w).$$

We also consider the interior boundary value problem

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

Taking account of (6.2), we define the interior D-N map by

$$\hat{\Lambda}^{(\pm)}_{int, V}(\lambda) \hat{f}(v) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \partial_{\hat{\Delta}_{int, \lambda}} \hat{u}^{(\pm)}_{int, V} = -\frac{1}{\deg_{\hat{\Delta}_{int, \lambda}}(v)} \sum_{w \sim v, w \in V_{int}} \hat{u}^{(\pm)}_{int, V}(w).$$

Note that by virtue of Lemma 3.3, if $\hat{u}$ satisfies the edge Schrödinger equation $(\hat{H}_E - \lambda) \hat{u} = 0$ and the Kirchhoff condition, $\hat{u}|_{V}$ satisfies the vertex Schrödinger equation $( -\hat{\Delta}_{V, \lambda} + \hat{Q}_{V, \lambda} ) \hat{u}|_{V} = 0$. Therefore, if the exterior boundary value problem (6.9) for the edge model is solvable, so is the interior boundary value problem (6.9) for the vertex model. The same remark applies to the interior boundary value problem.

If $\varphi(z)$ satisfies $-\varphi''(z) - \lambda \varphi(z) = 0$ in $(0, 1)$, 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 $\hat{u}|_{V}$, where $\hat{u}$ is the solution to the edge Schrödinger equation, this implies, by (6.4), (6.7), (6.10) and (6.12), the following formulas between the D-N maps of edge-Laplacian and vertex Laplacian.

We put

$$I_{ext} = (\text{Int } \sigma_c(\hat{H}_E)) \setminus (\sigma^{(0)}_V \cup \sigma^{(0)}_{\tau}),$$

and let $I_{int}$ be the set of $\lambda \in \mathbb{C} \setminus \sigma(-\hat{\Delta}_{int, E} + q_E)$ for which there exists $(-\hat{\Delta}_{V, \lambda} + \hat{Q}_{V, \lambda})^{-1}$. Let us note that

$$\sigma_c(-\hat{\Delta}_E) = \sigma_c(-\hat{\Delta}_{ext, E}).$$

**Lemma 6.1.** The following equalities hold:

$$\hat{\Lambda}^{(\pm)}_{ext, V}(\lambda) = \cos \sqrt{\lambda} - \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Lambda^{(\pm)}_{ext, E}(\lambda), \quad \lambda \in I_{ext},$$

$$\hat{\Lambda}_{int, V}(\lambda) = -\cos \sqrt{\lambda} - \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Lambda_{int, E}(\lambda), \quad \lambda \in I_{int}.$$
Therefore, the D-N map for the edge model and the D-N map for the vertex model determine each other.

We put
\[ \Sigma = \partial V_{\text{int}} = \partial V_{\text{ext}}, \]
and define an operator \( \tilde{S}_\Sigma : \ell^2(\Sigma) \to \ell^2(\Sigma) \) by
\[
(\tilde{S}_\Sigma \hat{f})(v) = \frac{1}{\deg_{V}(v)} \sum_{w \sim v, w \in \Sigma} \hat{f}(w),
\]
where
\[ \deg_{V}(v) = \deg(v) = \# \{ w \in V : w \sim v \} \]
is the degree on \( V \). Let \( \chi_{\Sigma} \) be the characteristic function of \( \Sigma \). We use \( \chi_{\Sigma} \) to mean both of the operator of restriction
\[ \chi_{\Sigma} : \ell^2_{\text{loc}}(V) \ni \hat{f} \to \hat{f}_{\mid \Sigma}, \]
and the operator of extension
\[ \chi_{\Sigma} : \ell^2(\Sigma) \ni \hat{f} \to \begin{cases} \hat{f}, & \text{on } \Sigma, \\ 0, & \text{otherwise}. \end{cases} \]
Then, we have for \( \hat{f} \in \ell^2(\Sigma) \)
\[ \tilde{\Delta}_V \chi_{\Sigma} \hat{f} = \tilde{S}_\Sigma \hat{f}. \]
We also introduce multiplication operators by
\[
(M_{\text{int}} \hat{f})(v) = \frac{\deg_{V_{\text{int}}}(v)}{\deg_{V}(v)} \hat{f}(v),
\]
\[
(M_{\text{ext}} \hat{f})(v) = \frac{\deg_{V_{\text{ext}}}(v)}{\deg_{V}(v)} \hat{f}(v).
\]

Given \( \hat{f} \in \ell^2(\Sigma) \), let \( \hat{u}_{\text{ext},E}^{(\pm)} \) be the solution to the exterior boundary value problem
\[
\begin{cases}
-\tilde{\Delta}_{\text{ext},E} - \lambda \hat{u}_{\text{ext},E}^{(\pm)} = 0, & \text{in } E_{\text{ext}}, \\
\hat{u}_{\text{ext},E}^{(\pm)} = \hat{f}, & \text{on } \partial E_{\text{ext}}
\end{cases}
\]
satisfying the radiation condition. Let \( \hat{u}_{\text{int},E}^{(\pm)} \) be the solution to the interior problem
\[
\begin{cases}
-\tilde{\Delta}_{\text{int},E} + q_{\text{E}} - \lambda \hat{u}_{\text{int},E}^{(\pm)} = 0, & \text{in } E_{\text{int}}, \\
\hat{u}_{\text{int},E}^{(\pm)} = \hat{f}, & \text{on } \partial E_{\text{int}}
\end{cases}
\]
We put
\[ \hat{u}_{E}^{(\pm)} = \begin{cases} \hat{u}_{\text{ext},E}^{(\pm)} & \text{on } E_{\text{ext}} \setminus \Sigma, \\ \hat{f} & \text{on } \Sigma, \\ \hat{u}_{\text{int},E}^{(\pm)} & \text{on } E_{\text{int}} \setminus \Sigma. \end{cases} \]
Then, \( \hat{u}_{E}^{(\pm)} \) satisfies
\[ \hat{u}_{E}^{(\pm)} \in B^*_{1}(E) \cap H_{\text{loc}}^1(E) \cap H_{\text{loc}}^2(E_{\text{ext}}) \cap H^2(E_{\text{int}}), \]
and on any edge \( e \in E \)
\[
(-\tilde{\Delta}_E + q_{E} - \lambda)\hat{u}_{E}^{(\pm)} = 0
\]
We then have
\[ \hat{f}^{(\pm)}(\lambda) = \hat{f}^{(\pm)}(\lambda, v) = (-\hat{\Delta}_{V,\lambda} + \hat{Q}_{V,\lambda}) \left( \hat{u}^{(\pm)}|_V \right), \quad v \in V. \]

Then, since \( \hat{u}^{(\pm)} \) satisfies the Kirchhoff condition outside \( \Sigma \), we have
\[ \text{supp} \hat{f}^{(\pm)}(\lambda) \subset \Sigma. \]

Define a bounded operator \( B_{\Sigma}^{(\pm)}(\lambda) : \ell^2(\Sigma) \to \ell^2(\Sigma) \) by
\[ B_{\Sigma}^{(\pm)}(\lambda) = \frac{\sqrt{\lambda}}{\sin \sqrt{\lambda}} \left( M_{\text{int}} \lambda^{\text{int},V}(\lambda) - M_{\text{ext}} \lambda^{\text{ext},V}(\lambda) - \hat{S}_\Sigma + \cos \sqrt{\lambda} \right). \]

We have, using (3.23), (3.24) and (6.13),
\[ \text{Then, since} \quad \hat{f}^{(\pm)}(\lambda) = B_{\Sigma}^{(\pm)}(\lambda) \hat{f}, \quad \text{on} \quad \Sigma. \]

We put an edge function \( \hat{w}^{(\pm)}_e \) by
\[ \hat{w}^{(\pm)}_e(z) = \hat{c}_e^{(\pm)}(1, \lambda) \frac{\phi_0(z, \lambda)}{\phi_0(1, \lambda)} + \hat{c}_e^{(\pm)}(0, \lambda) \frac{\phi_1(z, \lambda)}{\phi_1(1, \lambda)}, \quad e \in \mathcal{E}, \]
where \( \hat{c}_e^{(\pm)}(p, \lambda) \) is defined by
\[ \hat{c}_e^{(\pm)}(p, \lambda) = \left( -\hat{\Delta}_{V,\lambda \pm 0} + \hat{Q}_{V,\lambda \pm 0} \right)^{-1} \hat{f}^{(\pm)}(\lambda), \quad p = 0, 1, \]
at the end point of an edge \( e \), and
\[ \left( -\hat{\Delta}_{V,\lambda \pm 0} + \hat{Q}_{V,\lambda \pm 0} \right)^{-1} = \lim_{\epsilon \to 0} \left( -\hat{\Delta}_{V,\lambda \pm \epsilon} + \hat{Q}_{V,\lambda \pm \epsilon} \right)^{-1}. \]

We then have
\[ \hat{w}^{(\pm)}_e = \hat{T}_{\mathcal{E}}^{(0)}(\lambda) \left( -\hat{\Delta}_{V,\lambda \pm 0} + \hat{Q}_{V,\lambda \pm 0} \right)^{-1} \hat{f}^{(\pm)}(\lambda). \]

Note that outside \( \mathcal{E}_{\text{int}} \)
\[ \hat{w}^{(\pm)}_e(z) = \hat{c}_e^{(\pm)}(1, \lambda) \frac{\sin \sqrt{\lambda} z}{\sqrt{\lambda}} + \hat{c}_e^{(\pm)}(0, \lambda) \frac{\sin \sqrt{\lambda}(1 - z)}{\sqrt{\lambda}}. \]

Moreover, \( \hat{w}^{(\pm)}_e \) satisfies the Kirchhoff condition on \( V \setminus \Sigma \).

We prepare one more notation. Let the operator of restriction \( r|_V : H^1(\mathcal{E}) \to L^2(V) \) be defined by
\[ \left( r|_V \hat{u} \right)(v) = \hat{u}(v), \quad v \in V. \]
The adjoint : \( \left( r|_V \right)^* : L^2(V) \to H^{-1}(\mathcal{E}) \) is defined by
\[ \left( r|_V \hat{u}, \hat{v} \right)_{L^2(V)} = \left( \hat{u}, \left( r|_V \right)^* \hat{v} \right)_{L^2(\mathcal{E})}. \]

We then have in view of (2.16)
\[ \left( r|_V \right)^* = \frac{1}{d_g} \sum_{v \in V} \delta_v, \]
where \( \delta_v \) denotes the Dirac distribution on \( \mathcal{E} \) supported at \( v \in V \). By the elliptic regularity
\[ \hat{R}_\mathcal{E}(\lambda \pm \epsilon) \in B(L^2(\mathcal{E}); H^2(\mathcal{E})). \]

Taking the adjoint
\[ \hat{R}_\mathcal{E}(\lambda \pm \epsilon) \in B(H^{-2}(\mathcal{E}); L^2(\mathcal{E})). \]
By an interpolation, we then have
\[ \hat{R}_\varepsilon(\lambda \pm ie) \in \mathcal{B}(H^{-1}(\varepsilon); H^{2-i}(\varepsilon)), \quad 0 \leq t \leq 2, \]
which implies
\[ \hat{R}_\varepsilon(\lambda \pm ie) \in \mathcal{B}(H_0^{-1}(\varepsilon); H_{loc}^{2-i}(\varepsilon)), \quad 0 \leq t \leq 2, \]
where \( H_0^{-1}(\varepsilon) \) is the set of the compactly supported distributions in \( H^{-1}(\varepsilon) \). Therefore
\[ \hat{R}_\varepsilon(\lambda \pm i0)(r|_\varepsilon) \ast \chi_\Sigma \in \mathcal{B}(L^2(\varepsilon); H_{loc}^1(\varepsilon)) \]
is well-defined.

**Lemma 6.2.** Let \( \hat{u}_{\varepsilon}^{(\pm)} \) be defined by
\[
(6.23) \quad \hat{u}_{\varepsilon}^{(\pm)} = \begin{cases} \chi_{\text{ext}} \hat{u}_{\text{ext},\varepsilon}^{(\pm)} + \chi_{\text{int}} \hat{u}_{\text{int},\varepsilon}^{(\pm)} & \text{outside } \Sigma, \\ \hat{f} & \text{on } \Sigma, \end{cases}
\]
where \( \hat{f} \in L^2(\Sigma) \), \( \chi_{\text{ext}} \) and \( \chi_{\text{int}} \) are the characteristic functions of \( \varepsilon_{\text{ext}} \) and \( \varepsilon_{\text{int}} \), and \( \hat{u}_{\text{ext},\varepsilon}^{(\pm)}, \hat{u}_{\text{int},\varepsilon}^{(\pm)} \) are the solutions of the boundary value problems \( (6.14), (6.15) \), respectively. Let \( \hat{w}_{\varepsilon}^{(\pm)} \) be as in \( (6.20) \). Then we have
\[
(6.24) \quad \hat{u}_{\varepsilon}^{(\pm)} = \hat{w}_{\varepsilon}^{(\pm)} = \hat{R}_\varepsilon(\lambda \pm i0)(r|_\varepsilon) \ast \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \hat{f} \quad \text{on } \varepsilon.
\]
In particular, we have
\[
(6.25) \quad \hat{u}_{\text{ext},\varepsilon}^{(\pm)} = \hat{R}_\varepsilon(\lambda \pm i0)(r|_\varepsilon) \ast \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \hat{f} = \hat{T}_\varepsilon(\lambda) \left( -\hat{\Delta}_{\varepsilon,\lambda} + \hat{Q}_{\varepsilon,\lambda} \right)^{-1} \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \hat{f} \quad \text{on } \varepsilon_{\text{ext}},
\]
\[
(6.26) \quad \hat{f} = \left( -\hat{\Delta}_{\varepsilon,\lambda} + \hat{Q}_{\varepsilon,\lambda} \right)^{-1} \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \hat{f} \quad \text{on } \Sigma.
\]

Proof. By definition, for any edge \( e \),
\[
\left( -\frac{d^2}{dz^2} + q_\varepsilon(z) - \lambda \right) \hat{u}_{\varepsilon,e}^{(\pm)}(z) = 0, \quad \text{on } e.
\]
In view of \( (6.16) \) and \( (6.20) \), we have
\[
\left( -\hat{\Delta}_{\varepsilon,\lambda} + \hat{Q}_{\varepsilon,\lambda} \right) \left( \hat{w}_{\varepsilon}^{(\pm)}|_\varepsilon \right) = \hat{f}^{(\pm)}(\lambda) = \left( -\hat{\Delta}_{\varepsilon,\lambda} + \hat{Q}_{\varepsilon,\lambda} \right) \left( \hat{u}_{\varepsilon}^{(\pm)}|_\varepsilon \right),
\]
where we use
\[
(6.27) \quad r|_\varepsilon \hat{T}_\varepsilon(\lambda) = 1_\varepsilon,
\]
\( 1_\varepsilon \) being the identity on \( \varepsilon \). These two formulas imply that \( u_{\varepsilon}^{(\pm)} - \hat{w}_{\varepsilon}^{(\pm)} \) satisfies the equation
\[
\left( -\frac{d^2}{dz^2} + q_\varepsilon(z) - \lambda \right) \left( u_{\varepsilon,e}^{(\pm)}(z) - \hat{w}_{\varepsilon,e}^{(\pm)}(z) \right) = 0, \quad \text{on } e,
\]
and the Kirchhoff condition
\[
\left( -\hat{\Delta}_{\varepsilon,\lambda} + \hat{Q}_{\varepsilon} \right) 
\left( u_{\varepsilon}^{(\pm)}|_\varepsilon - \hat{w}_{\varepsilon}^{(\pm)}|_\varepsilon \right) = 0.
\]
Then, \( \hat{u}_{\varepsilon}^{(\pm)} - \hat{w}_{\varepsilon}^{(\pm)} = 0 \) since it satisfies the radiation condition.

Again using \( (6.27) \) and Lemma 3.5
\[
1_\varepsilon = \hat{T}_\varepsilon(\lambda)(r|_\varepsilon)\ast.
\]
Note that
\[ r|_{\nu} r_\Sigma(\lambda) = 0, \]
hence taking the adjoint,
\[ r_\Sigma(\lambda)(r|_{\nu})^* = 0. \]
In view of (3.18), we have
\[ \chi_{\Sigma} r|_{\nu} \hat{R}^{(0)}(\lambda - i0) = B^{(\pm)}_{\Sigma}(\lambda) \chi_{\Sigma} \]
\[ = \hat{T}_\Sigma(\lambda)(-\Delta_{\Sigma} + \hat{Q}_{\Sigma} + \hat{V}_{\Sigma})^{-1} \hat{T}_\Sigma(\lambda)(r|_{\nu})^* B^{(\pm)}_{\Sigma}(\lambda) \chi_{\Sigma} \]
\[ = \hat{T}_\Sigma(\lambda)(-\Delta_{\Sigma} + \hat{Q}_{\Sigma} + \hat{V}_{\Sigma})^{-1} \chi_{\Sigma} B^{(\pm)}_{\Sigma}(\lambda) \chi_{\Sigma}. \]
Using (6.17), (6.19) and (6.20), we have proven (6.24) and (6.25). By (6.27), one can prove (6.26).

6.3. Spectral representation in an exterior domain. Note that
\[ \chi_{\Sigma} r|_{\nu} \hat{R}^{(0)}(\lambda - i0) \in \mathcal{B}(B(\Sigma); \ell^2(\Sigma)), \]
which yields
\[ \hat{R}^{(0)}(\lambda - i0)(r|_{\nu})^* \chi_{\Sigma} \in \mathcal{B}(\ell^2(\Sigma); B^*(\Sigma)). \]
With this in mind, we prove the following lemma.

Lemma 6.3. The following equalities hold
(6.28)
\[ \hat{R}_{\Sigma}(\lambda - i0) = \chi_{\Sigma} \left( I - \hat{R}_\Sigma(\lambda - i0)(r|_{\nu})^* B^{(\pm)}_{\Sigma}(\lambda) \chi_{\Sigma} r |_{\nu} \right) \hat{R}^{(0)}(\lambda - i0) \chi_{\Sigma}, \]
(6.29)
\[ \hat{R}_{\Sigma}(\lambda - i0) = \chi_{\Sigma} \left( I - (r|_{\nu})^* B^{(\pm)}_{\Sigma}(\lambda) r |_{\nu} \hat{R}_\Sigma(\lambda - i0) \right) \chi_{\Sigma}. \]

Proof. Take \( \hat{f} \in B(\Sigma) \) arbitrarily, and replace \( \hat{f} \) in (6.14), (6.15) and (6.23) by \( \chi_{\Sigma} r|_{\nu} \hat{R}^{(0)}(\lambda - i0) \hat{f} \). Then, letting
\[ \hat{u}_0 = \hat{R}_\Sigma(\lambda - i0)(r|_{\nu})^* \chi_{\Sigma} B^{(\pm)}_{\Sigma}(\lambda) \chi_{\Sigma} r|_{\nu} \hat{R}^{(0)}(\lambda - i0) \hat{f} \]
and using (6.24), we have
\[ \hat{u}_0^{(\pm)} = \hat{u}_0. \]
This implies \( \hat{u}_0 = \hat{u}_0^{(\pm)} \) in \( \mathcal{E}_{\Sigma} \), hence
\[ \begin{cases} (-\hat{\Delta}_\Sigma - \lambda) \hat{u}_0 = 0, & \text{in } \mathcal{E}_{\Sigma}, \\ \hat{u}_0 = r |_{\nu} \hat{R}^{(0)}(\lambda - i0) \hat{f}, & \text{on } \Sigma. \end{cases} \]
Let \( \hat{w} = \hat{u}_0 - \hat{R}^{(0)}(\lambda - i0) \hat{f} \). Then
\[ \begin{cases} (-\hat{\Delta}_\Sigma - \lambda) \hat{w} = -\hat{f}, & \text{in } \mathcal{E}_{\Sigma}, \\ \hat{w} = 0, & \text{on } \Sigma. \end{cases} \]
Taking account of the radiation condition, we then have \( \hat{w} = -\hat{R}_{\Sigma}(\lambda - i0) \chi_{\Sigma} \hat{f} = \hat{u}_0 - \hat{R}^{(0)}(\lambda - i0) \hat{f} \), which implies (6.28). By taking the adjoint, we obtain (6.29). □
By virtue of (5.5) and (5.9), \( \widehat{\mathcal{F}}^{(0)}(\lambda) \) is extended to a bounded operator from \( \ell^2(\Sigma) \) to \( h_\lambda \). We then define a spectral representation for \( \widehat{H}_{ext} = -\widehat{\Delta}_{ext, \mathcal{E}} \) by
\[
\widehat{F}_{ext}^{(\pm)}(\lambda) = \widehat{\mathcal{F}}^{(0)}(\lambda) \left( 1 - (r|_\Sigma)^* \chi_\Sigma (B^{(\mp)}_\Sigma(\lambda)) \chi_\Sigma r|_\Sigma \widehat{R}_{\mathcal{E}}(\lambda \pm i0) \right) \chi_{ext}.
\]
Taking the adjoint, we also have
\[
(6.30) \quad \widehat{F}_{ext}^{(\pm)}(\lambda)^* = \chi_{ext} \left( 1 - \widehat{R}_{\mathcal{E}}(\lambda \mp i0)(r|_\Sigma)^* \chi_\Sigma B^{(\mp)}_\Sigma(\lambda) \chi_\Sigma r|_\Sigma \right) \widehat{\mathcal{F}}^{(0)}(\lambda)^*.
\]
By (6.29), we have
\[
\widehat{F}_{ext}^{(\pm)}(\lambda) = \widehat{\mathcal{F}}^{(0)}(\lambda)(-\widehat{\Delta}_{\mathcal{E}} - \lambda) \widehat{R}_{ext, \mathcal{E}}(\lambda \pm i0).
\]
Therefore, \( \widehat{F}_{ext}^{(\pm)}(\lambda) \) is independent of the perturbation \( q_\mathcal{E} \).

**Lemma 6.4.** For any \( \phi \in h_\lambda \), \( \widehat{F}_{ext}^{(-)}(\lambda)^* \phi \) satisfies the equation
\[
\begin{cases}
(-\widehat{\Delta}_{ext, \mathcal{E}} - \lambda) \widehat{F}_{ext}^{(-)}(\lambda)^* \phi = 0, & \text{in } \mathcal{E}_{ext}, \\
\widehat{F}_{ext}^{(-)}(\lambda)^* \phi = 0 & \text{on } \Sigma.
\end{cases}
\]
Moreover, \( \widehat{F}_{ext}^{(-)}(\lambda)^* \phi - \widehat{\mathcal{F}}^{(0)}(\lambda)^* \phi \) is outgoing.

**Proof.** We put \( \widehat{v} = \widehat{R}_{\mathcal{E}}(\lambda + i0)(r|_\Sigma)^* \chi_\Sigma B^{(\mp)}_\Sigma(\lambda) \chi_\Sigma r|_\Sigma \widehat{\mathcal{F}}^{(0)}(\lambda)^* \phi \). Then,
\[
(-\widehat{\Delta}_{\mathcal{E}} - \lambda) \widehat{v} = 0, \quad \text{in } \mathcal{E}_{ext}.
\]
Letting \( \widehat{f} = \chi_\Sigma r|_\Sigma \widehat{\mathcal{F}}^{(0)}(\lambda)^* \phi \), and using (6.24), we have \( \widehat{v} = \widehat{u}_{ext}^{(+)}(\lambda)^* \). Then, by (6.23), \( \widehat{v} = \widehat{f} = \widehat{\mathcal{F}}^{(0)}(\lambda)^* \phi \) on \( \Sigma \). Since \( \widehat{v} \) is outgoing, we obtain the lemma.

---

### 6.4. Imbedding of \( \ell^2(\Sigma) \) to \( h_\lambda \)

We put
\[
\widehat{F}^{(\pm)}(\lambda) = \widehat{\mathcal{F}}^{(\pm)}(\lambda)(r|_\Sigma)^* \chi_\Sigma B^{(\pm)}_\Sigma(\lambda) : \ell^2(\Sigma) \to h_\lambda.
\]
Then, by (5.10) and (6.24),
\[
\widehat{F}^{(\pm)}(\lambda)(r|_\Sigma)^* \chi_\Sigma B^{(\pm)}_\Sigma(\lambda) \widehat{f} = \widehat{\mathcal{F}}^{(0)}(\lambda)(1 - q_\mathcal{E} \widehat{R}_{\mathcal{E}}(\lambda \pm i0))(r|_\Sigma)^* \chi_\Sigma B^{(\pm)}_\Sigma(\lambda) \widehat{f} = \widehat{\mathcal{F}}^{(0)}(\lambda)(-\widehat{\Delta}_{\mathcal{E}} - \lambda) \widehat{u}_{ext}^{(\pm)}(\lambda)^*.
\]
This formula shows that \( \widehat{F}^{(\pm)}(\lambda) \) does not depend on the perturbation \( q_\mathcal{E} \).

**Lemma 6.5.** (1) \( \widehat{F}^{(\pm)}(\lambda) : \ell^2(\Sigma) \to h_\lambda \) is 1 to 1.

(2) \( \widehat{F}^{(\pm)}(\lambda)^* : h_\lambda \to \ell^2(\Sigma) \) is onto.

**Proof.** Assume \( \widehat{F}^{(\pm)}(\lambda) \widehat{f} = 0 \), and let \( \widehat{u}_{ext, \mathcal{E}}^{(\pm)} \) be the solution of the exterior problem (6.3). Then, by virtue of (6.24)
\[
\widehat{u}_{ext, \mathcal{E}}^{(\pm)} = \widehat{R}_{\mathcal{E}}(\lambda \pm i0)\widehat{g}, \quad \widehat{g} = (r|_\Sigma)^* \chi_\Sigma B^{(\pm)}_\Sigma(\lambda) \chi_\Sigma \widehat{f}.
\]

Theorem 5.6 yields
\[
U_{\mathcal{E}, i} \widehat{R}_{\mathcal{E}}(\lambda \pm i0)\widehat{g} \simeq \Pi(\lambda) D^{(0)}(\lambda \pm i0) \widehat{F}^{(\pm)}(\lambda) \widehat{g}.
\]
Since \( \widehat{F}^{(\pm)}(\lambda) \widehat{f} = \widehat{\mathcal{F}}^{(\pm)}(\lambda) \widehat{g} \), this implies \( \widehat{u}_{ext, \mathcal{E}}^{(\pm)} \in \mathcal{B}^*_0 \). Using the Rellich type theorem (Theorem 4.1) and the unique continuation property, we obtain \( \widehat{u}_{ext, \mathcal{E}}^{(\pm)} = 0 \), which implies \( \widehat{f} = 0 \). This proves (1). To prove the assertion (2), let us note the
following fact: Let \( X, Y \) be Hilbert spaces, and assume that a bounded operator \( A : X \to Y \) is injective, and \( \dim X < \infty \). Then

- \( A : X \to \text{Ran}(A) \) is bijective,
- \( A^* : \text{Ran}(A) \to X \) is surjective.

(The first assertion is elementary. The second assertion follows from the fact that \( A^* A : X \to X \) is injective, hence surjective.)

6.5. **Scattering amplitude in the exterior domain.** We define the scattering amplitude in the exterior domain by

\[
A_{\text{ext}}(\lambda) = \tilde{F}^{(+)}(\lambda)(r|_\Sigma)^* \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \chi_\Sigma r|_\Sigma \tilde{F}^{(0)}(\lambda)^*.
\]

Using Theorem 6.3 and (6.30), and extending \( \tilde{F}_{\text{ext}}^{(\pm)}(\lambda)^* \phi - \tilde{F}^{(0)}(\lambda)^* \phi \) to be 0 on \( E_{\text{int}} \), we have

\[
\mathcal{U}_{E,F} \left( \tilde{F}_{\text{ext}}^{(\pm)}(\lambda)^* \phi - \tilde{F}^{(0)}(\lambda)^* \phi \right) = -\mathcal{U}_{E,F} \chi_{\text{ext}} \hat{R}_E(\lambda + i0)(r|_\Sigma)^* \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \chi_\Sigma r|_\Sigma \hat{F}^{(0)}(\lambda)^* \phi \\
\simeq -\Pi_\ell(\lambda)D^{(0)}(\lambda + i0)A_{\text{ext}}(\lambda) \phi.
\]

This shows that \( A_{\text{ext}}(\lambda) \) depends only on \( E_{\text{ext}} \).

6.6. **Single layer and double layer potentials.** The operator

\[
\hat{R}_E(\lambda + i0)(r|_\Sigma)^* \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \chi_\Sigma : \ell^2(\Sigma) \to B^*(E)
\]

is an analogue of the double layer potential. The operator \( M_{\Sigma}^{(\pm)}(\lambda) : \ell^2(\Sigma) \to \ell^2(\Sigma) \) defined by

\[
M_{\Sigma}^{(\pm)}(\lambda) \hat{f} := (\hat{R}_E(\lambda \pm i0) \chi_\Sigma \hat{f})|_\Sigma
\]

is an analogue of the single layer potential.

**Lemma 6.6.** (1) \( M_{\Sigma}^{(\pm)}(\lambda) = \chi_\Sigma \left( -\hat{\Delta}_{V,\lambda \pm i0} + \hat{Q}_{V,\lambda \pm i0} \right)^{-1} \chi_\Sigma \).

(2) \( M_{\Sigma}^{(\pm)}(\lambda)B_{\Sigma}^{(\pm)}(\lambda) = 1 \) on \( \ell^2(\Sigma) \).

**Proof.** In view of (3.18) and (6.27), we have

\[
\chi_\Sigma \hat{R}_E(\lambda \pm i0) \hat{f} = \chi_\Sigma \left( -\hat{\Delta}_{V,\lambda \pm i0} + \hat{Q}_{V,\lambda \pm i0} \right)^{-1} \hat{T}_V(\lambda) \chi_\Sigma \hat{f}.
\]

This proves (1). By (6.26),

\[
\hat{f} = \left( -\hat{\Delta}_{V,\lambda \pm i0} + \hat{Q}_{V,\lambda \pm i0} \right)^{-1} B_{\Sigma}^{(\pm)}(\lambda) \hat{f}.
\]

The assertion (2) then follows from these equalities. □

6.7. **S-matrix and interior D-N map.**

**Theorem 6.7.** The following equality holds:

\[
A_{\text{ext}}(\lambda) - A(\lambda) = \hat{R}^{(+)}(\lambda)(r|_\Sigma)^* \left( B_{\Sigma}^{(\pm)}(\lambda) \right)^{-1} r|_\Sigma \hat{F}^{(-)}(\lambda)^*.
\]

**Proof.** For \( \phi \in \mathfrak{h}_\lambda \), we put

\[
\tilde{u} = \tilde{F}^{(-)}(\lambda)^* \phi - \tilde{F}^{(-)}(\lambda)^* \phi.
\]

By (5.10) and (6.30), we have

\[
\tilde{u} = (\chi_{\text{ext}} - 1)(1 - \hat{R}_E(\lambda + i0)q_E) \hat{F}^{(0)}(\lambda)^* \phi \\
+ \chi_{\text{ext}} \hat{R}_E(\lambda + i0) \left( (r|_\Sigma)^* \chi_\Sigma B_{\Sigma}^{(\pm)}(\lambda) \chi_\Sigma r|_\Sigma - q_E \right) \hat{F}^{(0)}(\lambda)^* \phi.
\]
The first term of the right-hand side is a smooth function when passed to the Fourier series. Theorem 5.6 then implies
\[ \mathcal{U}_{\mathcal{E}, \ell} \tilde{u} \simeq \Pi_{\ell}(\lambda) D^{(0)}(\lambda + i0) \mathcal{F}^{(+)}(\lambda) \left( \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) \chi_{\Sigma} r_{\mathcal{V}} - q_{\mathcal{E}} \right) \mathcal{F}^{(0)}(\lambda)^* \phi. \]

By Lemma 6.4, \( \tilde{u} \) is the outgoing solution of the equation
\[ (\mathcal{D}_{\mathcal{E}} - \lambda) \tilde{u} = 0, \quad \text{in} \quad \mathcal{E}_{\text{ext}}, \quad \tilde{u}\big|_{\Sigma} = \mathcal{F}^{(-)}(\lambda)^* \phi. \]

In view of (6.25), we have
\[ \tilde{u} = \bar{R}_{\mathcal{E}}(\lambda + i0) \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) \chi_{\Sigma} \mathcal{F}^{(-)}(\lambda)^* \phi. \]

Again using Theorem 5.6
\[ \mathcal{U}_{\mathcal{E}, \ell} \tilde{u} \simeq \Pi_{\ell}(\lambda) D^{(0)}(\lambda + i0) \mathcal{F}^{(+)}(\lambda) \left( \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) \chi_{\Sigma} \mathcal{F}^{(-)}(\lambda)^* \phi. \]

This implies
\[ A_{\text{ext}}(\lambda) - A(\lambda) = \mathcal{F}^{(+)}(\lambda) \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) \chi_{\Sigma} \mathcal{F}^{(-)}(\lambda)^* \phi. \]

Let us note here that \( 1 = B_{\Sigma}^{(-)}(\lambda) M_{\Sigma}^{(-)}(\lambda) \) by virtue of Lemma 6.6 Since \( M_{\Sigma}^{(+)}(\lambda) = \chi_{\Sigma} r_{\mathcal{V}} \bar{R}(\lambda + i0) \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} \), we have \( (M_{\Sigma}^{(-)}(\lambda))^* = M_{\Sigma}^{(+)}(\lambda) \), which implies
\[ (6.31) \quad 1 = M_{\Sigma}^{(+)}(\lambda)(B_{\Sigma}^{(-)}(\lambda))^*. \]

Inserting (6.31) between \( B_{\Sigma}^{(+)}(\lambda) \) and \( \mathcal{F}^{(-)}(\lambda)^* \phi \), we obtain
\[ \mathcal{F}^{(+)}(\lambda) \left| r \right|_{\mathcal{V}}^* \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) M_{\Sigma}^{(-)}(\lambda)(B_{\Sigma}^{(+)\ast}(\lambda))^* \chi_{\Sigma} r_{\mathcal{V}} \mathcal{F}^{(-)}(\lambda)^* \]
\[ = \mathcal{F}^{(+)}(\lambda)(r_{\mathcal{V}}^*) \chi_{\Sigma} B_{\Sigma}^{(+)}(\lambda) M_{\Sigma}^{(-)}(\lambda) B_{\Sigma}^{(-)}(\lambda))^* \chi_{\Sigma} r_{\mathcal{V}} r_{\mathcal{V}} \mathcal{F}^{(-)}(\lambda)^* \]
\[ = \bar{F}^{(+)}(\lambda)(r_{\mathcal{V}}^*) M_{\Sigma}^{(+)}(\lambda) r_{\mathcal{V}} r_{\mathcal{V}} \bar{F}^{(-)}(\lambda)^*. \]

We have thus proven Theorem 6.4. \( \square \)

6.8. The operator \( \bar{F}^{(+)}(\lambda) \). To construct \( A(\lambda) \) from \( B_{\Sigma}^{(+)}(\lambda) \), we need to invert \( \bar{F}^{(+)}(\lambda) \) and its adjoint. To compute them, we first construct a solution \( \bar{u}_{\text{ext}}^{(\pm)} \) to the exterior Dirichlet problem satisfying (6.3) and the radiation condition in the form
\[ \bar{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \tilde{\psi}, \]
where \( \tilde{\psi} \in l^2(\Sigma) \). Then it is the desired solution if and only if
\[ (6.32) \quad \bar{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \tilde{\psi} = \bar{f} \quad \text{on} \quad \Sigma. \]

Suppose \( \bar{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \tilde{\phi} = 0 \) on \( \Sigma \). Then, \( \tilde{\phi} = \bar{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \tilde{\phi} \) is the solution to the equation (6.3) with 0 boundary data. Since \( \tilde{\phi}^{(\pm)} \) satisfies the radiation condition, and Lemma 4.6 holds also for the exterior problem, it vanishes identically in \( \mathcal{E}_{\text{ext}} \) hence on all \( \mathcal{E} \). It then follows that \( \tilde{\phi}^{(\pm)} = 0 \). Therefore, the equation (6.32) is uniquely solvable for any \( \tilde{f} \in l^2(\Sigma) \). Let \( \tilde{\psi} = \bar{r}_{\Sigma}^{(\pm)}(\lambda) \tilde{f} \) be the solution. Then, we have
\[ (6.33) \quad \bar{u}_{\text{ext}}^{(\pm)} = \bar{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \bar{r}_{\Sigma}^{(\pm)}(\lambda) \tilde{f}, \]
which is a potential theoretic solution to the boundary value problem (6.3).

Let \( \hat{g}_n, n = 1, \cdots, N \), be a basis of \( l^2(\Sigma) \) and put
\[ v_n^{(\pm)} = \bar{f}^{(\pm)}(\lambda) \hat{g}_n = \mathcal{F}^{(0)}(\lambda) \mathcal{U}_{\mathcal{E}}(\bar{R}_{\mathcal{E}}^{(0)} - \lambda) \hat{R}_{\text{ext}}^{(0)}(\lambda \pm i0) \bar{r}_{\Sigma}^{(\pm)}(\lambda) \hat{g}_n \in h_\lambda. \]
Let $M_\Sigma$ be the linear hull of $v_1^{(\pm)}, \cdots, v_N^{(\pm)}$. Then, the mapping $g_n \to v_n^{(\pm)}$ induces a bijection

$$\tilde{j}^{(\pm)}(\lambda) : \ell^2(\Sigma) \nrightarrow \sum_{n=1}^N c_n g_n \to \sum_{n=1}^N c_n v_n^{(\pm)} \in M_\Sigma^{(\pm)}.$$ 

In view of Theorem 6.7, we have the following theorem.

**Theorem 6.8.** The following equality holds:

$$(B_\Sigma^{(\pm)}(\lambda))^{-1} = \left|_r \right|_V (\tilde{j}^{(+))(\lambda)})^{-1} (A_{ext}(\lambda) - A(\lambda)) (\tilde{j}^{(-)(\lambda)^*})^{-1} (\left|_V \right)^*.$$ 

Theorems 6.7 and 6.8 imply that the S-matrix and the D-N map determine each other.

7. **Inverse Scattering**

7.1. **Hexagonal parallelogram.** We are now in a position to considering the inverse scattering problem. As was discussed in Subsection 2.6, the choice of fundamental domain of the lattice $\mathcal{L}$ is not unique. However, different choice gives rise to unitarily equivalent Hamiltonians. In this section, we take $p^{(1)}, p^{(2)}$ and $\mathbf{v}_1, \mathbf{v}_2$ as in (2.15) in order 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 $n = n_1 + in_2 \in \mathbb{Z}[i] = \mathbb{Z} + i\mathbb{Z}$, let

$$\mathcal{L}_0 = \{v(n); n \in \mathbb{Z}[i]\}, \quad v(n) = n_1 \mathbf{v}_1 + n_2 \mathbf{v}_2,$$

$$v_1 = 1 + \omega, \quad v_2 = \sqrt{3}i,$$

$$p_1 = \omega^{-1} = \omega^5, \quad p_2 = 1,$$

and define the vertex set $\mathcal{V}_0$ by

$$\mathcal{V}_0 = \mathcal{V}_{01} \cup \mathcal{V}_{02}, \quad \mathcal{V}_{0i} = p_i + \mathcal{L}_0.$$ 

The adjacent points of $a_1 \in \mathcal{V}_{01}$ and $a_2 \in \mathcal{V}_{02}$ are given by

$$\mathcal{N}_{a_1} = \{z \in \mathbb{C}; |a_1 - z| = 1\} \cap \mathcal{V}_{02}$$

$$= \{a_1 + \omega, a_1 + \omega^3, a_1 + \omega^5\},$$

$$\mathcal{N}_{a_2} = \{z \in \mathbb{C}; |a_2 - z| = 1\} \cap \mathcal{V}_{01}$$

$$= \{a_2 + 1, a_2 + \omega^2, a_2 + \omega^4\}.$$ 

By virtue of the formula (6.18) and Theorem 6.8, given an S-matrix and a bounded domain $\mathcal{E}_{int}$, we can compute the D-N map associated with $\mathcal{E}_{int}$. Let $\mathcal{V}_{int}$ be the set of the vertices in $\mathcal{E}_{int}$. By Lemma 6.1, we can compute the D-N map associated with $\mathcal{V}_{int}$. 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.

As $\mathcal{V}_{int}$, we use the following domain which is different from the one in Figure 5. Let $D_0$ 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 $D_N = \{n \in \mathbb{Z}[i]; 0 \leq n_1 \leq N, 0 \leq n_2 \leq N\}$, where $N$ is chosen large enough, and put

$$D_N = \bigcup_{n \in D_N} (D_0 + v(n)).$$ 

This is a parallelogram in the hexagonal lattice (see Figure 6). The interior angle...
Figure 6. Hexagonal parallelogram \((N = 2)\)

of each vertex on the periphery of \(D_N\) is either \(2\pi/3\) or \(4\pi/3\). Let \(A\) be the set of the former, and for each \(z \in A\), 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 \(D_N\). Let

\[\Omega = \{v \in V_0; v \in D_N\}\]

be the set of vertices in the inside of the resulting graph. The boundary \(\partial \Omega = \{t(e_{z, \zeta}); z \in A\}\) 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.

\[
\begin{align*}
(\partial \Omega)_T &= \{\alpha_0, \cdots, \alpha_N\}, \\
(\partial \Omega)_B &= \{2\omega^5 + k(1 + \omega); 0 \leq k \leq N\}, \\
(\partial \Omega)_R &= \{2 + N(1 + \omega) + k\sqrt{3}i; 1 \leq k \leq N\} \cup \{2 + N(1 + \omega) + N\sqrt{3}i + 2\omega^2\}, \\
(\partial \Omega)_L &= \{2\omega^4\} \cup \{\beta_0, \cdots, \beta_N\},
\end{align*}
\]

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

7.2. **Special solutions to the vertex Schrödinger equation.** Taking \(N\) large enough so that \(D_N\) contains all the supports of the potentials \(q_e(z)\) in its interior, we consider the following Dirichlet problem for the vertex Schrödinger equation

\[
\begin{cases}
(\widehat{\Delta}_{V, \lambda} + \widehat{Q}_{V, \lambda})\widehat{u} = 0, & \text{in} \quad \overset{\circ}{\Omega}, \\
\widehat{u} = \widehat{f}, & \text{on} \quad \partial \Omega.
\end{cases}
\]
Let $\Lambda_{\hat{Q}}$ be the associated D-N map. The key to the inverse procedure is the following partial data problem.

**Lemma 7.1.** (1) Given a partial Dirichlet data $\hat{f}$ on $\partial \Omega \setminus (\partial \Omega)_R$, and a partial Neumann data $\hat{g}$ on $(\partial \Omega)_L$, there is a unique solution $\hat{u}$ on $\bar{\Omega} \cup (\partial \Omega)_R$ to the equation

$$
\begin{cases}
(\Delta_{V,-} + \hat{Q}_{V,-})\hat{u} = 0, & \text{in } \bar{\Omega}, \\
\hat{u} = \hat{f}, & \text{on } \partial \Omega \setminus (\partial \Omega)_R, \\
\partial_D^N \hat{u} = \hat{g}, & \text{on } (\partial \Omega)_L.
\end{cases}
$$

(2) Given the D-N map $\Lambda_{\hat{Q}}$, 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 $\Lambda_{\hat{Q}} \hat{f} = \hat{g}$ on $(\partial \Omega)_L$.

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

**Figure 7.** Line $A_k$

Now, for $0 \leq k \leq N$, let us consider a diagonal line $A_k$ (see Figure 7):

$$
A_k = \{ x_1 + ix_2 : x_1 + \sqrt{3}x_2 = a_k \},
$$

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

$$
\alpha_{k,\ell} = \alpha_k + \ell(1 + \omega^5), \quad \ell = 0, 1, 2, \ldots.
$$
Lemma 7.2. Let \( A_k \cap \partial \Omega = \{ \alpha_{k,0}, \alpha_{k,m} \} \). Then, there exists a unique solution \( \hat{u} \) to the equation

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

with partial Dirichlet data \( \hat{f} \) such that

\[
\hat{f}(\alpha_{k,0}) = 1, \quad \hat{f}(z) = 0 \quad \text{for} \quad z \in \partial \Omega \setminus (\partial \Omega) \cup \alpha_{k,0} \cup \alpha_{k,m}
\]

and partial Neumann data \( \hat{g} = 0 \) on \( \partial \Omega \). 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

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

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 8. Then, evaluating the equation (7.9) at \( v = a \) and using (3.11), (3.12),

we obtain

\[
\frac{1}{\psi_{ba}(1, \lambda)} \hat{u}(b) + \frac{1}{\psi_{b' a}(1, \lambda)} \hat{u}(b') = 0.
\]

Here, for any edge \( e \in \mathcal{E} \), we associate an edge \([e]\) without orientation and a function \( \phi_{[e]}(z, \lambda) \) satisfying

\[
\begin{align*}
\left( -\frac{d^2}{dz^2} + q_e(z) - \lambda \right) \phi_{[e]}(z, \lambda) &= 0, \quad \text{for} \quad 0 < z < 1, \\
\phi_{[e]}(0, \lambda) &= 0, \quad \phi_{[e]}'(0, \lambda) = 1.
\end{align*}
\]
By the assumption (Q-3), \( \phi_{[e]}(z, \lambda) \) is determined by \( e \) and independent of the orientation of \( e \). Then, the equation (7.10) is rewritten as

\[
\hat{u}(b) = -\frac{\phi_{[e]}(1, \lambda)}{\phi_{[e']}^{\prime}(1, \lambda)} \hat{u}'(b).
\]

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

\[
f_{k,m}(\lambda) = -\frac{\phi_{[e_{k,m}]}(1, \lambda)}{\phi_{[e_{k,m}']}^{\prime}(1, \lambda)}.
\]

Then, we obtain the following lemma.

**Lemma 7.3.** The solution \( \hat{u} \) in Lemma 7.2 satisfies

\[
\hat{u}(\alpha_k, \ell) = f_{k,1}(\lambda) \cdots f_{k,\ell}(\lambda).
\]

7.3. **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 6 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 7 and take the boundary data \( f \) having the properties in Lemma 7.2.

3rd step. Compute the values of the associated solution \( \hat{u} \) to the boundary value problem in Lemma 7.2 at the points \( \alpha_k, \ell, \ell = 0, 1, 2, \ldots \).

4th step. Look at Figure 6. 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 8). Take two \( A_k' \)-adjacent edges \( e \) and \( e' \) between \( A_k \) and \( A_k' \), and use the formula (7.12) to compute the ratio of \( \phi_{[e]}(1, \lambda) \) and \( \phi_{[e']}^{\prime}(1, \lambda) \).

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 \( \phi_{[e']}^{\prime}(1, \lambda) \) 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 \( \phi_{[e']}^{\prime}(1, \lambda) \).

6th step. Take a zigzag line on the hexagonal lattice (see Figure 9), 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 \( \phi_{[e']}^{\prime}(1, \lambda) \) by computing the ratio for two successive edges between \( e \) and \( e' \).

7th step. For a sufficiently remote edge \( e' \), one knows \( \phi_{[e']}^{\prime}(1, \lambda) \) 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 \( -(d/dz)^2 + q_e(z) \) on \((0, 1)\). Since the potential is symmetric, by Borg’s theorem (see e.g. [14], 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 $q_{\ell}(z)$. The knowledge of the D-N map is used in the 2nd step (in the proof of Lemma 7.1). In the 3rd step, one uses the equation (7.6) 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 $(-\frac{d}{dz})^2 + q_{0}(z) - \lambda)\varphi = 0$.

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