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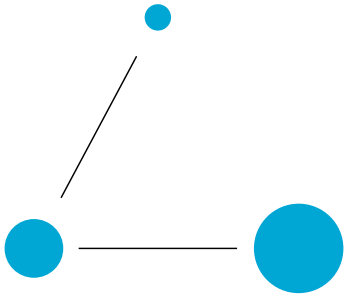

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INVERSE PROBLEMS FOR LOCALLY PERTURBED LATTICES – DISCRETE HAMILTONIAN AND QUANTUM GRAPH

PROBLÈMES INVERSES POUR TREILLIS LOCALEMENT PERTURBÉS – HAMILTONIEN DISCRET ET GRAPHE QUANTIQUE

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Abstract. — We consider the inverse scattering problems for two types of Schrödinger operators on locally perturbed periodic lattices. For the discrete Hamiltonian, the knowledge of the S-matrix for all energies determines the graph structure and the coefficients of the Hamiltonian. For locally perturbed equilateral metric graphs, the knowledge of the S-matrix for all energies determines the graph structure.

Résumé. — Nous considérons les problèmes de scattering inverse pour deux types d'opérateurs de Schrödinger sur des réseaux périodiques localement perturbés. Pour le hamiltonien discret, la connaissance de la S-matrice pour toutes les énergies détermine la structure du graphe et les coefficients du hamiltonien. Pour les graphes métriques équilatéraux localement perturbés, la connaissance de la S-matrice pour toutes les énergies détermine la structure du graphe.

1. Introduction

1.1. The goal of this work

There are two basic models for describing the motion of quantum mechanical particles on a periodic lattice. In the first model, the configuration space consists of graph vertices only and the Hamiltonian is written as a difference operator which is determined by the adjacency matrix. We refer to this operator as the discrete Schrödinger operator in this paper. In the other model, the wave functions are supported on the graph edges and the Hamiltonian is a differential operator on the edges. This model is called the quantum (or metric) graph.

The aim of this paper is twofold. The first topic concerns a locally perturbed periodic lattice, for instance, square, hexagonal or triangular. We analyze the discrete Schrödinger operator having the form

$$\widehat{H}_\Gamma : \widehat{u} \to \frac{1}{\mu_v} \sum_{w \sim v,\, w \in \Gamma} g_{vw}\widehat{u}(w) + q(v)\widehat{u}(v), \quad v \in \Gamma, \tag{1.1}$$

on a finite part of the graph Γ and prove the following result (Theorem 5.11):

- Given a locally perturbed periodic lattice of certain class and the associated discrete Hamiltonian $\widehat{H}_\Gamma$, from the knowledge of the S-matrix for all energies, we can determine the graph structure, that is, there exists an isomorphism between two such lattices. Moreover, if μ_v is equal to the degree of v (see (2.1)), we can determine g_{vw} and $q(v)$.

Here, a local perturbation of lattice means replacing a finite number of edges and vertices by a finite number of other edges and vertices and changing the weights g_{vw} and the potentials $q(v)$ on a finite number of edges and vertices, respectively. The S-matrix is introduced by observing the behavior at infinity of solutions to the Schrödinger equation on the lattice (Theorem 5.4).

As usual, we assume that our discrete graph is simple, i.e. for two vertices v, w there is at most one edge having v, w as end points, and in addition, that each edge has different end points. The main assumptions are (**C-1**), (**C-2**) (see also **C-1'**), (**D-1**)–(**D-4**), and (E-1) given in § 3 and § 5.

With regards to concrete examples, we can include the square, triangular, hexagonal lattices and their ladders. For the sake of definiteness, let us speak of a connected

infinite hexagonal lattice, on a finite part of which horizontal edges are arbitrarily removed, and a Schrödinger operator $\widehat{H}_\Gamma$ with a compactly supported scalar potential $q(v)$. Then, we can determine the graph structure, g_{vw} and $q(v)$ from the S-matrix for all energies.

The other topic of this paper concerns the Schrödinger operator on a metric graph $\Gamma = \{\mathcal{V}, \mathcal{E}\}$, with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$, and the topology determined by an appropriate adjacency matrix. The metric character of the graph means that each edge is identified with a line segment, in our case finite, and parametrized by its arclength. This makes it possible to endow Γ naturally with the metric defined as the length of the shortest path between two points. We do not fix the orientation of a given edge e, that is, the graph is undirected. As in the discrete case, we assume that for $v, v' \in \mathcal{V}$, there exists at most one edge with end points v, v', and that Γ has no loops. This can be assumed without loss of generality, since otherwise one can insert a 'dummy' vertex of degree 2 to any 'superfluous' edge. By a function $\widehat{f}$ on Γ, we mean a collection of functions $\widehat{f} = \{\widehat{f}_e\}_{e\in\mathcal{E}}$, each $\widehat{f}_e$ being a function on the edge e with a parametrization $e(\cdot) : [0, \ell_e] \to e$ such that $\widehat{f}(p) = \widehat{f}_e(e(z))$ for $p = e(z)$. We often denote $\widehat{f}_e(z)$ instead of $\widehat{f}_e(e(z))$. We fix the parametrization $e(\cdot)$ for each e. Hence ℓ_e is a given positive constant, which we say to be the length of e. With each edge $e \in \mathcal{E}$, we associate a one-dimensional Schrödinger operator

$$h_e := -\frac{d^2}{dz^2} + V_e(z), \quad z \in [0, \ell_e] =: I_e. \tag{1.2}$$

To convert the collection of operators (1.2) into a self-adjoint Schrödinger operator on the whole graph, one has to impose conditions matching the functions at the vertices. In general, self-adjoint operators referring to the differential expression in question are parametrized by $\deg v \times \deg v$ unitary matrices, cf. [KS99] or [BK13, Theorem 1.4.4]. If we require continuity of the functions at the vertices, however, this multitude is reduced to a one-parameter family, which we adopt in our case. To be concrete, for $\widehat{f} \in H^2_{loc}(\mathcal{E})$, we impose the generalized Kirchhoff condition, otherwise known as δ-coupling: if $\widehat{f} = \{\widehat{f}_e\}_{e\in\mathcal{E}}$ such that $\widehat{f} \in C(\mathcal{E})$ and $\widehat{f}_e \in C^1(I_e)$, it holds that

$$\sum_{v\in e} \widehat{f}'_e(v) = C_v \widehat{f}(v), \quad v \in \mathcal{V}, \tag{1.3}$$

where $\widehat{f}'_e(v)$ is given by (2.2) and $v \in e$ means that v is an endpoint of the edge e, C_v is a real constant, $\widehat{f}(v) = \widehat{f}_e(0)$ if $e(0) = v$. Here $\widehat{f} \in C(\mathcal{E})$ means that $\widehat{f}_e(v) = \widehat{f}_{e'}(v)$ if $v \in e \cap e'$ and that $\widehat{f}$, thus defined globally on $\mathcal{E}$, is continuous on the whole graph Γ. One should be careful about the definition of the Sobolev space $H^m(\mathcal{E})$. In this paper, we do not assume the continuity for $\widehat{f} \in H^m(\mathcal{E})$ at the junctions $\mathcal{V}$. See (2.3). Note that such a Hamiltonian can be defined as the norm-resolvent limit as $\kappa \to \infty$ of the following operators,

$$\widetilde{h}_{e,\kappa} = -\frac{d^2}{dz^2} + V_e(z) + \kappa W_e(\kappa z),$$

with the usual Kirchhoff condition $\sum_{v\in e} \widehat{f}'_e(v) = 0$ for any $v \in \mathcal{V}$, where $C_v := \sum_{v\in e} \int_e W_e(z)\, dz$ and $W_e \in L^1(e)$ is a fixed function, cf. [Exn96]. Note also that the

singular vertex couplings with functions discontinuous at the vertex also allow for an interpretation, but the corresponding approximation procedure is considerably more complicated, see [CET10].

We develop an inverse spectral and scattering theory associated with such quantum graphs which would facilitate a recovery of the graph structure, potentials $V_e(z)$, and constants C_v. Roughly speaking, we consider a locally perturbed periodic graph. More precisely, we consider equilateral metric graphs with identical potentials on the edges, and prove the following result (Theorem 7.2):

- Consider an infinite quantum graph $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ on which all ℓ_e, $V_e(z)$ coincide for all $e \in \mathcal{E}$, and $C_v/\deg v$ coincide for all $v \in \mathcal{V}$. If Γ is a local perturbation of a periodic lattice of a certain class, then we can determine the graph structure of Γ from the S-matrix for all energies.

Using this result, one can deal with the square, triangular, hexagonal lattices and their ladders, for which the coupling constant C_v in (1.3) and the degree d_v in (2.1) of each vertex v is determined from the S-matrix of all energies. An application of this result we have in mind is a network of semicondutor nanowires the width of which is changing along the edge; the transverse contribution to energy gives rise to an effective potential.

The proof will be done by showing the equivalence of the S-matrix and the Dirichlet-to-Neumann (D-N) map in a bounded domain, and by reducing the problem to inverse problems for discrete Schrödinger operators of the type (1.1).

1.2. Plan of the work

We proceed in the following steps.

(1) Preliminaries on metric graphs (§ 2).
(2) Inverse boundary value problem with the D-N map for a finite graph (§ 3): Use the results from [BILL23a] to determine the structure of finite discrete graphs and quantum graphs from the knowledge of the corresponding D-N map.
(3) Inverse scattering for discrete Hamiltonians (§ 5): Show that the S-matrix and the D-N map are equivalent and thus reduce the inverse scattering problem to the inverse boundary value problem.
(4) Inverse scattering for quantum graphs (§ 6, § 7): Develop the spectral and scattering theory for locally perturbed periodic graph Laplacians, show that the S-matrix and the D-N map are equivalent, and recover the perturbations from the D-N map.

Since we use a number of assumptions and the notation is not always simple, we add for the reader's convenience their overview in the following table:

Assumptions			
(M-1) - (M-5)	§2	(A-1) - (A-4)	[AIM18, §2.3]
(B-1) - (B-3)	[AIM18, §2.3]	(**C-1**), (**C-2**), (**C-1'**)	§ 3.1, § 3.2
(**D-1**) - (**D-4**)	§ 5.1	(E-1)	§ 5.4

Notations									
h_e	(1.2)	C_v	(1.3)	d_v	(2.1)	$\phi_{e0}(z,\lambda)$	(2.6)	$\phi_{e1}(z,\lambda)$	(2.7)
$r_e(\lambda)$	(2.8)	$\widehat{\Delta}_{\mathcal{V},\lambda}$	(2.11)	$\widehat{Q}_{\mathcal{V},\lambda}$	(2.12)	$\widehat{T}_{\mathcal{V},\lambda}$	(2.13)	$\Lambda_{\mathcal{V}}(\lambda)$	(3.5)
$\Lambda_{\mathcal{E}}(\lambda)$	(3.3)	$\ell_{\mathcal{E}}, V_{\mathcal{E}}(z)$	(4.1)	$\kappa_{\mathcal{V}}$	(4.2)	$\mathcal{U}_{\mathcal{V}}$	(5.3)	$\widehat{\Delta}_{\Gamma_0}$	(5.4)
$\mathcal{T}_1$	(**D-1**)	$\mathcal{T}_0$	(**D-2**)	$\widehat{P}_{ext}$	(5.8)	$\simeq$	(5.15)	Σ	(3.1)
$E(\lambda)$	(6.4)	$\sigma^{(0)}(h^{(0)})$	(6.6)	$\sigma^{(0)}(-\widehat{\Delta}_{\mathcal{V}})$	(6.7)	$\sigma^{(0)}_{\mathcal{T}}$	(6.8)	$\mathcal{T}$	(6.9)

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2. Metric graph and the associated discrete operator

Rephrasing the treatment of a Schrödinger operator, with or without a potential, on a *metric* graph to the analogous problem on a *combinatorial* (or discrete) graph is a well-known procedure that has been discussed in many papers, e.g. [BER15, Cat97, Exn97, Pan13]. We repeat it here mainly to fix notations. Let $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ be a metric graph with the vertex set $\mathcal{V}$ and edge set $\mathcal{E}$. Note that for the metric graph, an edge $e \in \mathcal{E}$ is a segment between two vertices while for the discrete graph, an edge is a pair of vertices. To avoid the complexity of notation, we use the same symbol e_{vw} for an edge with endpoints v, w for both graphs, often omitting v, w. However, we will make a distinction between them in the arguments in §2 following Definition 2.1 and those in §3.1. For $v, w \in \mathcal{V}$, we say that v and w are adjacent, denoted by $v \sim w$, if there exists an edge having v and w as its endpoints. For an edge $e \in \mathcal{E}$ and $v \in \mathcal{V}$, $v \in e$ means that v is an end point of e. The degree of a vertex $v \in \mathcal{V}$ is defined as

$$d_v := \deg v = \sharp\{e \in \mathcal{E}\,;\, v \in e\}. \tag{2.1}$$

Recall that for adjacent $v, v' \in \mathcal{V}$, the edge joining v and v' is unique by assumption. For a function $\widehat{f} = \{\widehat{f}_e\}_{e\in\mathcal{E}}$ on Γ, with $\widehat{f}_e : I_e \to \mathbf{C}$, and $e \in \mathcal{E}$ with $v \in e$, we define

$$\frac{d\widehat{f}}{d\nu_e}(v) := \widehat{f}'_e(v). \tag{2.2}$$

When computing the right-hand side, we parametrize e as $e(z)$, $z \in [0, \ell_e]$ with $e(0) = v$, and the boundary derivative is taken in the *outward* direction with respect to v, see [BK13, § I.4]. Equivalently, the boundary derivatives can be written as

$$\frac{d\widehat{f}}{d\nu_e}(e(0)) = \widehat{f}'_e(0), \quad \frac{d\widehat{f}}{d\nu_e}(e(\ell_e)) = -\widehat{f}'_e(\ell_e),$$

where ℓ_e is the length of the edge e. For the sake of brevity, we use the following shorthand notation:

$$\int_e \widehat{u} = \int_0^{\ell_e} \widehat{u}(z)dz.$$

Then the following Green's formula holds:

$$-\int_e (\widehat{u}')'\widehat{w} = \frac{d\widehat{u}}{d\nu_e}\widehat{w}\bigg|_{e(0)} + \frac{d\widehat{u}}{d\nu_e}\widehat{w}\bigg|_{e(\ell_e)} + \int_e \widehat{u}'\widehat{w}'.$$

For an edge $e \in \mathcal{E}$, let $L^2(e)$ be the set of all L^2-functions on e, conventionally understood as equivalence classes of functions coinciding a.e., and put

$$L^2(\mathcal{E}) = \bigoplus\nolimits_{e\in\mathcal{E}} L^2(e).$$

For $\widehat{u} = \{\widehat{u}_e\}_{e\in\mathcal{E}}$ and $\widehat{w} \in \{\widehat{w}_e\}_{e\in\mathcal{E}}$, let $(\widehat{u},\widehat{w})_{\mathcal{E}}$ be the inner product:

$$(\widehat{u},\widehat{w})_{\mathcal{E}} = \sum_{e\in\mathcal{E}} (\widehat{u}_e,\widehat{w}_e)_e = \sum_{e\in\mathcal{E}} \int_e \widehat{u}_e\overline{\widehat{w}_e}.$$

The Sobolev spaces are defined by

$$H^m(\mathcal{E}) = \bigoplus\nolimits_{e\in\mathcal{E}} H^m(e). \tag{2.3}$$

Note that different conventions are used and sometimes the definition may involve the continuity at the vertices, see [BK13, Definition I.3.6].

Given a real-valued function $V_e \in L^1(e)$ on each $e \in \mathcal{E}$, we define a multiplication operator V by

$$\left(V\widehat{u}\right)_e(z) = V_e(z)\widehat{u}_e(z).$$

Let C_v be as in (1.3). Throughout the paper we impose the following requirements:

(M-1) $0 < \inf_e \ell_e \leqslant \sup_e \ell_e < \infty$,
(M-2) $\sup_{v\in\mathcal{V}} d_v < \infty$,
(M-3) $\sup_{e\in\mathcal{E}} \|V_e\|_{L^1(e)} < \infty$,
(M-4) $V_e(z) = V_e(\ell_e - z)$,
(M-5) $\sup_{v\in\mathcal{V}} |C_v| < \infty$.

Naturally all of these requirements except the symmetry condition (M-4) are satisfied automatically if the graph Γ is finite. We define the operator $\widehat{H}_{\mathcal{E}}$ by

$$\left(\widehat{H}_{\mathcal{E}}\widehat{u}\right)_e(z) = -\widehat{u}_e''(z) + V_e(z)\widehat{u}_e(z) \tag{2.4}$$

acting on I_e, with the domain consisting of functions

$$\widehat{u} \in D(\widehat{H}_{\mathcal{E}}) \Longleftrightarrow \begin{cases} \widehat{u} \in H^2(\mathcal{E}), \quad \widehat{u} \in C(\mathcal{E}), \\ \sum_{v\in e} \widehat{u}_e'(v) = C_v\widehat{u}(v), \quad v \in \mathcal{V}. \end{cases} \tag{2.5}$$

It is straightforward to check that $\widehat{H}_{\mathcal{E}}$ is self-adjoint.

Let $\lambda \in \mathbb{C}\setminus\mathbb{R}$. For any edge $e \in \mathcal{E}$, let $\phi_{e0}(z,\lambda)$ and $\phi_{e1}(z,\lambda)$ be the solutions of $-\phi'' + V_e\phi = \lambda\phi$ on I_e satisfying the boundary conditions

$$\phi_{e0}(0,\lambda) = 0, \quad \phi_{e0}'(0,\lambda) = 1, \tag{2.6}$$

$$\phi_{e1}(\ell_e,\lambda) = 0, \quad \phi_{e1}'(\ell_e,\lambda) = -1. \tag{2.7}$$

Note that $\phi_{e1}(z,\lambda) = \phi_{e0}(\ell_e - z, \lambda)$ by the symmetry condition (M-4). Let $r_e(\lambda)$ be the Green operator of $-d^2/dz^2 + V_e(z) - \lambda$ on e with the Dirichlet boundary condition:

$$r_e(\lambda)\widehat{f}_e = \left(-\frac{d^2}{dz^2} + V_e(z) - \lambda\right)^{-1} \widehat{f}_e = \int_{I_e} r_e(z,z',\lambda)\widehat{f}_e(z')dz', \tag{2.8}$$

where the integral kernel is given by

$$r_e(z,z',\lambda) = -\frac{1}{W_e(\lambda)} \begin{cases} \phi_{e0}(z,\lambda)\phi_{e1}(z',\lambda), & 0 < z < z', \\ \phi_{e1}(z,\lambda)\phi_{e0}(z',\lambda), & 0 < z' < z, \end{cases}$$

$$W_e(\lambda) = \phi_{e0}(z,\lambda)\phi'_{e1}(z,\lambda) - \phi'_{e0}(z,\lambda)\phi_{e1}(z,\lambda).$$

Note that the Wronskian for the system ϕ_{e0} and ϕ_{e1} is independent of z. Let $\widehat{u} = (\widehat{H}_{\mathcal{E}} - \lambda)^{-1}\widehat{f}$. Then on each edge e, the function $\widehat{u}_e(z,\lambda)$ can be written as

$$\widehat{u}_e(z,\lambda) = c_e(\ell_e,\lambda)\frac{\phi_{e0}(z,\lambda)}{\phi_{e0}(\ell_e,\lambda)} + c_e(0,\lambda)\frac{\phi_{e1}(z,\lambda)}{\phi_{e1}(0,\lambda)} + r_e(\lambda)\widehat{f}_e, \tag{2.9}$$

where the constants $c_e(\ell_e,\lambda), c_e(0,\lambda)$ are determined by the δ-coupling condition (1.3). Since $\phi'_{e0}(0,\lambda) = 1$, we infer that

$$\frac{d}{dz} r_e(\lambda)\widehat{f}_e\Big|_{z=0} = -\int_{I_e} \frac{\phi_{e1}(z',\lambda)}{W_e(\lambda)}\widehat{f}_e(z')\,dz',$$

and consequently we have using $\phi'_{e1}(0,\lambda) = -\phi'_{e0}(\ell_e,\lambda)$ and $\phi_{e1}(0,\lambda) = \phi_{e0}(\ell_e,\lambda)$

$$\widehat{u}'_e(0,\lambda) = \frac{1}{\phi_{e0}(\ell_e,\lambda)}\Big(c_e(\ell_e,\lambda) - \phi'_{e0}(\ell_e,\lambda)c_e(0,\lambda)\Big) - \int_{I_e} \frac{\phi_{e1}(z',\lambda)}{W_e(\lambda)}\widehat{f}_e(z')\,dz'.$$

Since $\widehat{u}_e(0,\lambda) = c_e(0,\lambda)$, the δ-coupling condition (1.3) can be rewritten as

$$\sum_{e(0)=v} \left(\frac{1}{\phi_{e0}(\ell_e,\lambda)}\Big(c_e(\ell_e,\lambda) - \phi'_{e0}(\ell_e,\lambda)c_e(0,\lambda)\Big) - \frac{C_v}{d_v}c_e(0,\lambda)\right) = \sum_{e(0)=v} \int_{I_e} \frac{\phi_{e1}(z',\lambda)}{W_e(\lambda)}\widehat{f}_e(z')\,dz'. \tag{2.10}$$

To make the dependence on the edge parametrization more visible, we alternatively write $\widehat{f}_e(e(z))$ instead of a function $\widehat{f}_e(z)$ on I_e.

From here until the end of § 3.1, we denote the functions on the metric graph by $\underline{\widehat{u}}$, $\underline{\widehat{u}}_e$ and those of the discrete graph by $\widehat{u}$, $\widehat{u}_e$.

Let us begin with recalling relations between Schrödinger operators h_e on edges and the discrete Laplacian on vertices (Lemmas 2.2 and 2.3) which have been already found in [Cat97, Exn97, Pan06, Pan13].

Definition 2.1. — *The weighted discrete graph Laplacian* $\widehat{\Delta}_{\mathcal{V},\lambda} : \ell^2(\mathcal{V}) \to \ell^2(\mathcal{V})$ *on* $\mathcal{V}$*, associated with the Schrödinger operator on* Γ *specified by* (1.2) *and* (1.3),

acts on a function $\widehat{u}(v)$ *on* $\mathcal{V}$ *as*

$$\begin{aligned}\left(\widehat{\Delta}_{\mathcal{V},\lambda}\widehat{u}\right)(v) &= \frac{1}{d_v}\sum_{e(0)=v,\, e\in\mathcal{E}} \frac{1}{\phi_{e0}(\ell_e,\lambda)}\widehat{u}(e(\ell_e)) \\ &= \frac{1}{d_v}\sum_{w\sim v,\, w\in\mathcal{V}} \frac{1}{\phi_{e0}(w,\lambda)}\widehat{u}(w).\end{aligned} \tag{2.11}$$

We introduce the discrete scalar potential $\widehat{Q}_{\mathcal{V},\lambda} = \{\widehat{Q}_{v,\lambda}\}_{v\in\mathcal{V}}$ *by*

$$\widehat{Q}_{v,\lambda} = \frac{1}{d_v}\sum_{v\in e,\, e\in\mathcal{E}} \frac{\phi'_{e0}(\ell_e,\lambda)}{\phi_{e0}(\ell_e,\lambda)} + \frac{C_v}{d_v}. \tag{2.12}$$

Note that $e(0) = v$ *and* $e(\ell_e) = w$ *hold in the definitions* (2.11) *and* (2.12).

Furthermore, defining

$$\left(\widehat{T}_{\mathcal{V},\lambda}\underline{\widehat{f}}\right)(v) := \frac{1}{d_v}\sum_{e(0)=v}\int_{I_e}\frac{\phi_{e0}(z,\lambda)}{\phi_{e0}(\ell_e,\lambda)}\underline{\widehat{f}}_e(z)\,dz, \tag{2.13}$$

we can rewrite the coupling condition (2.10) in the following way.

LEMMA 2.2. — *The* δ*-coupling condition* (1.3) *can be expressed as*

$$\left(-\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda}\right)\underline{\widehat{u}}(v) = \widehat{T}_{\mathcal{V},\lambda}\underline{\widehat{f}}(v), \quad v\in\mathcal{V}. \tag{2.14}$$

Assuming that the equation (2.14) is solvable, we write $\underline{\widehat{u}} = \{\underline{\widehat{u}}_e\}_{e\in\mathcal{E}}$ in the form of (2.9) with $c_e(0,\lambda)$, $c_e(\ell_e,\lambda)$ being the vertex values of $\underline{\widehat{u}}(v)$ at $v = e(0)$ and $v = e(\ell_e)$, respectively. Then we have

$$\underline{\widehat{u}}\big|_{\mathcal{V}} = \left(-\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda}\right)^{-1}\widehat{T}_{\mathcal{V},\lambda}\underline{\widehat{f}}.$$

Note further that the adjoint operator $(\widehat{T}_{\mathcal{V},\lambda})^*$ acts as

$$\begin{aligned}\left(\left(\widehat{T}_{\mathcal{V},\lambda}\right)^*\underline{\widehat{g}}\right)_e(z) &= \sum_{v=e(0)}\frac{1}{d_v}\frac{\phi_{e0}(z,\overline{\lambda})}{\phi_{e0}(\ell_e,\overline{\lambda})}\,\underline{\widehat{g}}(v) \\ &= \frac{1}{d_{e(0)}}\frac{\phi_{e0}(z,\overline{\lambda})}{\phi_{e0}(\ell_e,\overline{\lambda})}\underline{\widehat{g}}(e(0)) + \frac{1}{d_e(\ell_e)}\frac{\phi_{e1}(z,\overline{\lambda})}{\phi_{e1}(0,\overline{\lambda})}\,\underline{\widehat{g}}(e(\ell_e)),\end{aligned} \tag{2.15}$$

where in the first line we consider both orientations of the edge e, while in the second line we fix one orientation. Now we define the operator $r_{\mathcal{E}}(\lambda)$ on $\mathcal{E}$ by

$$r_{\mathcal{E}}(\lambda)\underline{\widehat{f}} = r_e(\lambda)\underline{\widehat{f}}_e \quad \text{on } e,$$

and we arrive at the following Krein-type formula expressing the resolvent through its comparison to that of the Dirichlet-decoupled graph.

LEMMA 2.3. — *The resolvent* $\widehat{R}_{\mathcal{E}}(\lambda) = (\widehat{H}_{\mathcal{E}} - \lambda)^{-1}$ *is expressed as*

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

Let us note here that for $\lambda\notin\mathbb{R}$, the coefficients of $\widehat{\Delta}_{\mathcal{V},\lambda}$ and $\widehat{Q}_{\mathcal{V},\lambda}$ are not real and hence the existence of the inverse $(-\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda})^{-1}$ is not obvious. We postpone its justification until § 6, and admit Lemma 2.3 as a formal formula for the moment.

3. Inverse boundary value problem for a finite graph

3.1. The D-N maps

In this section, we consider a finite graph $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ with boundary. Assume that

(**C-1**) The vertex set $\mathcal{V}$ consists of two disjoint parts called boundary $\partial\mathcal{V}$ and interior $\mathcal{V}^o$. Each boundary vertex is connected to only one interior vertex. Moreover, there are no edges between the boundary vertices.

Under the assumption (**C-1**), we write $\{\mathcal{V}^o, \partial\mathcal{V}, \mathcal{E}\}$ instead of $\{\mathcal{V}, \mathcal{E}\}$. Note that, topologically speaking, the notion of the graph boundary is not trivial; here we use the freedom to determine it *ad hoc* to suit our purposes.

Let $\widehat{H}_{\mathcal{E}}$ be the quantum graph Schrödinger operator on the finite graph Γ as in the previous section with Dirichlet boundary condition on the boundary $\partial\mathcal{V}$. We put

$$\sigma' := \left(\bigcup_{e\in\mathcal{E}} \sigma(h_e)\right) \cup \left\{\lambda \in \mathbb{C}\,;\, \det\left(-\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda}\right) = 0\right\}, \tag{3.1}$$

which is discrete in $\mathbb{C}$, as Γ is a finite graph. Note $\sigma(\widehat{H}_{\mathcal{E}}) \subset \sigma'$. Let h_e be the differential operator on e as in (1.2). Then for any $\lambda \notin \sigma(\widehat{H}_{\mathcal{E}})$ and given boundary data $\underline{\widehat{f}}$, there is a unique solution $\underline{\widehat{u}} = \{\underline{\widehat{u}}_e\}_{e\in\mathcal{E}}$ to the equation

$$\begin{cases} (h_e - \lambda)\underline{\widehat{u}}_e = 0 \quad \text{on} \quad \forall\, e \in \mathcal{E}, \\ \underline{\widehat{u}} = \underline{\widehat{f}} \quad \text{on} \quad \partial\mathcal{V}, \\ \delta\text{-coupling condition (1.3)}. \end{cases} \tag{3.2}$$

Here, as in (2.5), $\underline{\widehat{u}}$ is assumed to be in $C(\Gamma)$. Using the solution $\underline{\widehat{u}}$, we define the D-N map $\Lambda_{\mathcal{E}}(\lambda) : \mathbb{C}^m \to \mathbb{C}^m$, $m = \sharp\partial\mathcal{V}$, by

$$\Lambda_{\mathcal{E}}(\lambda) : \underline{\widehat{f}} \to \underline{\widehat{u}}'_e(v), \quad e(0) = v \in \partial\mathcal{V}. \tag{3.3}$$

Recall for $v \in \partial\mathcal{V}$ the edge with end point v is unique by our assumption.

Under the Dirichlet boundary condition on the boundary $e(0)$ and $e(\ell_e)$, h_e has discrete spectrum, and for any $\lambda \notin \cup_{e\in\mathcal{E}}\sigma(h_e)$, we have $\phi_{e0}(\ell_e, \lambda) \neq 0$. Hence the weighted discrete Laplacian (2.11) is well defined. We consider the boundary value problem for the corresponding Schrödinger-type operator $\widehat{H}_{\mathcal{V},\lambda} =: -\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda}$ on the vertex set $\mathcal{V}$ with the boundary value $\widehat{f}$ on $\partial\mathcal{V}$, namely

$$\begin{cases} \left(-\widehat{\Delta}_{\mathcal{V},\lambda} + \widehat{Q}_{\mathcal{V},\lambda}\right)\widehat{u}(v) = 0, \quad v \in \mathcal{V}^o = \mathcal{V} \setminus \partial\mathcal{V}, \\ \widehat{u}(v) = \widehat{f}(v), \quad v \in \partial\mathcal{V}. \end{cases} \tag{3.4}$$

Note that $\underline{\widehat{u}} = \{\underline{\widehat{u}}_e\}_{e\in\mathcal{E}}$ is the solution to the edge Schrödinger equation (3.2) if and only if $\underline{\widehat{u}}|_{\mathcal{V}}$ is the solution to the vertex Schrödinger equation (3.4) (cf. [Exn97]).

Using the solution $\widehat{u}_{\mathcal{V}}$, which depends also on λ and is denoted by $\widehat{u}_{\mathcal{V}}(v, \lambda)$, we next define the D-N map for $\widehat{H}_{\mathcal{V},\lambda} : \mathbb{C}^m \to \mathbb{C}^m$ by

$$\Lambda_{\mathcal{V}}(\lambda) : \widehat{f} \to \frac{1}{\phi_{e0}(w, \lambda)}\widehat{u}_{\mathcal{V}}(w, \lambda), \quad w = e(\ell_e), \quad v = e(0) \in \partial\mathcal{V}. \tag{3.5}$$

Therefore, $\Lambda_{\mathcal{E}}(\lambda)$ and $\Lambda_{\mathcal{V}}(\lambda)$ are meromorphic functions of λ with poles in the discrete set σ'. Recall that given a subset $A \subset \mathcal{V}$ and an edge $e \in \mathcal{E}$, we say that e is adjacent to A, if $e(0) \in A$ and $e(\ell_e) \notin A$.

LEMMA 3.1. — *Assuming that we know ℓ_e and $V_e(z)$ for all e adjacent to $\partial\mathcal{V}$, then $\Lambda_{\mathcal{E}}(\lambda)$ and $\Lambda_{\mathcal{V}}(\lambda)$ determine each other for any $\lambda \notin \sigma'$.*

Proof. — Given the solution $\underline{\widehat{u}}$ to (3.2), the corresponding $\underline{\widehat{u}}|_{\mathcal{V}}$ solves (3.4). Conversely, given the solution $\widehat{u}_{\mathcal{V}}$ of (3.4), we define $\underline{\widehat{u}}$ by

$$\underline{\widehat{u}}_e(z) = c_e(\ell_e,\lambda)\frac{\phi_{e0}(z,\lambda)}{\phi_{e0}(\ell_e,\lambda)} + c_e(0,\lambda)\frac{\phi_{e1}(z,\lambda)}{\phi_{e1}(0,\lambda)},$$

where on the edge with the initial vertex $v = e(0) \in \partial\mathcal{V}$, we put

$$c_e(0,\lambda) = \underline{\widehat{f}}(v).$$

The function $\widehat{u}$ defined in this way solves (3.2). The D-N map for $\widehat{H}_{\mathcal{E}}$ is

$$\Lambda_{\mathcal{E}}(\lambda) : \underline{\widehat{f}} \to c_e(\ell_e,\lambda)\frac{1}{\phi_{e0}(\ell_e,\lambda)} + \underline{\widehat{f}}(v)\frac{\phi'_{e1}(0,\lambda)}{\phi_{e1}(0,\lambda)}, \quad v = e(0) \in \partial\mathcal{V}.$$

The D-N map for $\widehat{H}_{\mathcal{V},\lambda}$ is, by (3.5), taking $w = e(\ell_e)$,

$$\Lambda_{\mathcal{V}}(\lambda) : \underline{\widehat{f}} \to \frac{1}{\phi_{e0}(\ell_e,\lambda)}\left(c_e(\ell_e,\lambda) + \frac{\underline{\widehat{f}}(v)}{\phi_{e1}(0,\lambda)}\right). \tag{3.6}$$

Since we know $\phi_{e0}(z,\lambda)$, $\phi_{e1}(z,\lambda)$ for edges e adjacent to $\partial\mathcal{V}$, the knowledge of the D-N maps for both the $\widehat{H}_{\mathcal{E}}$ and $\widehat{H}_{\mathcal{V},\lambda}$ is thus equivalent to that of the initial value problem or the two-point boundary value problem for $h_e - \lambda$ on each edge e. Consequently, the two D-N maps are equivalent. □

3.2. A reminder: inverse problem for the discrete graph Laplacian.

To make this paper self-contained, let us recall a result obtained in [BILL23a] as follows. We say that the collection $\Gamma = \{\mathcal{V}^o, \partial\mathcal{V}, \mathcal{E}, \mu, g\}$ is a weighted discrete graph with boundary, if it satisfies the following conditions.

- $\{\mathcal{V}^o \cup \partial\mathcal{V}, \mathcal{E}\}$ *is an undirected simple discrete graph satisfying* (**C-1**).
- $\mu : \mathcal{V}^o \cup \partial\mathcal{V} \to \mathbb{R}_+$ *is a weight function on vertices.*
- $g : \mathcal{E} \to \mathbb{R}_+$ *is a weight function on edges.*

We say Γ is finite (resp. connected) if $\{\mathcal{V}^o \cup \partial\mathcal{V}, \mathcal{E}\}$ is finite (resp. connected). When the weights μ, g are not relevant in a specific context, we write $\{\mathcal{V}^o, \partial\mathcal{V}, \mathcal{E}\}$ for short. In § 3.2 and § 5.4, we use x, y, z to refer to vertices in $\mathcal{V}$.

Given a subset $S \subset \mathcal{V}^o$, we say that $x_0 \in S$ is an *extreme point* of S with respect to $\partial\mathcal{V}$ if

$$\exists\, z \in \partial\mathcal{V} \text{ such that } d(x_0,z) < d(x,z),\ \forall\, x \in S,\ x \neq x_0,$$

where $d(x,y)$ is the distance of $x, y \in \mathcal{V}^o \cup \partial\mathcal{V}$ understood as the minimum number of edges forming a path connecting the two points x, y. The following *Two-Points Condition* for $\{\mathcal{V}^o, \partial\mathcal{V}, \mathcal{E}\}$ is imposed:

(**C-2**) For any subset $S \subset \mathcal{V}^o$ with $\sharp S \geqslant 2$, there exist at least two extreme points of S with respect to $\partial\mathcal{V}$.

We consider the set of points adjacent to the boundary defined as

$$N(\partial\mathcal{V}) = \{x \in \mathcal{V}^o\,;\, \exists\, z \in \partial\mathcal{V},\ \text{such that } x \sim z\} \cup \partial\mathcal{V}.$$

We say that two weighted graphs with boundary Γ, Γ' are *boundary isomorphic* if there exists a bijection $\Phi_0 : N(\partial\mathcal{V}) \to N(\partial\mathcal{V}')$ with the following properties.

(i) $\Phi_0|_{\partial\mathcal{V}} : \partial\mathcal{V} \to \partial\mathcal{V}'$ is bijective.
(ii) For any $z \in \partial\mathcal{V}$, $y \in N(\partial\mathcal{V})$ the equivalence $y \sim z \Longleftrightarrow \Phi_0(y) \sim' \Phi_0(z)$ holds, where $x' \sim' y'$ means that x', y' are adjacent in $\mathcal{V}' \cup \partial\mathcal{V}'$.

The graph Laplacian $\widehat{\Delta}_\Gamma$ is defined by

$$\left(\widehat{\Delta}_\Gamma u\right)(x) = \frac{1}{\mu_x} \sum_{y \sim x,\, y \in \mathcal{V}^o \cup \partial\mathcal{V}} g_{xy}\Big(u(y) - u(x)\Big), \quad x \in \mathcal{V}^o,$$

and the Neumann derivative at the boundary is defined by

$$(\partial_\nu u)(z) = \frac{1}{\mu_z} \sum_{x \sim z,\, x \in \mathcal{V}^o} g_{xz}\Big(u(x) - u(z)\Big), \quad z \in \partial\mathcal{V}. \tag{3.7}$$

Moreover, adding a potential function q on $\mathcal{V}^o$ to $\widehat{\Delta}_\Gamma$, we can define the D-N map in the same way as in the previous section.

The following result is valid, cf. [BILL23a, Theorems 1 and 2].

THEOREM 3.2. — *Let $\Gamma = \{\mathcal{V}^o, \partial\mathcal{V}, \mathcal{E}, \mu, g\}$ and $\Gamma' = \{\mathcal{V}^{o\prime}, \partial\mathcal{V}', \mathcal{E}', \mu', g'\}$ be two finite weighted graphs with boundary satisfying* (**C-1**), (**C-2**), *and let q, q' be real-valued potential functions on $\mathcal{V}^o, \mathcal{V}^{o\prime}$. Suppose Γ and Γ' are boundary isomorphic via Φ_0, and their D-N maps coincide for all energies. Then, there exists a bijection $\Phi : \mathcal{V}^o \cup \partial\mathcal{V} \to \mathcal{V}^{o\prime} \cup \partial\mathcal{V}'$ such that*

(1) $\Phi\big|_{\partial\mathcal{V}} = \Phi_0\big|_{\partial\mathcal{V}}$.
(2) $x \sim y \Longleftrightarrow \Phi(x) \sim' \Phi(y), \quad \forall\ x, y \in \mathcal{V}^o \cup \partial\mathcal{V}$.

Identifying vertices of Γ with those of Γ' by this bijection, assume furthermore that $\mu_z = \mu'_z$, $g_{xz} = g'_{xz}$ for all $z \in \partial\mathcal{V}$, $x \in \mathcal{V}^o$ such that $z \sim x$. Then we have

(3) *If $\mu = \mu'$, then $g = g'$, $q = q'$.*
(4) *If $q = q' = 0$, then $\mu = \mu'$ and $g = g'$.*

In particular, if $\mu(v) = \deg v$ and $\mu'(v') = \deg v'$ holds for all $v \in \mathcal{V}^o$ and $v' \in \mathcal{V}^{o\prime}$, respectively, then $g = g'$, $q = q'$.

Remark 3.3. — Let us add three remarks.

(1) The theorems in [BILL23a] that we refer to were formulated in terms of Neumann boundary spectral data; however, the claims hold for the Dirichlet boundary spectral data as well with a minor modification of the proof.

(2) Under the conditions (**C-1**), (**C-2**), the Neumann boundary spectral data determine the N-D maps for all energies, that is, the N-D map of $-\widehat{\Delta}_\Gamma - \lambda$ for all λ, and vice versa, see Lemma 5.8 below. In the same way, the Dirichlet boundary spectral data and the D-N maps for all energies determine each other.

(3) We can replace the assumption (**C-1**) by

(**C-1'**) For any $z \in \partial\mathcal{V}$ and any $x, y \in \mathcal{V}^o$, if $x \sim z$, $y \sim z$, then $x \sim y$.

cf. [BILL23a]. Inspecting Figures 5.1 – 5.4 in § 5 below, we see that (**C-1**) is satisfied for the hexagonal lattice, but not, e.g., for the triangular lattice. The latter, however, is covered by (**C-1'**). All the arguments below work under the assumption (**C-1'**) with minor modification. For the sake of simplicity, we adopt (**C-1**) in this paper.

For a similar result for trees, we refer to [GR22].

4. Equilateral graphs

Suppose we are given a finite quantum graph $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ satisfying (**C-1**), (**C-2**). We further assume that there exist a number $\ell_{\mathcal{E}}$ and a function $V_{\mathcal{E}}(z)$ such that

$$\ell_e = \ell_{\mathcal{E}}, \quad V_e(z) = V_{\mathcal{E}}(z), \quad \forall\, e \in \mathcal{E}. \tag{4.1}$$

Moreover, assume that

$$k_{\mathcal{V}} := \frac{C_v}{d_v} \text{is independent of } v \in \mathcal{V}. \tag{4.2}$$

Let $\phi_0(z,\lambda)$ and $\phi_1(z,\lambda)$ be $\phi_{e0}(z,\lambda)$, $\phi_{e1}(z,\lambda)$ in § 2. By (2.11) and (2.12), the discrete graph Laplacian $\widehat{\Delta}_{\mathcal{V},\lambda}$ and the vertex potential $\widehat{Q}_{\mathcal{V},\lambda}$ can be rewritten as

$$\big(\widehat{\Delta}_{\mathcal{V},\lambda}\widehat{u}\big)(v) = \frac{1}{d_v}\frac{1}{\phi_0(\ell_{\mathcal{E}},\lambda)}\sum_{w\sim v}\widehat{u}(w), \quad v \in \mathcal{V}, \tag{4.3}$$

$$\widehat{Q}_{\mathcal{V},\lambda} = \frac{1}{\phi_0(\ell_{\mathcal{E}},\lambda)}E_{\mathcal{E}}(\lambda), \quad E_{\mathcal{E}}(\lambda) = \phi_0'(\ell_{\mathcal{E}},\lambda) + k_{\mathcal{V}}\phi_0(\ell_{\mathcal{E}},\lambda). \tag{4.4}$$

Thus (4.3) and (4.4) differ by a multiplicative constant $\phi_0(\ell_{\mathcal{E}},\lambda)$ from the discrete operator with the graph Laplacian $(\widehat{\Delta}_{\mathcal{V}}\widehat{u})(v) := \frac{1}{d_v}\sum_{w\sim v}\widehat{u}(w)$ and potential $E_{\mathcal{E}}(\lambda)$.

This amounts to considering a graph $\widetilde{\Gamma}$ with the same edge set $\mathcal{E}$ and the vertex set $\mathcal{V}$ as our original Γ, and $\mu_v = d_v$, $g_{vw} = 1$. We let λ vary and use analytic continuation: if we are given the D-N map for the original quantum graph Γ for all energies, we can obtain the D-N map of the above discrete operator $\widehat{\Delta}_{\mathcal{V}}$ for all energies, and, *mutatis mutandis*, the Dirichlet boundary spectral data for $\widehat{\Delta}_{\mathcal{V}}$ under the conditions (**C-1**), (**C-2**). Note that the D-N map for the operator $\widehat{\Delta}_{\mathcal{V}}$ acts as

$\widehat{u}(v)\mapsto\widehat{u}(w)$, $w\sim v\in\partial\mathcal{V}$, $w\in\mathcal{V}^o$; by (3.6) it can be computed from the D-N map of $\widehat{\Delta}_{\mathcal{V},\lambda}$ if we know $\phi_0(z,\lambda)$, i.e. $\ell_{\mathcal{E}}$ and $V_{\mathcal{E}}(z)$.

Suppose now that we are given two such graphs $\widetilde{\Gamma}=\{\mathcal{V},\mathcal{E}\}$ and $\widetilde{\Gamma}'=\{\mathcal{V}',\mathcal{E}'\}$. Applying then Theorem 3.2 with $\mu_x=d_x$, $g_{xy}=1$, we infer that there is a bijection

$$\Phi:\widetilde{\Gamma}\to\widetilde{\Gamma}' \tag{4.5}$$

preserving the graph structure. Setting $v'=\Phi(v)$, we conclude that

$$d_v=d_{v'},\quad\forall\, v\in\mathcal{V}^o,$$

and consequently

$$C_v=C'_{v'},\quad\forall\, v\in\mathcal{V}^o.$$

In this way, we have proven the following theorem:

THEOREM 4.1. — *Let $\Gamma=\{\mathcal{V},\mathcal{E}\}$ and $\Gamma'=\{\mathcal{V}',\mathcal{E}'\}$ be two finite quantum graphs satisfying assumptions* (**C-1**), (**C-2**), (4.1), (4.2) *and $\ell_{\mathcal{E}}=\ell_{\mathcal{E}'}, V_{\mathcal{E}}(z)=V_{\mathcal{E}'}(z)$, $k_{\mathcal{V}}=k_{\mathcal{V}'}$. Suppose that Γ and Γ' are boundary isomorphic and that the D-N maps for the Schrödinger operator for the two quantum graphs coincide for all energies. Then there is a bijection $\Phi:\Gamma\to\Gamma'$ preserving the graph structure, and $d_v=d_{v'}$, $C_v=C'_{v'}$ hold for all $v\in\mathcal{V}^o$ and $v'=\Phi(v)$.*

5. Inverse scattering for the discrete Hamiltonian

It is known that the potential of the discrete Schrödinger operator on periodic square or hexagonal lattices can be uniquely recovered from the knowledge of the scattering matrix of all energies, see [And13, IK12]. Furthermore, the forward and inverse scattering problems have been considered for infinite graphs that are local perturbations of periodic lattices in [AIM16, AIM18]. For several standard types of lattices, it was shown in [AIM18] that the scattering matrix for the discrete Schrödinger operator on locally perturbed lattices determines the Dirichlet-to-Neumann map for the discrete Schrödinger equation on the perturbed subgraph. In this section, we apply Theorem 3.2 to recover the potential on locally perturbed lattices, as well as to recover the structure of the perturbed subgraph (see Theorem 5.11). This result may be applied, in particular, to probe graphene defects from the knowledge of the scattering matrix, see Figures 5.1 and 5.2.

5.1. Periodic lattices and local perturbations

To begin with, we review a framework of the scattering theory on perturbed periodic lattices used in [AIM16, AIM18]. A periodic graph in $\mathbb{R}^d$ is a triple $\Gamma_0=\{\mathcal{L}_0,\mathcal{V}_0,\mathcal{E}_0\}$, where $\mathcal{E}_0$ is the edge set, and $\mathcal{L}_0$ is a lattice of rank d in $\mathbb{R}^d$ with a basis $\mathbf{v}_j, j=1,\cdots,d$, in other words

$$\mathcal{L}_0=\Big\{\mathbf{v}(n):\,n\in\mathbb{Z}^d\Big\},\quad\mathbf{v}(n)=\sum_{j=1}^{d}n_j\mathbf{v}_j,\quad n=(n_1,\cdots,n_d)\in\mathbb{Z}^d. \tag{5.1}$$

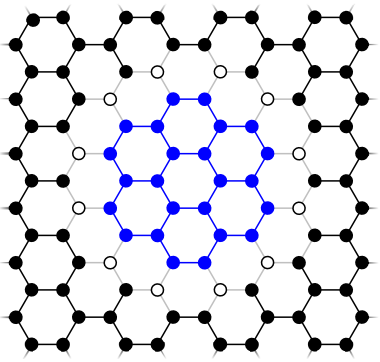

Figure 5.1. Periodic hexagonal lattice. The white vertices are considered to be the boundary vertices for the subgraph of the blue (interior) vertices.

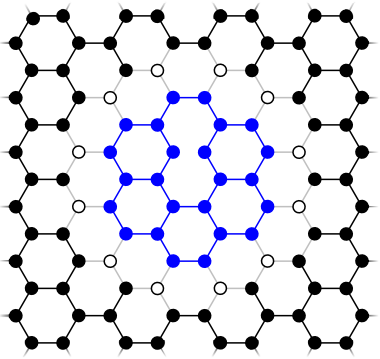

Figure 5.2. A hexagonal lattice of Figure 5.1 with one blue edge removed. By Theorem 5.11, the exact structure of such graphs and the potential can be uniquely recovered from the scattering matrix.

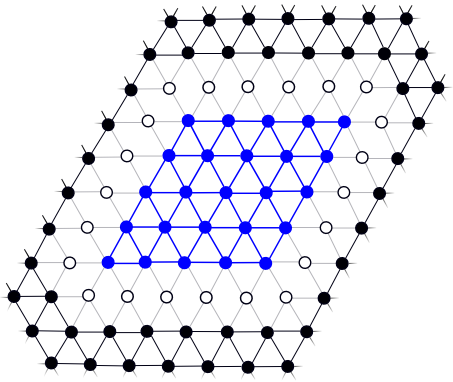

Figure 5.3. A triangular lattice satisfying (**C-1'**).

The vertex set $\mathcal{V}_0$ is defined by

$$\mathcal{V}_0 = \bigcup_{j=1}^{s} \left(p_j + \mathcal{L}_0\right), \tag{5.2}$$

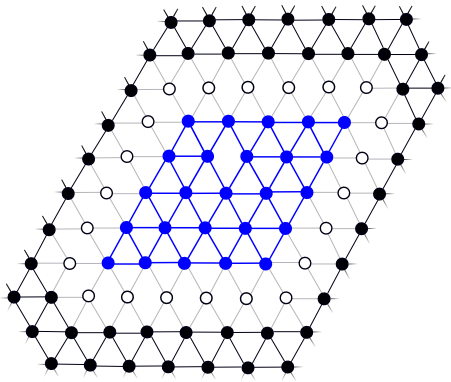

Figure 5.4. A triangular lattice satisfying (**C-1'**) *of Figure 5.3 with one blue edge removed. By Theorem 5.11, the exact structure of such graphs and the potential can be uniquely recovered from the scattering matrix.*

where p_j, $j = 1, \cdots, s$, are points in $\mathbb{R}^d$ satisfying $p_i - p_j \notin \mathcal{L}_0$ if $i \neq j$. We assume that the degree of vertices are equal for all vertices $v \in \mathcal{V}_0$ and denote it by $\deg_{\mathcal{V}_0}$. From (5.2), we know that any function $\widehat{f}$ on $\mathcal{V}_0$ can be written as $\widehat{f}(n) = (\widehat{f}_1(n), \cdots, \widehat{f}_s(n))$, $n \in \mathbb{Z}^d$, where $\widehat{f}_j(n)$ is a function on $p_j + \mathcal{L}_0$. Hence the associated Hilbert space is $\ell^2(\mathcal{V}_0) = \ell^2(\mathbb{Z}^d)^s$, and it is unitarily equivalent to $L^2(\mathbb{T}^d)^s$, where $\mathbb{T}^d$ is the flat torus $\mathbb{R}^d/(2\pi\mathbb{Z})^d$, by means of the discrete Fourier transformation

$$\left(\mathcal{U}_{\mathcal{V}}\widehat{f}\right)(x) = \sqrt{\deg_{\mathcal{V}_0}}\,(2\pi)^{-d/2} \sum_{n\in\mathbb{Z}^d} \widehat{f}(n)\, e^{in\cdot x}, \quad x \in \mathbb{T}^d. \tag{5.3}$$

The Laplacian $\widehat{\Delta}_{\Gamma_0}$ on the lattice Γ_0 is defined by

$$\left(\widehat{\Delta}_{\Gamma_0} u\right)(v) = \frac{1}{\deg_{\mathcal{V}_0}} \sum_{w\in\mathcal{V}_0,\, e_{vw}\in\mathcal{E}_0} u(w), \quad v \in \mathcal{V}_0, \tag{5.4}$$

where, e_{vw} denotes an edge $\in \mathcal{E}_0$ with end points $v, w \in \mathcal{V}_0$, and we will use the symbol $\widehat{H}_0 = -\widehat{\Delta}_{\Gamma_0}$.

On the torus $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z})^d$, the Floquet image of the Laplacian $\widehat{H}_0$ is an $s \times s$ matrix operator $H_0(x)$, where $x \in \mathbb{T}^d$ is the quasimomentum variable. We denote the matrix by H_0; its entries are trigonometric functions. Let $\lambda_1(x) \leqslant \cdots \leqslant \lambda_s(x)$ be the eigenvalues of $H_0(x)$. We put

$$p(x,\lambda) := \det(H_0(x) - \lambda), \qquad M_\lambda := \left\{x \in \mathbb{T}^d : p\,(x,\lambda) = 0\right\},$$

$$M_{\lambda,j} := \left\{x \in \mathbb{T}^d : \lambda_j(x) = \lambda\right\}, \qquad M_\lambda^{\mathbb{C}} := \left\{z \in \mathbb{C}^d/(2\pi\mathbb{Z})^d : p(z,\lambda) = 0\right\},$$

$$M_{\lambda,reg}^{\mathbb{C}} := \left\{z \in M_\lambda^{\mathbb{C}} : \nabla_z p(z,\lambda) \neq 0\right\}, \qquad M_{\lambda,sng}^{\mathbb{C}} := \left\{z \in M_\lambda^{\mathbb{C}} : \nabla_z p(z,\lambda) = 0\right\}.$$

In the spirit of § 3.1, we define

$$\partial_{\Gamma_0}\Omega := \left\{v \in \mathcal{V}_0 \setminus \Omega \,\middle|\, e_{vw} \in \mathcal{E}_0 \text{ for some } w \in \Omega\right\}, \tag{5.5}$$

where Ω is any subset in $\mathcal{V}_0$.

We impose the following assumptions on the periodic lattice Γ_0.

(**D-1**) *There exists a subset* $\mathcal{T}_1 \subset \sigma(H_0)$ *such that for* $\lambda \in \sigma(H_0) \setminus \mathcal{T}_1$, $M^{\mathbb{C}}_{\lambda,sng}$ *is discrete, and each connected component of* $M^{\mathbf{C}}_{\lambda,reg}$ *intersects with* $\mathbb{T}^d$, *the intersection being a* $(d-1)$*-dimensional real analytic submanifold of* $\mathbb{T}^d$.

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

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

(**D-3**) $\nabla_x p\ (x,\lambda) \neq 0$ *holds on* M_λ *for* $\lambda \in \sigma(H_0) \setminus \mathcal{T}_0$.

(**D-4**) *The last assumption consists of two requirements:*

(a) *On the unperturbed lattice* Γ_0, *there exist finite connected subsets* $\{\Omega_k\}_{k=1}^\infty$ *of* $\mathcal{V}_0$ *such that* $\Omega_k \subset \Omega_{k+1}$, $\mathcal{V}_0 = \cup_{k=1}^\infty \Omega_k$, *and the triple* $(\Omega_k, \partial_{\Gamma_0}\Omega_k, \mathcal{E}_0)$ satisfies assumptions (**C-1**), (**C-2**) for all k, and

(b) *the unique continuation from infinity holds on* $\Omega_k^{ext} := \mathcal{V}_0 \setminus \Omega_k$ *for all* k.

Assumption (**D-4**) requires a little explanation. For a subset $U \subset \mathcal{V}_0$ satisfying $\sharp(\mathcal{V}_0 \setminus U) < \infty$, by the unique continuation from infinity on U, we mean the following claim. If $\widehat{u}$ satisfies $(-\widehat{\Delta}_{\Gamma_0} - \lambda)\widehat{u} = 0$ on U for some λ and $\widehat{u} = 0$ near infinity, then $\widehat{u}$ vanishes on whole U. Namely, if $\widehat{u}$ satisfies $(-\widehat{\Delta}_{\Gamma_0} - \lambda)\widehat{u} = 0$ on U and $\widehat{u} = 0$ on $|v| > R$ for some $R > 0$, then $\widehat{u} = 0$ on U.

On the other hand, the unique continuation from the boundary in the finite domain Ω_i follows from the first part of (**D-4**). Namely, if $(-\widehat{\Delta}_{\Gamma_0} - \lambda)\widehat{u} = 0$ in Ω_i and $\widehat{u} = \partial_\nu \widehat{u} = 0$ on $\partial_{\Gamma_0}\Omega_i$, then $\widehat{u} = 0$ in Ω_i. This claim also holds for $-\widehat{\Delta}_{\Gamma_0} + q(v)$ with any potential q, see [BILL23a, Lemma 3.5] or [BILL23b, Lemma 2.4].

In particular, part (**D-4**a) implies the unique continuation property on $\mathcal{V}_0$ from infinity.

LEMMA 5.1. — *If part* (**D-4**a) *is satisfied for* Γ_0, *then the unique continuation from infinity holds for the unperturbed equation* $(-\widehat{\Delta}_{\Gamma_0} - \lambda)\widehat{u} = 0$ *on* Γ_0.

Proof. — If a solution $\widehat{u}$ is finitely supported in $\mathcal{V}_0$, we can find Ω_k such that $\mathrm{supp}\,(\widehat{u}) \subset \Omega_k$ by assumption (**D-4**a). Then $\widehat{u}$ vanishes outside Ω_k on the unperturbed lattice Γ_0 for some k. By definition (5.4), we know for any $z \in \partial_{\Gamma_0}\Omega_k$,

$$\begin{aligned}\sum_{x\sim z,\, x\in\Omega_k} \big(\widehat{u}(x) - \widehat{u}(z)\big) &= \sum_{x\sim z,\, x\in\mathcal{V}_0} \big(\widehat{u}(x) - \widehat{u}(z)\big) \\ &= \deg_{\mathcal{E}_0}(z)\, \widehat{\Delta}_{\Gamma_0}\widehat{u}(z) = -\deg_{\mathcal{E}_0}(z)\, \lambda \widehat{u}(z) = 0.\end{aligned}$$

This indicates that $\widehat{u}$ is a solution of the Schrödinger equation on $(\Omega_k, \partial_{\Gamma_0}\Omega_k, \mathcal{E}_0)$ satisfying simultaneously the Dirichlet and Neumann boundary conditions. Hence $\widehat{u}$ vanishes everywhere by [BILL23b, Lemma 2.4], provided that the subgraph $(\Omega_k, \partial_{\Gamma_0}\Omega_k, \mathcal{E}_0)$ satisfies the assumptions (**C-1**) and (**C-2**). □

The assumption (**D-2**) implies that the eigenvalues $\lambda_j(x)$ are simple for $\lambda \notin \mathcal{T}_0$. For $\lambda \notin \mathcal{T}_1$, (**D-1**) guarantees the Rellich type theorem (cf. [AIM16, Theorems 5.1 and 5.7]). Therefore, (**D-1**) and (**D-4**) yield the non-existence of embedded eigenvalues for $H_0(x)$ and its perturbation for the energy $\lambda \notin \mathcal{T}_0 \cup \mathcal{T}_1$.

For the square, triangular, hexagonal, Kagome, and diamond lattices, as well as for subdivisions of square lattices, the subset $\mathcal{T}_1$ is finite. On the other hand, for the ladder and "layered" graphite lattices, $\mathcal{T}_1$ fills closed intervals, cf. [AIM16, § 5].

By virtue of [BILL23a, Proposition 1.10], our result applies to several standard types of lattices and their perturbations. As for examples illustrating (**D-4**a), see Example 5.12 of the present paper. The unique continuation from infinity on Ω_i^{ext} is seen to be satisfied for e.g. the square, hexagonal, triangular lattices by directly examining the figures.

Referring to the papers [AIM16, AIM18], we note that their authors employed four assumptions, (A-1)–(A-4), of which the first three coincided with (**D-1**)–(**D-3**) above. The fourth assumption there, (A-4), follows from part (**D-4**a) by Lemma 5.1.

Now let us consider an infinite connected graph $\Gamma = \{\mathcal{V}, \mathcal{E}\}$, which is a local perturbation of the periodic lattice $\Gamma_0 = \{\mathcal{L}_0, \mathcal{V}_0, \mathcal{E}_0\}$ satisfying the assumptions (**D-1**)–(**D-4**) above. We assume that the lattice Γ_0 is perturbed only in a finite subset $\Omega \subset \mathcal{V}_0$ and the potential function is supported in the perturbed region. Later we will further assume (**C-1**) and (**C-2**) for the perturbed part in Ω. Lemma 5.1 then holds also for the perturbed system by the same proof, see Lemma 5.10.

For a subgraph $\{\Omega,\ \{e_{vw} \in \mathcal{E}_0 : v, w \in \Omega\}\}$ of Γ_0, we consider its perturbation $\{\widetilde{G}, E_{pert}\}$, which is a finite connected graph with vertex set $\widetilde{G}$ and edge set E_{pert}. Without loss of generality, we may assume Ω is chosen sufficiently large so that the perturbation does not remove the vertices (of Ω) which are connected to the subgraph boundary $\partial_{\Gamma_0}\Omega$. We add an unperturbed layer of edges to E_{pert} defining

$$E \ := \ E_{pert} \cup \left\{ e_{vw} \in \mathcal{E}_0 \,\middle|\, v \in \Omega, w \in \partial_{\Gamma_0}\Omega \right\}. \tag{5.6}$$

Remark 5.2. — Let us remark here that when perturbing an infinite lattice on a finite set, we must be careful about the boundary points for the exterior and interior domains. We remove the edges between the boundary points. See Figures 5.2, 5.4.

For the scattering problem in this section, we set

$$\partial G = \partial_{\Gamma_0}\Omega, \quad G = \widetilde{G} \setminus \partial_{\Gamma_0}\Omega.$$

Then the weighted graph

$$\mathbb{G}_\Gamma := \{G, \partial G, E, \mu, g\}, \tag{5.7}$$

where $\mu = \{\mu_v\,;\, v \in G\}$, $g = \{g_{vw}\,;\, v, w \in G,\ v \sim w\}$ are the vertex weight and edge weight, fits into our setting for finite graphs in § 3.2.

Observe that the edges connecting ∂G and G are known, and that by construction there are no edges between vertices in ∂G.

In particular, we can simply choose the perturbed vertex set Ω to be Ω_k for some k as assumed in part (**D-4**a). We define the following sets:

$$\begin{aligned} \mathcal{V}_{int} &:= G \cup \partial G, & \mathcal{V}_{int}^{\circ} &:= G, & \partial\mathcal{V}_{int} &:= \partial G; \\ \mathcal{V}_{ext} &:= \mathcal{V} \setminus G, & \mathcal{V}_{ext}^{\circ} &:= (\mathcal{V} \setminus G) \setminus \partial G, & \partial\mathcal{V}_{ext} &:= \partial G. \end{aligned}$$

Then the unique continuation from infinity holds on $\mathcal{V}_{ext}$ due to part (**D-4**b). Hence $\mathcal{V}_{int}$ and $\mathcal{V}_{ext}$ satisfy assumptions (B-1)–(B-3) imposed in [AIM18], and consequently, the Hilbert space $\ell^2(\mathcal{V})$ admits an orthogonal decomposition

$$\ell^2(\mathcal{V}) = \ell^2\left(\mathcal{V}_{ext}^{\circ}\right) \oplus \ell^2\left(\mathcal{V}_{int}\right).$$

Denote by $\widehat{P}_{ext}$ the orthogonal projection:

$$\widehat{P}_{ext} : \ell^2(\mathcal{V}) \to \ell^2\left(\mathcal{V}^\circ_{ext}\right). \tag{5.8}$$

The Laplacian $\widehat{\Delta}_\Gamma$ on the graph Γ is defined in analogy with (5.4), replacing $\mathcal{V}_0, \mathcal{E}_0$ by $\mathcal{V}, \mathcal{E}$. Adding then a bounded self-adjoint perturbation of $\widehat{V}$, which is assumed to vanish on $\mathcal{V}_{ext}$, we consider Hamiltonian $\widehat{H}$ of the form

$$\widehat{H} = -\widehat{\Delta}_\Gamma + \widehat{V} \colon \ell^2(\mathcal{V}) \to \ell^2(\mathcal{V}).$$

Note that in the forward scattering problem, following the arguments of [AIM16] and those from [AIM18, § 2–§ 5], one can allow arbitrary structure modification on the finite part of the graph.

5.2. Spectral representation and the S-matrix

Let us keep reviewing the needed results from [AIM16, AIM18]. In general, scattering is a time-dependent phenomenon, and the S-matrix is defined through the wave operators. However, it has the stationary counterpart which we employ here. Let us recall how it looks for a Schrödinger operator in $\mathbb{R}^n$. We introduce a Banach space $\mathcal{B}(\mathbb{R}^n)^*$ consisting of $L^2_{loc}(\mathbb{R}^n)$ functions $f(x)$ such that

$$\|f\|^2_{\mathcal{B}(\mathbb{R}^n)^*} := \sup_{R>1} \frac{1}{R} \int_{|x|<R} |f(x)|^2 dx < \infty, \tag{5.9}$$

which is the dual space of the Banach space $\mathcal{B}(\mathbb{R}^n)$ defined as follows,

$$\|f\|_{\mathcal{B}(\mathbb{R}^n)} = \sum_{j=0}^{\infty} R_j \left(\int_{\Omega_j} |f(x)|^2 dx \right)^{1/2} < \infty, \tag{5.10}$$

where $R_j = 2^j$ and $\Omega_j = \{x \in \mathbb{R}^d\,;\, R_{j-1} \leqslant |x| < R_j\}$; for $j = 0$ we put $R_{-1} := 0$. These spaces give rise to a rigged structure of $L^2(\mathbb{R}^n)$, namely

$$\mathcal{B} \subset L^2\left(\mathbb{R}^n\right) \subset \mathcal{B}^*$$

with continuous inclusions. Given $u, v \in \mathcal{B}(\mathbb{R}^n)^*$, we define

$$u \simeq v \Longleftrightarrow \lim_{R\to\infty} \frac{1}{R} \int_{|x|<R} |u(x) - v(x)|^2 dx = 0. \tag{5.11}$$

We consider the Helmholtz equation

$$(-\Delta + V(x) - \lambda)u = 0 \quad \text{in} \quad \mathbb{R}^n, \tag{5.12}$$

where $\lambda > 0$ and $V(x)$ is a real function decaying sufficiently rapidly at infinity. Then, for any $\phi^{in} \in L^2(S^{n-1})$, there exist a unique $u \in \mathcal{B}(\mathbb{R}^n)^*$ satisfying (5.12) and $\phi^{out} \in L^2(S^{n-1})$ such that

$$u \simeq \frac{e^{i\sqrt{\lambda}r}}{r^{(n-1)/2}}\phi^{out} - \frac{e^{-i\sqrt{\lambda}r}}{r^{(n-1)/2}}\phi^{in}. \tag{5.13}$$

The operator

$$S(\lambda) : L^2\left(S^{n-1}\right) \ni \phi^{in} \to \phi^{out} \in L^2\left(S^{n-1}\right)$$

is unitary and can be identified, up to a unitary operator, with the on-shell S-matrix obtained by the direct-integral decomposition of the scattering operator defined in the time-dependent theory.

As for scattering on perturbed periodic lattices, in some cases one can argue in the same way as above, e.g., when a square lattice is concerned [IM15]. However, to deal with general lattices, it is more convenient to pass the problem on the torus by the discrete Fourier transform and to observe the singularities of solutions to the Helmholtz equation.

On the torus $\mathbb{T}^d$, the counterpart of the above space $\mathcal{B}(\mathbb{R}^n)^*$ is defined as follows. Let ϕ be a distribution on $\mathbb{T}^d$. Multiplying it by a smooth cut-off function, passing to the Fourier transform in the appropriate local chart, and denoting the resulting function by $\widetilde{\phi}$, we define $\mathcal{B}(\mathbb{T}^d)^*$ to be the set of distributions such that

$$\sup_{R>1} \frac{1}{R} \int_{|\xi|<R} \left|\widetilde{\phi}(\xi)\right|^2 d\xi < \infty\,; \tag{5.14}$$

for two distributions ϕ, ψ on $\mathbb{T}^d$, $\phi \simeq \psi$ means

$$\frac{1}{R} \int_{|\xi|<R} \left|\widetilde{\phi}(\xi) - \widetilde{\psi}(\xi)\right|^2 d\xi \to 0 \quad \text{as} \quad R \to \infty. \tag{5.15}$$

We also define the space $\mathcal{B}(\mathbb{T}^d)$ similarly to (5.10). See [AIM16, § 4] and [AIM18, § 2.4].

Assume that the unperturbed periodic lattice Γ_0 satisfies the above assumptions (**D-1**)–(**D-4**). The spectral representation of H_0 is nothing but the diagonalization of $H_0(x)$. Let $P_j(x)$ be the eigenprojection associated with the eigenvalue $\lambda_j(x)$. Let $I_j = \{\lambda_j(x)\,;\, x \in \mathbb{T}^d\} \setminus \mathcal{T}_0$, and

$$M_{\lambda,j} = \begin{cases} \left\{x \in \mathbb{T}^d\,;\, \lambda_j(x) = \lambda\right\}, & \lambda \in I_j, \\ \emptyset, & \lambda \notin I_j. \end{cases} \tag{5.16}$$

For $\lambda \in \sigma(H_0) \setminus \mathcal{T}_0$, we have $M_{\lambda,i} \cap M_{\lambda,j} = \emptyset$ if $i \neq j$, hence each of them is a C^∞-submanifold of $\mathbb{T}^d$. We define the Hilbert spaces $\mathbf{h}_{\lambda,j}$ equipped with the inner product

$$(\psi, \phi)_{L^2(M_{\lambda,j})} = \int_{M_{\lambda,j}} P_j(x)\psi(x) \cdot \overline{\phi(x)} \frac{dM_{\lambda,j}}{|\nabla \lambda_j(x)|},$$

and put

$$\mathbf{h}_\lambda = \mathbf{h}_{\lambda,1} \oplus \cdots \oplus \mathbf{h}_{\lambda,s}. \tag{5.17}$$

For $f \in \mathcal{B}(\mathbb{T}^d)$, we define

$$\mathcal{F}_{0,j}(\lambda) f = P_j(x) f(x)\Big|_{M_{\lambda,j}} \tag{5.18}$$

and

$$\mathcal{F}_0(\lambda) f = \Big(\mathcal{F}_{0,1}(\lambda) f, \ldots, \mathcal{F}_{0,s}(\lambda) f\Big); \tag{5.19}$$

in the spirit of the above orthogonal sum, we often write the right-hand side as $\sum_{j=1}^s \mathcal{F}_{0,j}(\lambda) f$. Then the operators

$$\mathcal{F}_0(\lambda) \in \mathbf{B}\left(\mathcal{B}\left(\mathbb{T}^d\right)\,;\, \mathbf{h}_\lambda\right) \tag{5.20}$$

provide us with a spectral representation (or a generalized Fourier transformation) associated with H_0. It is related to the resolvent of H_0 in the following way,

$$(H_0 - \lambda \mp i0)^{-1} f \simeq \sum_{j=1}^{s} \frac{\mathcal{F}_{0,j}(\lambda) f}{\lambda_j(x) - \lambda \mp i0}, \quad f \in \mathcal{B}\left(\mathbb{T}^d\right), \tag{5.21}$$

where the relation $\simeq$ is defined by (5.15). This shows that the generalized Fourier transform can be associated with the singular part of the resolvent of H_0 on the torus, which in turn describes the behavior at infinity of the resolvent of $\widehat{H}_0$ in the lattice space. Compared with the case of $\mathbb{R}^n$, the lattice and the torus here can be matched off against the position space and the momentum space, respectively.

The same fact holds for the perturbed operator $\widehat{H} = -\widehat{\Delta}_\Gamma + \widehat{V}$ on $\ell^2(\mathcal{V})$. One can easily check that $\sigma_e(\widehat{H}) = \sigma(\widehat{H}_0) = \sigma(H_0)$, and furthermore, that $\sigma_p(\widehat{H}) \cap \sigma_e(\widehat{H})$ is discrete in $\sigma_e(H_0) \setminus \mathcal{T}_0$ with possible accumulation points in $\mathcal{T}_0$ only [AIM16, Lemma 7.5]. In the following we consider $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \sigma_p(\widehat{H}))$. Define $\mathcal{B} = \mathcal{B}(\mathcal{V})$ and $\mathcal{B}^* = \mathcal{B}(\mathcal{V})^*$ as direct sums,

$$\mathcal{B}(\mathcal{V}) = \mathcal{B}(\mathcal{V}_{ext}) \oplus \ell^2\left(\mathcal{V}_{int}^\circ\right), \quad \mathcal{B}(\mathcal{V})^* = \mathcal{B}(\mathcal{V}_{ext})^* \oplus \ell^2\left(\mathcal{V}_{int}^\circ\right), \tag{5.22}$$

where the spaces $\mathcal{B}(\mathcal{V}_{ext})$ and $\mathcal{B}(\mathcal{V}_{ext})^*$ are defined on the torus in the way described above[(1)]. Denoting $\widehat{R}(z) := (\widehat{H} - z)^{-1}$ and assuming $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \sigma_p(\widehat{H}))$, we have

$$\widehat{R}(\lambda \pm i0) \in \mathbf{B}(\mathcal{B}\,;\, \mathcal{B}^*). \tag{5.23}$$

The generalized Fourier transformation $\mathcal{F}_\pm(\lambda)$ associated with $\widehat{H}$ is given by[(2)]

$$\mathcal{F}_\pm(\lambda) = \mathcal{F}_0(\lambda)\, \mathcal{U}_\mathcal{V} \widehat{Q}_1(\lambda \pm i0)\, \mathcal{U}_\mathcal{V}^*, \tag{5.24}$$

where

$$\widehat{Q}_1(z) = \widehat{P}_{ext} + \widehat{K}_1 \widehat{R}(z), \quad \widehat{K}_1 = \widehat{H}_0 \widehat{P}_{ext} - \widehat{P}_{ext} \widehat{H}. \tag{5.25}$$

It is related to the resolvent in the following way, see [AIM16, Theorems 7.7 and 7.15]:

THEOREM 5.3. — *Let $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \sigma_p(\widehat{H}))$. For $f \in \mathcal{B}$ we have the relation*

$$\mathcal{U}_\mathcal{V} \widehat{P}_{ext} \widehat{R}(\lambda \pm i0) f \simeq \sum_{j=1}^{s} \frac{\mathcal{F}_{\pm,j}(\lambda) f}{\lambda_j(x) - \lambda \mp i0}. \tag{5.26}$$

As in the case of $\mathbb{R}^n$, the S-matrix is defined by means of the Helmholtz equation.

THEOREM 5.4. —

(1) *For any solution $\widehat{u} \in \widehat{\mathcal{B}}$ to the equation*

$$\left(\widehat{H} - \lambda\right) \widehat{u} = 0, \tag{5.27}$$

(1) More explicitly, the norm of $\mathcal{B}(\mathcal{V}_0)^*$ is defined by $\|\widehat{u}\|^2_{\mathcal{B}(\mathcal{V}_0)^*} = \sup_{R>1} \frac{1}{R} \sum_{|n|<R} |\widehat{u}(n)|^2$, while in the case of $\mathcal{V}_{ext}$, the sum ranges over vertices of the set $\mathcal{V}_{ext}$ only.

(2) To get (5.24), we employ the resolvent equation, cf. the argument preceding Theorem 6.11 in § 6.6, in particular, the formula (6.45).

there exist unique pair of vectors $\phi^{in}, \phi^{out} \in \mathbf{h}_\lambda$ *such that*

$$\mathcal{U}_{\mathcal{V}} \widehat{P}_{ext} \widehat{u} \simeq \sum_{j=1}^{s} \frac{1}{2\pi i} \left(\frac{\phi_j^{out}}{\lambda_j(x) - \lambda - i0} - \frac{\phi_j^{in}}{\lambda_j(x) - \lambda + i0} \right). \tag{5.28}$$

Moreover, the operator $S(\lambda) \in \mathbf{B}(\mathbf{h}_\lambda\,;\, \mathbf{h}_\lambda)$ *defined by*

$$S(\lambda) = 1 - 2\pi i A(\lambda), \tag{5.29}$$

where

$$A(\lambda) := \mathcal{F}_+(\lambda)\, \mathcal{U}_{\mathcal{V}} \widehat{K}_2\, \mathcal{U}_{\mathcal{V}}^* \mathcal{F}_0(\lambda)^*, \quad \widehat{K}_2 := \widehat{H}\widehat{P}_{ext} - \widehat{P}_{ext}\widehat{H}_0, \tag{5.30}$$

is unitary on $\mathbf{h}_\lambda$*, and satisfies*

$$\phi^{out} = S(\lambda)\phi^{in}. \tag{5.31}$$

(2) *For any* $\phi^{in} \in \mathbf{h}_\lambda$*, there is a unique* $\widehat{u} \in \widehat{\mathcal{B}}$ *and* $\phi^{out} \in \mathbf{h}_\lambda$ *such that*

$$(\widehat{H} - \lambda)\widehat{u} = 0, \tag{5.32}$$

and relations (5.28), (5.31) *are satisfied.*

The operator $S(\lambda)$ is the S-matrix for our perturbed lattice, in the physics literature usually referred to as the on-shell S-matrix.

5.3. The S-matrix and Dirichlet-to-Neumann map

Now we consider eigenvalue equations separately on $\mathcal{V}_{ext}$ and $\mathcal{V}_{int}$, assuming that [AIM18, (B-1)–(B-3)] are satisfied. Suppose that there is no perturbation outside $\mathcal{V}_{int}$ and that the potential is also supported in $\mathcal{V}_{int}$ only. Let $\widehat{H}_{ext}$ be $-\widehat{\Delta}_\Gamma$ on $\mathcal{V}_{ext}^0$ with Dirichlet boundary condition on $\partial\mathcal{V}_{ext}$. For $\lambda \in \sigma_e(\widehat{H}_{ext}) \setminus (\mathcal{T}_0 \cup \mathcal{T}_1)$, there exists a unique solution $\widehat{u}_{ext}^{(\pm)} \in \widehat{\mathcal{B}}^*$ to the following equation,

$$\begin{cases} \left(-\widehat{\Delta}_{\Gamma_0} - \lambda\right) \widehat{u}_{ext}^{(\pm)} = 0 \quad \text{in} \quad \mathcal{V}_{ext}^\circ, \\ \widehat{u}_{ext}^{(\pm)} = \widehat{f} \quad \text{on} \quad \partial\mathcal{V}_{ext}, \end{cases}$$

satisfying the radiation condition[(3)] (outgoing for $\widehat{u}_{ext}^{(+)}$ and incoming for $\widehat{u}_{ext}^{(-)}$). We define the *exterior D-N map* $\Lambda_{ext}^{(\pm)}(\lambda)$ by

$$\Lambda_{ext}^{(\pm)}(\lambda)\widehat{f} = -\partial_\nu^{\mathcal{V}_{ext}} \widehat{u}_{ext}^{(\pm)}\Big|_{\partial\mathcal{V}_{ext}},$$

where the normal derivative of a function u at $z \in \partial\mathcal{V}_{ext}$ in $\mathcal{V}_{ext}^\circ$ is defined by

$$\begin{aligned} \left(\partial_\nu^{\mathcal{V}_{ext}} u\right)(z) &:= -\frac{1}{\deg_{\mathcal{E}}^{ext}(z)} \sum_{x \in \mathcal{V}_{ext}^\circ,\, \{x,z\} \in \mathcal{E}} u(x)\,, \\ \deg_{\mathcal{E}}^{ext}(z) &:= \sharp\,\{x \in \mathcal{V}_{ext}^\circ \,:\, \{x,z\} \in \mathcal{E}\}\,. \end{aligned} \tag{5.33}$$

(3) We speak here of the discrete analogue of the usual radiation condition, see [AIM18, § 2.6].

On the other hand, for $\lambda \notin \sigma(\widehat{H}_{int})$, where $\widehat{H}_{int}$ is $-\widehat{\Delta}_\Gamma + \widehat{V}$ in $\mathcal{V}_{int}$ with Dirichlet boundary condition, there exists a unique solution $\widehat{u}_{int}$ to the following equation,

$$\begin{cases} \left(-\widehat{\Delta}_\Gamma + \widehat{V} - \lambda\right)\widehat{u}_{int} = 0 \quad \text{in} \quad \mathcal{V}_{int}^\circ, \\ \widehat{u}_{int} = \widehat{f} \quad \text{on} \quad \partial\mathcal{V}_{int}. \end{cases}$$

The *interior D-N map* $\Lambda_{int}(\lambda)$ is defined by

$$\Lambda_{int}(\lambda)\widehat{f} = \partial_\nu^{\mathcal{V}_{int}}\widehat{u}_{int}\Big|_{\partial\mathcal{V}_{int}},$$

where the normal derivative at $\partial\mathcal{V}_{int}$ in $\mathcal{V}_{int}^\circ$ is defined in the analogous way, replacing all the exterior sets in (5.33) with the respective interior ones.

We denote

$$\Sigma = \partial\mathcal{V}_{int} = \partial\mathcal{V}_{ext} \tag{5.34}$$

and define the operator

$$B_\Sigma^{(\pm)}(\lambda) := \mathcal{M}_{int}\Lambda_{int}(\lambda) - \mathcal{M}_{ext}\Lambda_{ext}^{(\pm)}(\lambda) - \widehat{S}_\Sigma - \lambda\chi_\Sigma, \tag{5.35}$$

where the operators $\mathcal{M}_{int}$, $\mathcal{M}_{ext}$, $\widehat{S}_\Sigma$, χ_Σ in (5.35) contain only information referring to Σ; for their definitions we refer to relations [AIM18, (3.30)-(3.33)].

Next, letting χ_Ω be the characteristic function of a subset $\Omega \subset \mathcal{V}$, we put

$$\widehat{u}^{(\pm)} = \chi_{\mathcal{V}_{int}^\circ}\widehat{u}_{int} + \chi_{\mathcal{V}_{ext}^\circ}\widehat{u}_{ext} + \chi_\Sigma\widehat{f}.$$

Noting that, as above, the operators $\chi_{\mathcal{V}_{int}^\circ}$ and $\chi_{\mathcal{V}_{ext}^\circ}$ contain only information referring to $\mathcal{V}_{int}^\circ$ and $\mathcal{V}_{ext}^\circ$, we define another operator, $\widehat{I}^{(\pm)}(\lambda) : \ell^2(\Sigma) \to \mathbf{h}_\lambda$, by (see [AIM18, (4.7)]),

$$\widehat{I}^{(\pm)}(\lambda)\widehat{f} := \mathcal{F}_0(\lambda)\mathcal{U}(\widehat{H}_0 - \lambda)\widehat{P}_{ext}\widehat{u}^{(\pm)};$$

the right-hand side of this relation shows that the action of $I^{(\pm)}(\lambda)$ depends neither on $\mathcal{V}_{int}$ nor on $\widehat{V}$, in other words, it is independent of the perturbation.

Here, an important role is played by a Rellich-type result, [AIM16, Theorem 5.1], and the following unique continuation property: if a solution of $(-\widehat{\Delta}_{\Gamma_0} - \lambda)\widehat{u} = 0$ on $\mathcal{V}_0$ vanishes except for a finite number of vertices for $\lambda \in \mathbb{C}$, then this solution vanishes identically on $\mathcal{V}_0$. This is what was assumed as [AIM16, (A-4)], [AIM18]. The said Rellich-type theorem, together with the unique continuation property in the exterior domain $\mathcal{V}_{ext}$ (which follows from the assumption (**D-4**)), implies the following claim, cf. [AIM18, Lemma 4.3].

LEMMA 5.5. — *Let $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \mathcal{T}_1 \cup \sigma_p(\widehat{H}) \cup \sigma(\widehat{H}_{int}))$. Then*

(1) *the map $\widehat{I}^{(\pm)}(\lambda) : \ell^2(\Sigma) \to \mathbf{h}_\lambda$ is injective,*
(2) *its adjoint $\widehat{I}^{(\pm)}(\lambda)^* : \mathbf{h}_\lambda \to \ell^2(\Sigma)$ is surjective.*

The scattering amplitude $A(\lambda)$ is defined by (5.30). In a similar way one can define the scattering amplitude in the exterior domain which we denote as $A_{ext}(\lambda)$. These scattering amplitudes satisfy the following relation, cf. [AIM18, Theorem 4.5].

THEOREM 5.6. — *Let $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \mathcal{T}_1 \cup \sigma_p(\widehat{H}) \cup \sigma(\widehat{H}_{int}))$. Then we have*

$$A_{ext}(\lambda) - A(\lambda) = \widehat{I}^{(+)}(\lambda)\Big(B_\Sigma^{(+)}(\lambda)\Big)^{-1}\widehat{I}^{(-)}(\lambda)^*. \tag{5.36}$$

By assumption, the exterior domain is free of perturbations, therefore $\Lambda_{ext}^{(\pm)}(\lambda)$ and $A_{ext}(\lambda)$ are known. By virtue of (5.29), (5.35) and Theorem 5.6, the S-matrix $S(\lambda)$ and the D-N map $\Lambda_{int}(\lambda)$ determine each other on some interval in the spectrum, and the same is true for the N-D map. Since the S-matrix, the D-N map and the N-D map are all complex analytic, this mutual determination extends from the said interval to the whole spectrum. Thus we arrive at the following claim.

THEOREM 5.7. — *For any $\lambda \in \sigma_e(\widehat{H}) \setminus (\mathcal{T}_0 \cup \mathcal{T}_1 \cup \sigma_p(\widehat{H}) \cup \sigma(\widehat{H}_{int}))$, the S-matrix $S(\lambda)$ and the D-N map $\Lambda_{int}(\lambda)$ determine each other.*

Let us remark that the definition of the normal derivative used in [AIM18] differs from the present one given by (3.7), adopted from [BILL23a], by a constant only. Hence the corresponding Neumann-to-Dirichlet maps determine each other.

Note further that the formula (5.36) is a discrete analogue of the one derived by Isakov and Nachman in [IN95] for the Schrödinger operator in $\mathbb{R}^n$. For the discrete problem, it provides us with a constructive route from the S-matrix to the corresponding D-N map.

5.4. The inverse scattering problem

The aim of this subsection is to show that the graph structure and the potential can be uniquely recovered from the knowledge of the scattering matrix at all energies for the discrete Schrödinger operator.

First of all, let us recall the definition of the Neumann-to-Dirichlet (N-D) map for a finite weighted graph with boundary, $\mathbb{G} = \{G, \partial G, E, \mu, g\}$. Let q be a real-valued potential function on G, and denote by $\{\lambda_k\}_{k=1}^N$ the Neumann eigenvalues, with the multiplicity taken into account, of the discrete Schrödinger operator $-\Delta_G + q$, where $N = \sharp G$. We consider the following equation:

$$\begin{cases} (-\Delta_G + q - \lambda)\, u(x) = 0, \quad x \in G,\ \lambda \in \mathbb{C}, \\ \partial_\nu u\big|_{\partial G} = f, \end{cases} \tag{5.37}$$

where the Neumann boundary value $\partial_\nu u$ was defined in (3.7). For $\lambda \notin \{\lambda_k\}_{k=1}^N$, denote by u_λ^f the unique solution of the equation (5.37) with the Neumann boundary value equal to f. The Neumann-to-Dirichlet map Λ_λ (at a fixed energy λ) for the equation (5.37) is defined as $\Lambda_\lambda : f \mapsto u_\lambda^f|_{\partial G}$.

LEMMA 5.8. — *Let $\mathbb{G}$ be a finite connected weighted graph with boundary satisfying the assumptions* (**C-1**) *and* (**C-2**) *in § 3. Suppose the weights*[4] *$\mu|_{\partial G}$, $g|_{\partial G \times G}$ are given. Then knowing the Neumann-to-Dirichlet map at all energies for the equation* (5.37) *on $\mathbb{G}$ is equivalent to the knowledge the Neumann boundary spectral data for the discrete Schrödinger operator on $\mathbb{G}$.*

[4] We abuse the notation here writing $g|_{\partial G \times G}$ to indicate the weights of the edges connecting the boundary vertices with the interior vertices.

Proof. — The proof for the manifold case can be found in [KKLM04] or [KKL01, § 4.1]. The proof in our case, for finite graphs, is simpler. Let $\{\phi_k\}_{k=1}^N$ be a family of orthonormalized Neumann eigenfunctions of the discrete Schrödinger operator corresponding to eigenvalues $\{\lambda_k\}$. Recall from [BILL23a] that the $L^2(G)$-inner product is defined by

$$\langle u_1, u_2 \rangle_{L^2(G)} = \sum_{x \in G} \mu_x u_1(x) \overline{u_2(x)}.$$

By Green's formula [BILL23a, Lemma 2.1], we infer that

$$\begin{aligned} \left\langle (-\Delta_G + q)\, u_\lambda^f, \phi_k \right\rangle_{L^2(G)} &= \left\langle u_\lambda^f, (-\Delta_G + q)\, \phi_k \right\rangle_{L^2(G)} - \sum_{z \in \partial G} \mu_z \phi_k(z) \left(\partial_\nu u_\lambda^f\right)(z) \\ &= \lambda_k \langle u_\lambda^f, \phi_k \rangle_{L^2(G)} - \sum_{z \in \partial G} \mu_z \phi_k(z) f(z), \end{aligned}$$

which yields

$$(\lambda - \lambda_k) \left\langle u_\lambda^f, \phi_k \right\rangle_{L^2(G)} = - \sum_{z \in \partial G} \mu_z \phi_k(z) f(z).$$

Now take an arbitrary real-valued function w^f on $G \cup \partial G$ satisfying $\partial_\nu w^f|_{\partial G} = f$. Then the difference $u_\lambda^f - w^f$ lies in the domain of the Neumann graph Laplacian and we have

$$\begin{aligned} u_\lambda^f - w^f &= \sum_{k=1}^N \left\langle u_\lambda^f - w^f, \phi_k \right\rangle_{L^2(G)} \phi_k \\ &= - \sum_{k=1}^N \frac{1}{\lambda - \lambda_k} \left(\sum_{z \in \partial G} \mu_z \phi_k(z) f(z) \right) \phi_k - \sum_{k=1}^N \left\langle w^f, \phi_k \right\rangle_{L^2(G)} \phi_k. \end{aligned} \tag{5.38}$$

This shows that Λ_λ is a meromorphic operator-valued function of λ with simple poles at $\lambda = \lambda_k$ only, and this in turn means that $\{\Lambda_\lambda\}$ determines the set of eigenvalues $\{\lambda_k\}$. Moreover, the residue of Λ_λ at $\lambda = \lambda_k$ is known as a finite-dimensional linear operator. In particular, since $\mu|_{\partial G}$ is known, the data $\{\Lambda_\lambda\}$ determine

$$Q_k(z_1, z_2) = \sum_{l \in L_k} \phi_l(z_1) \phi_l(z_2), \quad \forall\ z_1, z_2 \in \partial G,$$

where $L_k = \{p_k + 1, \cdots, p_k + \sharp L_k\}$, $p_k \in \mathbb{N}$, denotes the set of integers l satisfying $\lambda_l = \lambda_k$. This function $Q_k(\cdot, \cdot)$ can be viewed as an $m \times m$ matrix Q_k defined by $(Q_k)_{ij} = Q_k(z_i, z_j)$, where $m = \sharp \partial G$, or in the matrix form

$$Q_k = \left(\phi_{p_k+1}, \cdots, \phi_{p_k+\sharp L_k}\right)_{m \times \sharp L_k} \left(\phi_{p_k+1}, \cdots, \phi_{p_k+\sharp L_k}\right)_{m \times \sharp L_k}^T.$$

By [BILL23b, Lemma 2.4], the eigenfunctions $\{\phi_l|_{\partial G}\}_{l \in L_k}$ are linearly independent on ∂G, hence the rank of Q_k is simply $\sharp L_k$.

When the eigenvalue λ_k is simple, the matrix Q_k determines $\phi_k|_{\partial G}$ up to the sign. In general, since Q_k is symmetric and positive semi-definite, it can be decomposed into $Q_k = BB^T$, where B is an $m \times \sharp L_k$ matrix of rank $\sharp L_k$. Moreover, the decomposition is unique up to an $\sharp L_k \times \sharp L_k$ orthogonal matrix. Thus we take the column vectors of B, and they are the boundary values of orthonormalized eigenfunctions found by applying the orthogonal matrix to $\{\phi_l\}_{l \in L_k}$. This shows Q_k determines the boundary

values of the orthonormalized eigenfunctions (referring to the choice of $\{\phi_k\}_{k=1}^N$ we made).

To check the converse: the Neumann boundary spectral data determine the N-D map in accordance with the formula (5.38). We choose w^f such that $w^f|_G = 0$ and $\partial_\nu w^f|_{\partial G} = f$ so that the last term in (5.38) vanishes. Since $g|_{\partial G \times G}$ is known, thus $w^f|_{\partial G}$ is uniquely determined by f, and consequently, the N-D map can be determined from the Neumann boundary spectral data. □

Without loss of generality, we assume that the perturbed vertex set $\Omega = \Omega_{k_0}$ for some k_0 as assumed in part (**D-4**a), cf. § 5.1. With our choice (5.8) of the domains, Theorem 5.6 and Lemma 5.1 yield the following statement.

Corollary 5.9. — *Let Γ_0 be an infinite periodic lattice satisfying assumptions* (**D-1**)–(**D-4**). *Let q be a finitely supported potential on Γ, and $\mathbb{G}_\Gamma$ be the perturbed finite subgraph given by* (5.7). *Then the knowledge of the scattering matrix of the discrete Schrödinger operator on Γ at an arbitrarily fixed energy determines the Neumann-to-Dirichlet map of the equation* (5.37) *on $\mathbb{G}_\Gamma$ with $\mu = \deg_E$, $g \equiv 1$ for the same energy.*

Now we impose the following assumption on the locally perturbed lattice Γ.

(**E-1**) With the perturbed vertex set $\Omega = \Omega_{k_0}$ for some k_0 as in part (**D-4**a), the perturbed finite subgraph $\mathbb{G}_\Gamma$ given by (5.7) is connected and satisfies (**C-1**), (**C-2**).

The assumption (**E-1**), together with part (**D-4**b), implies the unique continuation from infinity for the perturbed system.

Lemma 5.10. — *Assume* (**E-1**)*and part* (**D-4**b) *are satisfied. Then the unique continuation from infinity holds for the perturbed equation $(-\widehat{\Delta}_\Gamma - \lambda)\widehat{u} = 0$ on Γ.*

Proof. — By assumption (**E-1**), the system is unperturbed outside of Ω_{k_0}. If $\widehat{u}$ vanishes near infinity, then $\widehat{u}$ vanishes on $\mathcal{V}_0 \setminus \Omega_{k_0}$ due to part (**D-4**b). Then the lemma follows from the same argument as Lemma 5.1. □

Our main result of this section is stated as follows.

Theorem 5.11. — *Consider a periodic lattice satisfying assumptions* (**D-1**)–(**D-4**), *and suppose that Γ is an infinite graph obtained by a local perturbation of this lattice. Let the potential q be finitely supported on Γ, and $\mathbb{G}_\Gamma$ be the perturbed finite subgraph given by* (5.7). *Assume that $\mathbb{G}_\Gamma$ satisfies* (**E-1**). *Then the topology of $\mathbb{G}_\Gamma$ can be uniquely recovered from the knowledge of the scattering matrix for the discrete Schrödinger operator on Γ for all energies. Furthermore, if we assume that $\mu_x = \deg x$ for all vertex v, we can determine the weight of the edge and the potential $q(x)$ from the scattering matrix for all energies.*

Proof. — From our construction of $\mathbb{G}_\Gamma$ in § 5.1, the edges connecting ∂G and G are known, and hence the weight $\mu = \deg_E$ on ∂G is known. The theorem then follows from Corollary 5.9 and Theorem 3.2. □

Example 5.12. — Finite square, hexagonal (see Figure 5.1), triangular, graphene and square ladder lattices all satisfy the Two-Points Condition (**C-2**) with the set

of boundary vertices being the domain boundary. Moreover, any horizontal edges in these lattices can be removed and the obtained graphs still satisfy the Two-Points Condition, see Figure 5.2; the term "horizontal edges" here refers to the edges in the non-gradient directions with respect to the function h in [BILL23a, Proposition 1.8].

6. Spectral theory for periodic quantum graph

In this and the next sections, we study the spectral theory for the Schrödinger operator on a quantum (metric) graph. Let $\Gamma_0 = \{\mathcal{L}_0, \mathcal{V}_0, \mathcal{E}_0\}$ be a periodic lattice introduced in § 5, and let assumptions (**D-1**)–(**D-4**) be imposed. As in § 5.1, we consider a local perturbation $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ of Γ_0. On each edge $e \in \mathcal{E}$, we are given a one-dimensional Schrödinger operator $h_e = -d^2/dz^2 + V_e(z)$ satisfying the δ-coupling condition (1.3) together with the assumptions (M-1)–(M-5) in § 2. We assume that $V_e(z)$ is equal to a fixed potential $V_0(z)$ except for a finite number of edges e. For the sake of (mainly notational) simplicity, we further assume that $V_0(z) = 0$ and $\ell_e = 1$ for all edges e. The arguments below also works for the general case by replacing $\phi^{(0)}_{e0}(z,\lambda)$, $\phi^{(0)}_{e1}(z,\lambda)$ and $\sigma^{(0)}(h^{(0)})$ by those associated with $V_0(z)$. Let $\widehat{H}_{\mathcal{E}}$ be the resulting self-adjoint operator in $L^2(\mathcal{E})$. In the unperturbed case, when $V_e = 0$ holds for each $e \in \mathcal{E}_0$ and C_v/d_v is equal to a fixed constant $\kappa_{\mathcal{V}}$, that is,

$$\frac{C_v}{d_v} = \kappa_{\mathcal{V}}, \quad \forall\, v \in \mathcal{V}_0, \tag{6.1}$$

the operator $\widehat{H}_{\mathcal{E}}$ shall be denoted by $\widehat{H}^{(0)}_{\mathcal{E}}$. In what follows, we call $\widehat{H}_{\mathcal{E}}$ the "edge" Schrödinger operator, and $-\widehat{\Delta}_{\mathcal{V},\lambda}$ the "vertex" Schrödinger operator.

6.1. Spectrum of $\widehat{H}_{\mathcal{E}}$

Let us begin with the unperturbed operator $\widehat{H}^{(0)}_{\mathcal{E}}$. Amending all the symbols introduced in § 2 with the superscript (0), we have $\phi^{(0)}_{e0}(z,\lambda) = \frac{\sin(\sqrt{\lambda}z)}{\sqrt{\lambda}}$ and $\phi^{(0)}_{e1}(z,\lambda) = \frac{\sin(\sqrt{\lambda}(1-z))}{\sqrt{\lambda}}$, hence

$$\big(\widehat{\Delta}^{(0)}_{\mathcal{V},\lambda}\widehat{u}\big)(v) = \frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}\frac{1}{d_v}\sum_{w\sim v}\widehat{u}(w) = \frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}\big(\widehat{\Delta}_{\mathcal{V}}\widehat{u}\big)(v), \tag{6.2}$$

with $\widehat{\Delta}_{\mathcal{V}}$ being the vertex Laplacian on $\mathcal{V}_0$, and

$$\widehat{Q}^{(0)}_{\mathcal{V},\lambda} = \frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}\cos\sqrt{\lambda} + \kappa_{\mathcal{V}}. \tag{6.3}$$

We put

$$E(\lambda) = -\cos\sqrt{\lambda} - \kappa_{\mathcal{V}}\frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}}, \tag{6.4}$$

and then the resolvent $R^{(0)}_{\mathcal{E}}(\lambda) = (H^{(0)}_{\mathcal{E}} - \lambda)^{-1}$ can be, in view of Lemma 2.3, rewritten as

$$R^{(0)}_{\mathcal{E}}(\lambda) = \left(\widehat{T}^{(0)}_{\mathcal{V},\overline{\lambda}}\right)^* \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}}\Big(- \widehat{\Delta}_{\mathcal{V}} - E(\lambda)\Big)^{-1} \widehat{T}^{(0)}_{\mathcal{V},\overline{\lambda}} + r^{(0)}_{\mathcal{E}}(\lambda). \tag{6.5}$$

Furthermore, we put

$$\sigma^{(0)}(h^{(0)}) = \left\{(\pi j)^2\,;\, j = 1, 2, \dots\right\}, \tag{6.6}$$

$$\sigma^{(0)}(-\widehat{\Delta}_{\mathcal{V}}) = \left\{\lambda\,;\, E(\lambda) \in \sigma\left(-\widehat{\Delta}_{\mathcal{V}}\right)\right\}, \tag{6.7}$$

$$\sigma^{(0)}_{\mathcal{T}} = \left\{\lambda \in \operatorname{Int}\left(\sigma_e\left(\widehat{H}^{(0)}_{\mathcal{E}}\right)\right)\,;\, E(\lambda) \in \mathcal{T}\right\}, \tag{6.8}$$

where $\operatorname{Int} I$ for a subset $I \subset \mathbb{R}$ means the interior of I, and

$$\mathcal{T} = \mathcal{T}_0 \cup \mathcal{T}_1. \tag{6.9}$$

Relation (6.5) allows us to write the spectrum in the following way:

LEMMA 6.1. — $\sigma(\widehat{H}^{(0)}_{\mathcal{E}}) = \sigma^{(0)}(-\widehat{\Delta}_{\mathcal{V}}) \cup \sigma^{(0)}(h^{(0)})$.

For example, in the Kirchhoff coupling case, $\kappa_{\mathcal{V}} = 0$, we have $\sigma(\widehat{H}^{(0)}_{\mathcal{E}}) = [0, \infty)$ for square and hexagonal lattices. Note that $\sigma^{(0)}(h^{(0)})$ is the set of eigenvalues of infinite multiplicities embedded in $\sigma(\widehat{H}^{(0)}_{\mathcal{E}})$.

6.2. Function spaces

For an edge $e \in \mathcal{E}_0$ with the endpoints $v, w \in \mathcal{V}_0$, we define

$$|e_c| = \frac{1}{2}|v + w|, \tag{6.10}$$

i.e. the distance of its midpoint from the origin, where for $x = (x_1, \dots, x_d) \in \mathcal{V}_0 \subset \mathbb{R}^d$ we denote $|x| = \sqrt{x_1^2 + \cdots + x_d^2}$. It will serve as a radius-like variable allowing to define the needed function spaces. Recall that our graph $\Gamma = (\mathcal{V}, \mathcal{E})$ is a local perturbation of a periodic lattice $\Gamma_0 = (\mathcal{L}_0, \mathcal{V}_0, \mathcal{E}_0)$, which means that Γ and Γ_0 coincide in the exterior domain

$$\mathcal{E}_{ext,R} \ni e \Longleftrightarrow |e_c| > R, \tag{6.11}$$

provided R is chosen sufficiently large; without loss of generality we may suppose that $R > 1$. The interior domain

$$\mathcal{E}_{int,R} = \mathcal{E} \setminus \mathcal{E}_{ext,R} \tag{6.12}$$

in which all the perturbations are located is finite and the "radius" plays no role there. Hence we keep the definition (6.10) in the exterior domain, and for the interior domain $\mathcal{E}_{int,R}$ we put instead

$$|e_c| = 1 \quad \text{if} \quad e \in \mathcal{E}_{int,R}. \tag{6.13}$$

With this proviso we introduce the function spaces on $\mathcal{E}$: we put $r_j = 2^j$ and define

$$\widehat{L}^{2,s}(\mathcal{E}) \ni \widehat{f} \Longleftrightarrow \sum_{e \in \mathcal{E}} |e_c|^{2s} \left\|\widehat{f}_e\right\|^2_{L^2(e)} < \infty, \tag{6.14}$$

$$\widehat{\mathcal{B}}(\mathcal{E}) \ni \widehat{f} \Longleftrightarrow \sum_{e\in\mathcal{E}} r_j^{1/2} \left(\sum_{r_{j-1}\leqslant |e_c|<r_j} \left\|\widehat{f}_e\right\|^2_{L^2(e)} \right)^{1/2} < \infty, \tag{6.15}$$

$$\widehat{\mathcal{B}}^*(\mathcal{E}) \ni \widehat{f} \Longleftrightarrow \sup_{R>1} \frac{1}{R} \sum_{|e_c|<R} \left\|\widehat{f}_e\right\|^2_{L^2(e)} < \infty, \tag{6.16}$$

equipped with their obvious norms. As the notation suggests, $\widehat{\mathcal{B}}^*(\mathcal{E})$ can be identified with the dual space of $\widehat{\mathcal{B}}(\mathcal{E})$, and the following inclusions hold for $s > 1/2$:

$$\widehat{L}^{2,s}(\mathcal{E}) \subset \widehat{\mathcal{B}}(\mathcal{E}) \subset \widehat{L}^{2,1/2}(\mathcal{E}) \subset \widehat{L}^2(\mathcal{E}) \subset \widehat{L}^{2,-1/2}(\mathcal{E}) \subset \widehat{\mathcal{B}}^*(\mathcal{E}) \subset \widehat{L}^{2,-s}(\mathcal{E}), \tag{6.17}$$

where $\widehat{L}^2(\mathcal{E}) = \widehat{L}^{2,0}(\mathcal{E})$. Moreover, $\widehat{\mathcal{B}}^*_0(\mathcal{E})$ is a closed subspace of $\widehat{\mathcal{B}}^*(\mathcal{E})$ defined by

$$\widehat{\mathcal{B}}^*_0(\mathcal{E}) \ni \widehat{f} \Longleftrightarrow \lim_{R\to\infty} \frac{1}{R} \sum_{|e_c|<R} \left\|\widehat{f}_e\right\|^2_{L^2(e)} = 0. \tag{6.18}$$

Let us further note that for the "vertex" Laplacian, the spaces $\widehat{L}^{2,s}(\mathcal{V})$, $\widehat{\mathcal{B}}(\mathcal{V})$, $\widehat{\mathcal{B}}^*(\mathcal{V})$, $\widehat{\mathcal{B}}^*_0(\mathcal{V})$ are defined in the same way as above with the norms $\|\widehat{f}_e\|_{L^2(e)}$ at the right-hand sides of (6.14)–(6.16) replaced by $|\widehat{f}(v)|$. This is one more manifestation of the parallelism between the discrete graph and the quantum graph. In the former, we consider $\mathbb{C}$-valued functions on the discrete set $\mathcal{V}$, while in the latter, we deal with $L^2((0,1))$-valued functions on the discrete set $\{e_c\,;\, e\in\mathcal{E}_{ext,R}\}$. This correspondence is inherited, in particular, in the resolvent estimates.

6.3. Rellich-type theorem

THEOREM 6.2. — *Let $\lambda \in (\operatorname{Int}\sigma_e(\widehat{H}^{(0)}_{\mathcal{E}})) \setminus \sigma^{(0)}_{\mathcal{T}}$, and suppose that $\widehat{u} \in \widehat{\mathcal{B}}^*_0(\mathcal{E})$ satisfies $\widehat{H}^{(0)}_{\mathcal{E}}\widehat{u} = \lambda\widehat{u}$ and the δ-coupling condition in $\mathcal{E}_{ext,R}$ for some $R > 1$. Then $\widehat{u} = 0$ holds in $\mathcal{E}_{ext,R_1}$ for some $R_1 \geqslant R$.*

Proof. — Since R is chosen large enough so that all the perturbations are inside of $\mathcal{E}_{int,R}$, on each edge $e \in \mathcal{E}_{ext,R}$, the solution $\widehat{u}$ can be written as

$$\widehat{u}_e(z) = \widehat{u}_e(1)\frac{\sin\sqrt{\lambda}z}{\sqrt{\lambda}} + \widehat{u}_e(0)\frac{\sin\sqrt{\lambda}(1-z)}{\sqrt{\lambda}}.$$

As the functions $\frac{\sin\sqrt{\lambda}(1-z)}{\sqrt{\lambda}}$ and $\frac{\sin\sqrt{\lambda}z}{\sqrt{\lambda}}$ are linearly independent for such a λ, there exists a constant $C_\lambda > 0$ such that

$$C_\lambda^{-1}\Big(|\widehat{u}_e(0)| + |\widehat{u}_e(1)|\Big) \leqslant \|\widehat{u}_e\|_{L^2(e)} \leqslant C_\lambda\Big(|\widehat{u}_e(0)| + |\widehat{u}_e(1)|\Big) \tag{6.19}$$

for all $e \in \mathcal{E}_{ext,R}$. We put $\widehat{w} = \widehat{u}\big|_{\mathcal{V}}$, then in view of Lemma 2.2, we have

$$\Big(-\widehat{\Delta}_{\mathcal{V}} - E(\lambda)\Big)\widehat{w} = 0, \quad \text{on} \quad \mathcal{V}\cap\mathcal{E}_{ext,R}.$$

Since $\widehat{u} \in \widehat{\mathcal{B}}^*_0(\mathcal{E})$ holds by assumption, the inequality (6.19) implies $\widehat{w} \in \widehat{\mathcal{B}}^*_0(\mathcal{V})$. By the Rellich-type theorem for vertex Schrödinger operators [AIM16, Theorem 5.1], we have $\widehat{w}(v) = 0$ for $|v| > R'$ with a sufficiently large R'. This proves the theorem. □

Definition 6.3. — *We say that the operator $\widehat{H}_{\mathcal{E}} - \lambda$ has the unique continuation property if the following assertion holds: If $\widehat{u}$ satisfies $(\widehat{H}_{\mathcal{E}} - \lambda)\widehat{u} = 0$ on $\mathcal{E}$, and $\widehat{u} = 0$ on $\mathcal{E}_{ext,R}$ for a positive R, then $\widehat{u} = 0$ holds on $\mathcal{E}$.*

For the unperturbed system, by assumption (**D-4**) in § 5 (essentially coinciding with (**C-2**) in § 3), $\widehat{H}_{\mathcal{E}}^{(0)} - \lambda$ has the unique continuation property for all λ. Adding a potential, it is also true for the unperturbed operator $\widehat{H}_{\mathcal{E}}$.

Lemma 6.4. — *Under the assumptions* (**D-1**)–(**D-4**)*, we have*

$$\sigma_p\left(\widehat{H}_{\mathcal{E}}^{(0)}\right) \cap \sigma_e\left(\widehat{H}_{\mathcal{E}}^{(0)}\right) \subset \sigma_{\mathcal{T}}^{(0)}.$$

Proof. — Any eigenvector of $\widehat{H}_{\mathcal{E}}$ is in $\widehat{L}^2(\mathcal{V}) \subset \widehat{\mathcal{B}}_0^*(\mathcal{E})$, and therefore it vanishes 'at infinity' by Theorem 6.2. By the unique continuation property, it vanishes everywhere. □

As can be checked easily, the square and hexagonal lattices satisfy the unique continuation property.

6.4. Radiation condition

For systems having $\mathbb{R}^d$ as the configuration space, the radiation condition is introduced either by observing the asymptotic behavior at infinity, or, what is equivalent, from the singularities of the Fourier image of solutions to the Schrödinger equation. Dealing with lattice Schrödinger operators, we adopt the latter approach.

Definition 6.5. — *Given a distribution $u \in \mathcal{D}'(\mathbb{T}^d)$, its wave front set $WF^*(u)$ is defined as follows: a point $(x_0, \omega) \in \mathbb{R}^d \times S^{d-1}$ does not belong to $WF^*(u)$ 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*

$$\lim_{R\to\infty} \frac{1}{R} \int_{|\xi|<R} \left|C_{\omega,\delta}(\xi)(\widetilde{\chi u})(\xi)\right|^2 d\xi = 0, \tag{6.20}$$

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

Let $\lambda_j(x)$, $j = 1, 2, \ldots, s$, be the eigenvalues of $H_0(x)$ and $P_j(x)$ the associated eigenprojections, and let H_0 be the operator of multiplication by $H_0(x)$ on $\left(L^2(\mathbb{T}^d)\right)^s$. In [AIM16, Lemma 4.7], it was proven that the operator

$$\mathcal{B}\left(\mathbb{T}^d\right) \ni f \to \frac{f(x)}{\lambda_j(x) - \rho \mp i0} \in \mathcal{B}^*\left(\mathbb{T}^d\right)$$

is bounded if $\rho \notin \left(\operatorname{Int}\sigma(H_0)\right) \setminus \mathcal{T}$. Furthermore in [AIM16, Theorem 6.1] it was shown that for any $f \in \mathcal{B}(\mathbb{T}^d)$, $1 \leqslant j \leqslant s$ and $\rho \in \sigma(H_0) \setminus \mathcal{T}$, it holds that

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

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

where $\omega_x \in S^{d-1} \cap T_x(M_{\lambda,j})^\perp$ and $\omega(x) \cdot \nabla\lambda_j(x) < 0$. Moreover, for any $f \in \mathcal{B}(\mathbb{T}^d)$, the function $u = (H_0(x) - \lambda \mp i0)^{-1} f \in \mathcal{B}^*(\mathbb{T}^d)$ is the unique solution to the equation $(H_0(x) - \rho)u = f$ satisfying $(RC)_+$ or $(RC)_-$, respectively. These claims also extend to the case with compactly supported perturbations.

We put

$$\operatorname{sgn}(\lambda) = \begin{cases} 1 & \text{for} \quad \lambda > 0, \quad \sin\sqrt{\lambda} > 0, \\ -1 & \text{for} \quad \lambda > 0, \quad \sin\sqrt{\lambda} < 0, \end{cases} \tag{6.21}$$

and then we can write

$$\cos\sqrt{\lambda \pm i0} = \cos\sqrt{\lambda} \mp i\, 0 \operatorname{sgn}(\lambda), \quad \lambda > 0. \tag{6.22}$$

We recall the discrete Fourier transform $\mathcal{U}_\mathcal{V}$ defined by (5.3). Let $\widehat{P}_{ext,R}$ be the orthogonal projection : $L^2(\mathcal{E}) \to L^2(\mathcal{E}_{ext,R})$. Taking (6.22) into account, we define the radiation condition as follows.

Definition 6.6. — *A solution $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ of the equation $(-\widehat{\Delta}_\mathcal{E} + V - \lambda)\widehat{u} = \widehat{f}$ is said to satisfy the* outgoing radiation condition *if either*

(i) $\sin\sqrt{\lambda} > 0$, *and* $w = \mathcal{U}\widehat{P}_{ext,R}\widehat{u}\|_\mathcal{V}$ *satisfies* $(RC)_+$ *with* $\rho = E(\lambda)$, *or*

(ii) $\sin\sqrt{\lambda} < 0$, *and* $u = \mathcal{U}\widehat{P}_{ext,R}\widehat{u}|_\mathcal{V}$ *satisfies* $(RC)_-$ *with* $\rho = E(\lambda)$, *holds. Similarly, we define the* incoming radiation condition *with* $(RC)_\pm$ *replaced by* $(RC)_\mp$. *If $\widehat{u}$ satisfies either the outgoing radiation condition or the incoming one, we simply say that $\widehat{u}$ satisfies the radiation condition.*

In [AIM16], the radiation condition was also introduced for the vertex Laplacian, see Lemmata 4.8 and 6.2 there. Let $\widehat{f} \in \mathcal{B}(\mathcal{E})$. Given a solution $\widehat{u}$ to the edge Schrödinger equation $(-\widehat{\Delta}_\mathcal{E} + V - \lambda)\widehat{u} = \widehat{f}$, denote by $\widehat{u}|_\mathcal{V}$ its restriction to $\mathcal{V}$. Then $\widehat{u}|_\mathcal{V}$ satisfies the vertex Schrödinger equation

$$\Big(- \widehat{\Delta}_\mathcal{V} - E(\lambda)\Big)\widehat{u} = \widehat{g}, \tag{6.23}$$

where $\widehat{g} \in \mathcal{B}(\mathcal{V})$. Comparing these two definitions of the radiation condition, one can prove the following lemma.

Lemma 6.7. — *A solution $\widehat{u}$ of the edge Schrödinger equation satisfies the radiation condition if and only if the solution $\widehat{u}|_\mathcal{V}$ of the vertex Schrödinger equation satisfies the radiation condition.*

Lemma 6.8. — *Let $\lambda \in (\operatorname{Int}\sigma_e(\widehat{H}_\mathcal{E})) \setminus \sigma_\mathcal{T}^{(0)}$. Then the solution $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ of the equation $(-\widehat{\Delta}_\mathcal{E} + V - \lambda)\widehat{u} = \widehat{f}$ satisfying the radiation condition is unique.*

Proof. — For the vertex Schrödinger operator, such a result was proven in [AIM16, Lemma 7.6]; in combination with Lemma 6.7, it yields the claim for the edge Schrödinger operator. □

6.5. Limiting absorption principle

Let us first investigate the existence of the limits $(-\widehat{\Delta}_{\mathcal{V},\lambda\pm i0}+\widehat{Q}_{\mathcal{V},\lambda\pm i0})^{-1}$.

LEMMA 6.9. — *If $E(\lambda)\in\sigma_e(-\widehat{\Delta}_{\mathcal{V}})\setminus\mathcal{T}$, there exists a limit*

$$\Big(-\widehat{\Delta}_{\mathcal{V},\lambda\pm i0}+\widehat{Q}_{\mathcal{V},\lambda\pm i0}\Big)^{-1}\in\mathbb{B}\Big(\mathcal{B}(\mathcal{V});\mathcal{B}(\mathcal{V})^*\Big).$$

Proof. — We use the limiting absorption principle for the vertex Schrödinger operator proved in [AIM16]. Taking into account (6.2) and (6.3), we define $\widehat{W}_{\mathcal{V},\lambda}$ by

$$-\widehat{\Delta}_{\mathcal{V},\lambda}+\widehat{Q}_{\mathcal{V},\lambda}=\frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}\left(-\widehat{\Delta}_{\mathcal{V}}-E(\lambda)+\widehat{W}_{\mathcal{V},\lambda}\right), \tag{6.24}$$

where $\widehat{W}_{\mathcal{V},\lambda}$ is a self-adjoint, bounded, and compactly supported perturbation of $-\widehat{\Delta}_{\mathcal{V}}$. Then, regarding $E(\lambda)$ as the energy for $-\widehat{\Delta}_{\mathcal{V}}$, and arguing in the same way as in [AIM16], we can prove the existence of the limit

$$\Big(-\widehat{\Delta}_{\mathcal{V}}+\widehat{W}_{\mathcal{V},\lambda}-E(\lambda\pm i0)\Big)^{-1}.$$

Using the identity

$$\begin{aligned}-\widehat{\Delta}_{\mathcal{V}}+\widehat{W}_{\mathcal{V},\lambda\pm i\epsilon}-E(\lambda\pm i\epsilon)&\\ =-\widehat{\Delta}_{\mathcal{V}}+\widehat{W}_{\mathcal{V},\lambda}-E(\lambda\pm i\epsilon)+\Big(\widehat{W}_{\mathcal{V},\lambda\pm i\epsilon}-W_{\mathcal{V},\lambda}\Big)&,\end{aligned} \tag{6.25}$$

together with the fact that $\widehat{W}_{\mathcal{V},\lambda\pm i\epsilon}-\widehat{W}_{\mathcal{V},\lambda}\to 0$ as $\epsilon\to 0$, we can construct the inverse of the right-hand side by the Neumann series. This proves the lemma. □

For $\lambda\notin\cup_{e\in\mathcal{E}}\sigma_p(-(d/dz)^2_D+V_e(z))$, where $-(d/dz)^2_D$ denotes $-(d/dz)^2$ in $L^2(e)$ with Dirichlet boundary condition, the functions $\phi_{e0}(z,\lambda)$ and $\phi_{e1}(z,\lambda)$ are linearly independent, hence by (2.15) there is a constant $C_\lambda>0$ such that

$$C_\lambda^{-1}\Big(|\widehat{g}(e(0))|+|\widehat{g}(e(1))|\Big)\leqslant\Big\|\Big(\widehat{T}_{\mathcal{V},\lambda}\Big)^*\,\widehat{g}_e\Big\|_{L^2(e)}\leqslant C_\lambda\Big(|\widehat{g}(e(0))|+|\widehat{g}(e(1))|\Big) \tag{6.26}$$

holds for all $e\in\mathcal{E}$. This implies

$$(\widehat{T}_{\mathcal{V},\lambda})^*\in\mathbb{B}\Big(\mathcal{B}(\mathcal{V})^*\,;\,\mathcal{B}^*(\mathcal{E})\Big), \tag{6.27}$$

and

$$\widehat{T}_{\mathcal{V},\lambda}\in\mathbb{B}\Big(\mathcal{B}(\mathcal{E})\,;\,\mathcal{B}(\mathcal{V})\Big). \tag{6.28}$$

Combining Lemma 2.3 with (6.27), (6.28), we arrive at the following result.

THEOREM 6.10. — *Let I be a compact interval in $(\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}}))\setminus\sigma^{(0)}_{\mathcal{T}}$.*

(1) *There exists a constant $C>0$ such that*

$$\Big\|\Big(\widehat{H}_{\mathcal{E}}-\lambda\mp i\epsilon\Big)^{-1}\Big\|_{\mathbb{B}\left(\widehat{\mathcal{B}}(\mathcal{E});\widehat{\mathcal{B}}^*(\mathcal{E})\right)}\leqslant C \tag{6.29}$$

holds for any $\lambda\in I$ and $\epsilon>0$.

(2) *For any $\lambda\in I$ and $s>1/2$, there exist strong limits*

$$\operatorname*{s-lim}_{\epsilon\downarrow 0}\Big(\widehat{H}_{\mathcal{E}}-\lambda\mp i\epsilon\Big)^{-1}=:\Big(\widehat{H}_{\mathcal{E}}-\lambda\mp i0\Big)^{-1}\in\mathbb{B}\left(\widehat{L}^{2,s}(\mathcal{E});\widehat{L}^{2,-s}(\mathcal{E})\right). \tag{6.30}$$

(3) *For any* $\widehat{f} \in \widehat{L}^{2,s}(\mathcal{E})$, $(\widehat{H}_{\mathcal{E}} - \lambda \mp i0)^{-1}\widehat{f}$ *is an* $\widehat{L}^{2,-s}(\mathcal{E})$*-valued strongly continuous function of* $\lambda \in I$.

(4) *For any* $\widehat{f}, \widehat{g} \in \widehat{\mathcal{B}}(\mathcal{E})$, *there exist limits*

$$\lim_{\epsilon \downarrow 0} \Big(\big(\widehat{H}_{\mathcal{E}} - \lambda \mp i\epsilon\big)^{-1} \widehat{f}, \widehat{g}\Big) =: \Big(\big(\widehat{H}_{\mathcal{E}} - \lambda \mp i0\big)^{-1} \widehat{f}, \widehat{g}\Big), \tag{6.31}$$

and $((\widehat{H}_{\mathcal{E}} - \lambda \mp i0)^{-1}\widehat{f}, \widehat{g})$ *is a continuous function of* $\lambda \in I$.

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

6.6. Spectral representation

As we have noted in the paragraph following eq. (5.2), there are unitary equivalences

$$\ell^2(\mathcal{V}_0) \cong \left(\ell^2\left(\mathbb{Z}^d\right)\right)^s \cong \left(L^2\left(\mathbb{T}^d\right)\right)^s,$$

by means of the decomposition (5.2) and the discrete Fourier transformation (5.3) with $\deg \mathcal{E}_0(x) = d_{\mathcal{V}_0}$. In the following, we freely make use of the identification

$$\ell^2(\mathcal{V}_0) \ni \big(\widehat{f}(v)\big)_{v \in \mathcal{V}_0} \longleftrightarrow \widehat{f}(n) = \big(\widehat{f}_1(n), \ldots, \widehat{f}_s(n)\big) \in \left(\ell^2\left(\mathbb{Z}^d\right)\right)^s \tag{6.32}$$

and we put[(5)]

$$\Phi^{(0)}(\lambda) = \mathcal{U}_{\mathcal{V}} \widehat{T}^{(0)}_{\mathcal{V},\lambda}, \tag{6.33}$$

where $\widehat{T}^{(0)}_{\mathcal{V},\lambda}$ is the unperturbed $\widehat{T}_{\mathcal{V},\lambda}$ defined by (2.13). Let $P_{\mathcal{V},j}(x)$ be the eigenprojection associated with the eigenvalue $\lambda_j(x)$ of $H_0(x)$, and denote

$$\begin{aligned} D^{(0)}(\lambda \pm i0) &= \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} \mathcal{U}_{\mathcal{V}} \left(-\widehat{\Delta}_{\mathcal{V}} - E(\lambda \pm i0)\right)^{-1} \mathcal{U}_{\mathcal{V}}^* \\ &= \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} \sum_{j=1}^{s} \frac{1}{\lambda_j(x) - E(\lambda \pm i0)} P_{\mathcal{V},j}(x). \end{aligned} \tag{6.34}$$

By (6.5), the following formula holds:

$$\widehat{R}^{(0)}_{\mathcal{E}}(\lambda \pm i0) = \Phi^{(0)}(\lambda)^* D^{(0)}(\lambda \pm i0) \Phi^{(0)}(\lambda) + r^{(0)}_{\mathcal{E}}(\lambda). \tag{6.35}$$

To construct a spectral representation of $\widehat{H}^{(0)}_{\mathcal{E}}$, we put

$$\begin{aligned} M_{\mathcal{E},\lambda,j} &= \left\{ x \in \mathbb{T}^d ;\, \lambda_j(x) - E(\lambda) = 0 \right\}, \\ (\varphi, \psi)_{\lambda,j} &= \int_{M_{\mathcal{E},\lambda,j}} P_{\mathcal{V},j}(x) \varphi(x) \cdot \overline{\psi(x)}\, dS_j, \\ dS_j &= \frac{|\sin\sqrt{\lambda}|}{\sqrt{\lambda}} \frac{dM_{\mathcal{E},\lambda,j}}{|\nabla_x \lambda_j(x)|}. \end{aligned} \tag{6.36}$$

[(5)] To be more precise, one should insert the operator of identification $J : \ell^2(\mathcal{V}_0) \to (\ell^2(\mathbb{Z}^d))^s$ defined by (6.32) in front of $\widehat{T}^{(0)}_{\mathcal{V},\lambda}$. We omit it, however, for the sake of simplicity.

Combining (6.35) with the formula

$$\left(\widehat{R}_{\mathcal{V}}^{(0)}\left(-\cos\sqrt{\lambda+i0}\right)\widehat{f}-\widehat{R}_{\mathcal{V}}^{(0)}\left(-\cos\sqrt{\lambda-i0}\right)\widehat{f},\widehat{g}\right) = 2\pi i\sum_j\int_{M_{\mathcal{E},\lambda,j}} P_{\mathcal{V},j}\widehat{f}\cdot\overline{P_{\mathcal{V},j}\widehat{g}}\,\frac{dM_{\mathcal{E},\lambda,j}}{|\nabla\lambda_j(x)|}, \tag{6.37}$$

valid for $\lambda\in(\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}}^{(0)}))\setminus\sigma_{\mathcal{T}}^{(0)}$, for which we refer to [AIM16, eq. (6.7)], we obtain the relation

$$\frac{1}{2\pi i}\Big(\big(\widehat{R}_{\mathcal{E}}^{(0)}(\lambda+i0)-\widehat{R}_{\mathcal{E}}^{(0)}(\lambda-i0)\big)\widehat{f},\widehat{g}\Big) = \sum_{j=1}^{s}\Big(P_{\mathcal{V},j}\Phi^{(0)}(\lambda)\widehat{f},P_{\mathcal{V},j}\Phi^{(0)}(\lambda)\widehat{g}\Big)_{\lambda,j}. \tag{6.38}$$

Furthermore, we put

$$\widehat{\mathcal{F}}_j^{(0)}(\lambda)\widehat{f}=\Big(P_{\mathcal{V},j}\Phi^{(0)}(\lambda)\widehat{f}\Big)\Big|_{M_{\mathcal{E},\lambda,j}}, \tag{6.39}$$

in other words, the restriction to $M_{\mathcal{E},\lambda,j}$ with the components

$$\begin{aligned}\widehat{\mathcal{F}}^{(0)}(\lambda)&=\Big(\widehat{\mathcal{F}}_1^{(0)}(\lambda),\cdots,\widehat{\mathcal{F}}_s^{(0)}(\lambda)\Big),\\ \mathbf{h}_\lambda&=\bigoplus_{j=1}^{s}P_{\mathcal{V},j}\Big|_{M_{\mathcal{E},\lambda,j}}L^2\Big(M_{\mathcal{E},\lambda,j};dS_j\Big),\\ \mathbb{H}&=L^2\Big((0,\infty),\mathbf{h}_\lambda;d\lambda\Big).\end{aligned} \tag{6.40}$$

Then, by virtue of (6.38) we can write

$$\frac{1}{2\pi i}\Big(\big(\widehat{R}_{\mathcal{E}}^{(0)}(\lambda+i0)-\widehat{R}_{\mathcal{E}}^{(0)}(\lambda-i0)\big)\widehat{f},\widehat{g}\Big)=\Big(\widehat{\mathcal{F}}^{(0)}(\lambda)\widehat{f},\widehat{\mathcal{F}}^{(0)}(\lambda)\widehat{g}\Big)_{\mathbf{h}_\lambda}.$$

Let $E^{(0)}(\lambda)$ be the spectral measure for $\widehat{H}_{\mathcal{E}}^{(0)}$. Integrating the last equality and using Stone's formula, we get

$$\Big(E^{(0)}(I)\widehat{f},\widehat{g}\Big)=\int_I\Big(\widehat{\mathcal{F}}^{(0)}(\lambda)\widehat{f},\widehat{\mathcal{F}}^{(0)}(\lambda)\widehat{g}\Big)_{\mathbf{h}_\lambda}d\lambda,$$

for any interval $I\subset(\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}}^{(0)}))\setminus\sigma_{\mathcal{T}}^{(0)}$. Hence $\widehat{\mathcal{F}}^{(0)}$ extends uniquely to an isometry from the subspace[(6)] $\mathcal{H}_{ac}(\widehat{H}_{\mathcal{E}}^{(0)})$ to $\mathbb{H}$. Moreover, we define

$$\widehat{\mathcal{F}}^{(0)}=0,\quad\text{on}\quad\mathcal{H}_p\left(\widehat{H}_{\mathcal{E}}^{(0)}\right).$$

As one can see from (6.39), to obtain $\widehat{\mathcal{F}}^{(0)}(\lambda)$ one has in fact to diagonalize the matrix $H_0(x)$.

The spectral representation for $\widehat{H}_{\mathcal{E}}$ is constructed by the perturbation method well known in the stationary scattering theory. For the case of perturbation by a potential, we make use of the resolvent equation

$$\widehat{R}_{\mathcal{E}}(\lambda\pm i0)=\widehat{R}_{\mathcal{E}}^{(0)}(\lambda\pm i0)\left(1-V_{\mathcal{E}}\widehat{R}_{\mathcal{E}}(\lambda\pm i0)\right). \tag{6.41}$$

(6) For a self-adjoint operator A, $\mathcal{H}_{ac}(A)$ denotes conventionally its absolutely continuous subspace, while $\mathcal{H}_p(A)$ is the closure of the linear hull of eigenvectors of A.

Then, defining $\widehat{\mathcal{F}}^{(\pm)}(\lambda)$ by

$$\widehat{\mathcal{F}}^{(\pm)}(\lambda) = \widehat{\mathcal{F}}^{(0)}(\lambda)\Big(1 - V_{\mathcal{E}}\widehat{R}_{\mathcal{E}}(\lambda \pm i0)\Big) \in \mathbb{B}\left(\widehat{\mathcal{B}}(\mathcal{E})\,;\, \mathbf{h}_\lambda\right), \tag{6.42}$$

and using the resolvent equation [AIM16, Lemma 7.8], we have

$$\frac{1}{2\pi i}\Big(\Big(\widehat{R}_{\mathcal{E}}(\lambda + i0) - \widehat{R}_{\mathcal{E}}(\lambda - i0)\Big)\widehat{f}, \widehat{g}\Big) = \Big(\widehat{\mathcal{F}}^{(\pm)}(\lambda)\widehat{f}, \widehat{\mathcal{F}}^{(\pm)}(\lambda)\widehat{g}\Big)_{\mathbf{h}_\lambda}.$$

We define an operator $\widehat{\mathcal{F}}^{(\pm)}$ by $(\widehat{\mathcal{F}}^{(\pm)}\widehat{f})(\lambda) = \widehat{\mathcal{F}}^{(\pm)}(\lambda)\widehat{f}$, and we also put

$$\widehat{\mathcal{F}}^{(\pm)} = 0, \quad \text{on} \quad \mathcal{H}_p(\widehat{H}_{\mathcal{E}}); \tag{6.43}$$

this yields the sought spectral representation of $\widehat{H}_{\mathcal{E}}$.

On the other hand, concerning the perturbation of the lattice structure, we take a cut-off function χ_0 whose support contains all the perturbation, and put $\chi_\infty = 1 - \chi_0$. In that case the equality

$$\chi_\infty \widehat{R}_{\mathcal{E}}(\lambda \pm i0) = \widehat{R}^{(0)}_{\mathcal{E}}(\lambda \pm i0)\Big(\chi_\infty + [H^{(0)}_{\mathcal{E}}, \chi_\infty]\widehat{R}_{\mathcal{E}}(\lambda \pm i0)\Big) \tag{6.44}$$

plays the role of the resolvent equation, and $\widehat{\mathcal{F}}^{(\pm)}(\lambda)$ is defined by

$$\widehat{\mathcal{F}}^{(\pm)}(\lambda) = \widehat{\mathcal{F}}^{(0)}(\lambda)\Big(\chi_\infty + \Big[H^{(0)}_{\mathcal{E}}, \chi_\infty\Big]\,\widehat{R}_{\mathcal{E}}(\lambda \pm i0)\Big). \tag{6.45}$$

Summarizing this discussion, we obtain the following result.

THEOREM 6.11. —

(1) *The operator $\widehat{\mathcal{F}}^{(\pm)}$ extends uniquely to a unitary operator from $\mathcal{H}_{ac}(\widehat{H}_{\mathcal{E}})$ to $\mathbb{H}$ annihilating the subspace $\mathcal{H}_p(\widehat{H}_{\mathcal{E}})$.*

(2) *The operator diagonalizes $\widehat{H}_{\mathcal{E}}$, namely*

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

(3) *The adjoint operator $\widehat{\mathcal{F}}^{(\pm)}(\lambda)^* \in \mathbb{B}(\mathbf{h}_\lambda; \mathcal{B}^*(\mathcal{E}))$ satisfies the eigenequation*

$$\Big(\widehat{H}_{\mathcal{E}} - \lambda\Big)\,\widehat{\mathcal{F}}^{(\pm)}(\lambda)^*\phi = 0, \quad \forall\, \phi \in \mathbf{h}_\lambda.$$

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

$$\widehat{f} = \int_{\sigma_{ac}(\widehat{H}_{\mathcal{E}})} \widehat{\mathcal{F}}^{(\pm)}(\lambda)^*\Big(\widehat{\mathcal{F}}^{(\pm)}\widehat{f}\Big)(\lambda)d\lambda.$$

We omit the proof, as it is almost the same as that of [AIM16, Theorem 7.11].

6.7. Resolvent expansion

We look at the behavior at infinity of $\widehat{R}_{\mathcal{E}}(\lambda \pm i0)\widehat{f}$ in the sense of $\widehat{\mathcal{B}}^*(\mathcal{E})$, which is equivalent to observing the singularities of its Fourier transform in the sense of $\mathcal{B}^*(\mathcal{E})$.

LEMMA 6.12. — *For any compact interval $I \subset (\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}}^{(0)})) \setminus \sigma_{\mathcal{T}}^{(0)}$, there exists a constant $C > 0$ such that*

$$\left\| \left\{ r_{\mathbf{e}}^{(0)}(\lambda) \widehat{f}_{\mathbf{e}} \right\}_{\mathbf{e} \in \mathcal{E}} \right\|_{\ell^2(\mathcal{E})} \leqslant C \left\| \widehat{f} \right\|_{\ell^2(\mathcal{E})}$$

holds for all $\lambda \in I$ and $\mathbf{e} \in \mathcal{E}$.

Proof. — Since I is in the resolvent set of $-(d/dz)_D^2 + V_{\mathbf{e}}$, the claim follows. □

For a pair $\widehat{f}, \widehat{g} \in \widehat{\mathcal{B}}^*(\mathcal{E})$, we consider the following equivalence relation

$$\widehat{f} \simeq \widehat{g} \Longleftrightarrow \widehat{f} - \widehat{g} \in \widehat{\mathcal{B}}_0^*(\mathcal{E}).$$

LEMMA 6.13. — *For any $\lambda \in (\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}}^{(0)})) \setminus \sigma_{\mathcal{T}}^{(0)}$ and $\widehat{f} \in \mathcal{B}(\mathcal{E})$, we have*

$$\mathcal{U}_{\mathcal{E}} \widehat{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \widehat{f} \simeq \frac{\sin\sqrt{\lambda}}{\lambda} \sum_{j=1}^{s} \frac{\widehat{\mathcal{F}}_j^{(0)}(\lambda) \widehat{f}}{\lambda_j(x) - E(\lambda \pm i0)}.$$

Proof. — Lemma 6.12 in combination with (6.35) implies

$$\begin{aligned} \widehat{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \widehat{f} &\simeq \Phi^{(0)}(\lambda)^* D^{(0)}(\lambda \pm i0) \Phi^{(0)}(\lambda) \widehat{f} \\ &= \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} \sum_{j=1}^{s} \frac{1}{\lambda_j(x) - E(\lambda \pm i0)} P_{\mathcal{V},j}(x) \left(\Phi^{(0)}(\lambda) \widehat{f} \right)(x). \end{aligned} \tag{6.46}$$

By virtue of [AIM16, eq. (4.34)], we have, for $g \in \mathcal{B}(\mathbb{T}^d)$, the equivalence

$$\frac{1}{\lambda_j(x) - \mu \mp i0} g(x) \simeq \frac{1}{\lambda_j(x) - \mu \mp i0} g \Big|_M,$$

where $M = \{x \in \mathbf{T}^d ;\, \lambda_j(x) = \mu\}$. This proves the claim. □

Next, we extend this lemma to the perturbed case.

THEOREM 6.14. — *For any $\lambda \in (\operatorname{Int}\sigma_e(\widehat{H}_{\mathcal{E}})) \setminus \sigma_{\mathcal{T}}^{(0)}$ and $\widehat{f} \in \mathcal{B}(\mathcal{E})$, we have*

$$\mathcal{U}_{\mathcal{E}} \chi_\infty \widehat{R}_{\mathcal{E}}(\lambda \pm i0) \widehat{f} \simeq \frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} \sum_{j=1}^{s} \frac{1}{\lambda_j(x) - E(\lambda \pm i0)} \widehat{\mathcal{F}}_j^{(\pm)}(\lambda) \widehat{f}.$$

Proof. — For the case of lattice structure perturbations, we use the resolvent equation (6.44). By Lemma 6.44, the left-hand side is, modulo $\mathcal{B}_0^*(\mathbb{T}^d)$, equal to

$$\frac{\sin\sqrt{\lambda}}{\sqrt{\lambda}} \sum_{j=1}^{s} \frac{1}{\lambda_j(x) - E(\lambda \pm i0)} \widehat{\mathcal{F}}_j^{(0)}(\lambda) \left(\chi_\infty + \left[H_{\mathcal{E}}^{(0)}, \chi_\infty \right] \widehat{R}_{\mathcal{E}}(\lambda \pm i0) \right) \widehat{f},$$

and thus the claim follows from (6.45). For the case of potential perturbations, we note that

$$\mathcal{U}_{\mathcal{E}} \chi_\infty \widehat{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \widehat{f} \simeq \mathcal{U}_{\mathcal{E}} \widehat{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \widehat{f},$$

since passing to the Fourier series, we see that $(1 - \chi_\infty) \widehat{R}_{\mathcal{E}}^{(0)}(\lambda \pm i0) \widehat{f}$ is a smooth function on the torus $\mathbb{T}^d$. Then, using (6.42) and the resolvent equation (6.41), we obtain the sought result. □

6.8. Helmholtz equation and S-matrix

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

THEOREM 6.15. —

(1) *For any solution* $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ *of the equation*

$$\left(\widehat{H}_{\mathcal{E}} - \lambda\right)\widehat{u} = 0,$$

there is an incoming datum and an outgoing datum $\phi^{in}, \phi^{out} \in \mathbf{h}_\lambda$ *satisfying*

$$\mathcal{U}_{\mathcal{E}}\chi_\infty\widehat{u} \simeq -\sum_{j=1}^{s} \frac{\phi_j^{in}}{\lambda_j(x) - E(\lambda - i0)} + \sum_{j=1}^{s} \frac{\phi_j^{out}}{\lambda_j(x) - E(\lambda + i0)}. \tag{6.47}$$

(2) *For any incoming datum* $\phi^{in} = (\phi_1^{in}, \dots, \phi_s^{in}) \in \mathbf{h}_\lambda$, *there exist a unique solution* $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ *of the equation*

$$\left(\widehat{H}_{\mathcal{E}} - \lambda\right)\widehat{u} = 0$$

and an outgoing datum $\phi^{out} = (\phi_1^{out}, \dots, \phi_s^{ou}) \in \mathbf{h}_\lambda$ *satisfying the relation* (6.47). *The operator* $S(\lambda)$ *defined by*

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

is unitary on $\mathbf{h}_\lambda$.

Proof. — Let $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ be a solution to $(\widehat{H}_{\mathcal{E}} - \lambda)\widehat{u} = 0$ and put $\widehat{u}|_{\mathcal{V}} = \widehat{w}$. Then, $\widehat{w} \in \widehat{\mathcal{B}}^*(\mathcal{V})$ and satisfies $(-\widehat{\Delta}_{\mathcal{V},\lambda} + \cos\sqrt{\lambda})\widehat{w} = 0$. By virtue of Theorem 5.4 (1), this $\widehat{w}$ admits an asymptotic expansion[(7)] (5.28). As $\widehat{u} = \widehat{T}^*_{\mathcal{V},\lambda}\widehat{w}$, the first claim follows.

The existence part of (2) can be proven by the same argument as above, reducing it to the case of the vertex operator. To prove the uniqueness, we take $\phi^{in} = 0$, and consider the solution $\widehat{u} \in \widehat{\mathcal{B}}^*(\mathcal{E})$ of the equation $(\widehat{H}_{\mathcal{E}} - \lambda)\widehat{u} = 0$ such that

$$\mathcal{U}_{\mathcal{E}}\chi_\infty\widehat{u} \simeq \sum_{j=1}^{s} \frac{\phi_j^{out}}{\lambda_j(x) - E(\lambda + i0)}. \tag{6.48}$$

Then $\widehat{u}$ satisfies the outgoing radiation condition, and by Lemma 6.8, such a solution vanishes identically. □

As this argument shows, the S-matrix for $\widehat{H}_{\mathcal{E}}$ at the energy λ coincides with the S-matrix for $-\widehat{\Delta}_{\mathcal{V},\lambda}$ at the energy $\frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}E(\lambda)$, and hence the unitarity follows. Stated more explicitly, we conclude:

COROLLARY 6.16. — *The S-matrix for* $\widehat{H}_{\mathcal{E}}$ *at the energy* λ *coincides with the S-matrix for* $-\widehat{\Delta}_{\mathcal{V},\lambda}$ *at the energy* $\dfrac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}E(\lambda) = -\sqrt{\lambda}\cot\sqrt{\lambda} - \kappa_{\mathcal{V}}$.

(7) Note that we have to replace $-\widehat{\Delta}_\Gamma$ by $-\widehat{\Delta}_{\mathcal{V},\lambda}$ and the energy parameter λ by $E(\lambda)$ in (5.28).

Remark 6.17. — By checking the above proof, one can see that all the arguments in this section remain valid in the situation when C_v/d_v is a fixed constant except for a finite number of vertices $v \in \mathcal{V}$. Moreover, one can deal in the same way with the case where the unperturbed operator $h_e^{(0)}$ has the same potential $V_0(z)$ at all the edges, that is, $h_e^{(0)} = -(d^2/dz^2)_D + V_0(z)$, $\forall\, e \in \mathcal{E}$.

7. Inverse scattering for quantum graph

THEOREM 7.1. — *For the Schrödinger operator $\widehat{H}_\mathcal{E}$ on a quantum graph of the considered class, the S-matrix $S(\lambda)$ for the scattering problem and the D-N map $\Lambda_\mathcal{E}(\lambda)$ for the interior boundary value problem determine each other.*

Proof. — By Corollary 6.16, knowing the S-matrix $S(\lambda)$ for $\widehat{H}_\mathcal{E}$ is equivalent to knowing the S-matrix for $-\widehat{\Delta}_{\mathcal{V},\lambda}$ at the energy $\frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}E(\lambda)$. By Theorem 5.6, this is equivalent to knowing the D-N map for $-\widehat{\Delta}_{\mathcal{V},\lambda}$ at the energy $\frac{\sqrt{\lambda}}{\sin\sqrt{\lambda}}E(\lambda)$. Finally by Lemma 3.1, this is equivalent to knowing the D-N map for $\widehat{H}_\mathcal{E}$ at the energy λ. □

We have now arrived at our next main theorem.

THEOREM 7.2. — *Let $\Gamma = \{\mathcal{V}, \mathcal{E}\}$ and $\Gamma' = \{\mathcal{V}', \mathcal{E}'\}$ be two infinite quantum graphs as in § 5 satisfying* (4.1), (4.2), *and* (**D-1**)–(**D-4**), *whose perturbed finite subgraphs satisfy* (**C-1**), (**C-2**). *Assume further that $\ell_\mathcal{E} = \ell_{\mathcal{E}'}, V_\mathcal{E}(z) = V_{\mathcal{E}'}(z)$, $k_\mathcal{V} = k_{\mathcal{V}'}$. Suppose that the S-matrices for the Schrödinger operator for the two quantum graphs coincide for all energies. Then there is a bijection $\Phi : \Gamma \to \Gamma'$ preserving the graph structure, and $d_v = d_{v'}$, $C_v = C'_{v'}$ hold for all $v \in \mathcal{V}$ and $v' = \Phi(v)$.*

Proof. — This is a direct consequence of Theorems 4.1 and 7.1. □

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