

Inverse Scattering on the Metric Graph for Graphene

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1 Introduction

We denote by $\Gamma = (\mathcal{V}, \mathcal{E})$ the graph, where \mathcal{V} is the vertex set and \mathcal{E} is the edge set, respectively. We assume that Γ is periodic. We omit the definition of the general periodic graph Γ , as we only treat the hexagonal lattice whose definition will be given later. We can regard the edge as a segment; for convenience sake, we identify $e \in \mathcal{E}$ as a closed interval $[0, 1]$:

$$e = \{(1-x)e(0) + xe(1); x \in [0, 1]\}, \quad e(0), e(1) \in \mathcal{V}, \quad (1)$$

which means that e can be regarded as a directed edge. The metric graph is the graph equipped with one-dimensional Schrödinger operator $-d^2/dx^2 + q_e(x)$ on each edge $e \in \mathcal{E}$ for a real-valued function $q_e(x) \in L^2(0, 1)$ with suitable boundary conditions on every vertices. We assume that $q_e(x)$ is symmetric on any $e \in \mathcal{E}$, i.e., $q_e(x) = q_e(1-x)$, and $q_e = 0$ except for a finite number of edges. If $q_e = 0$ for all edges, the Schrödinger operator is the metric Laplacian on \mathcal{E} . It is worth mentioning that the choice of direction of each edge does not affect the results.

Let $u = \{u_e\}_{e \in \mathcal{E}}$, where $u_e(x)$ is defined on e , $0 \leq x \leq 1$. We define the Hilbert space $L^2(\mathcal{E}) = \oplus_{e \in \mathcal{E}} L^2_e$, where $L^2_e = L^2(0, 1)$, equipped with the following inner product:

$$(u, v)_{L^2(\mathcal{E})} = \sum_{e \in \mathcal{E}} (u_e, v_e)_{L^2(0,1)} = \sum_{e \in \mathcal{E}} \int_0^1 u_e(x) \overline{v_e(x)} dx.$$

The Sobolev spaces $H^s(\mathcal{E})$ on \mathcal{E} , $s \in \mathbb{R}$, are defined in a similar way:

$$H^s(\mathcal{E}) = \oplus_{e \in \mathcal{E}} H^s_e,$$

where $H^s_e = H^s(0, 1)$.

For $u = \{u_e\}_{e \in \mathcal{E}}$, we define the normal derivative $\partial_e u(p)$ at the boundaries $p = e(0), e(1) \in \mathcal{V}$ as follows:

$$\partial_e u(p) = \begin{cases} u'_e(0), & \text{if } p = e(0), \\ -u'_e(1), & \text{if } p = e(1), \end{cases} \quad \text{where } u'_e = \frac{du_e}{dx}.$$

For $u = \{u_e\}_{e \in \mathcal{E}}$, the Kirchhoff condition is given as follows:

(K-1) u is continuous at any vertex $v \in \mathcal{V}$,

(K-2) $\sum_{e \in \mathcal{E}} \partial_e u(v) = 0$ at any vertex $v \in \mathcal{V}$.

The Kirchhoff Laplacian $H_{\mathcal{E}}^{(0)}$ is a metric Laplacian which satisfies the Kirhhoff condition:

$$H_{\mathcal{E}}^{(0)} u = \{-u''_e\}_{e \in \mathcal{E}}, \quad \text{where } u''_e = \frac{d^2}{dx^2} u_e,$$

$$\text{Dom}(H_{\mathcal{E}}^{(0)}) = \{u \in H^2(\mathcal{E}); u \text{ satisfies (K-1) and (K-2)}\}.$$

It is easy to see that $H_{\mathcal{E}}^{(0)}$ is self-adjoint on $L^2(\mathcal{E})$.

For the Kirchhoff Schrödinger operator on the metric graph, we impose the following assumption on the potential $q = \{q_e\}_{e \in \mathcal{E}}$:

(Q-1) $q_e \in L^2(0, 1)$ is real-valued for every $e \in \mathcal{E}$,

(Q-2) $q_e = 0$ except for a finite number of edges in \mathcal{E} ,

(Q-3) q_e is symmetric, i.e., $q_e(1-x) = q_e(x)$ for every $e \in \mathcal{E}$.

Then the Kirhhoff Schrödinger operator $H_{\mathcal{E}}$ is defined as follows:

$$H_{\mathcal{E}} u = \{-u''_e + q_e u_e\}_{e \in \mathcal{E}} \quad \text{with } \text{Dom}(H_{\mathcal{E}}) = \text{Dom}(H_{\mathcal{E}}^{(0)}),$$

where $q = \{q_e\}_{e \in \mathcal{E}}$ satisfies (Q-1), (Q-2) and (Q-3). One can easily see that $H_{\mathcal{E}}$ is self-adjoint on $L^2(\mathcal{E})$; moreover, $\sigma_{ac}(H_{\mathcal{E}}) = \sigma_{ac}(H_{\mathcal{E}}^{(0)})$ (see [3]).

2 Schrödinger Operators on the Hexagonal Metric Graph

2.1 Hexagonal Lattice

From now on, we consider the hexagonal lattice $\Gamma = (\mathcal{V}, \mathcal{E})$ which is a two dimensional periodic graph. Let us define \mathcal{V} and \mathcal{E} as follows.

Take points $p^{(1)} = (1, 0)$ and $p^{(2)} = (2, 0)$, and the vectors $\mathbf{v}_1 = (3/2, -\sqrt{3}/2)$ and $\mathbf{v}_2 = (3/2, \sqrt{3}/2)$. Put $\mathbf{v}(n) = n_1 \mathbf{v}_1 + n_2 \mathbf{v}_2$, where $n = (n_1, n_2) \in \mathbb{Z}^2$. Then the vertex set \mathcal{V} of the hexagonal lattice is defined by

$$\mathcal{V} = \mathcal{V}_1 \cup \mathcal{V}_2, \quad \mathcal{V}_j = \{p^{(j)} + \mathbf{v}(n); n \in \mathbb{Z}^2\}, \quad j = 1, 2.$$

Take the edges $e_j = (e_j(0), e_j(1))$, $j = 1, 2, 3$, as follows:

$$\mathbf{e}_1 = (p^{(2)}, (5/2, -\sqrt{3}/2)), \quad \mathbf{e}_2 = (p^{(2)}, (5/2, \sqrt{3}/2)), \quad \mathbf{e}_3 = (p^{(1)}, p^{(2)}).$$

Put $e_j + [n] = (e_j(0) + \mathbf{v}(n), e_j(1) + \mathbf{v}(n))$, $j = 1, 2, 3$. The edge set \mathcal{E} of the hexagonal lattice is defined by

$$\mathcal{E} = \mathcal{E}_1 \cup \mathcal{E}_2 \cup \mathcal{E}_3, \quad \mathcal{E}_j = \{e_j + [n]; n \in \mathbb{Z}^2\}, \quad j = 1, 2, 3.$$

The fundamental domain \mathbf{F}_{Γ} of the hexagonal lattice is defined by

$$\mathbf{F}_{\Gamma} = \{y_1 \mathbf{v}_1 + y_2 \mathbf{v}_2; y_1, y_2 \in [0, 1)\},$$

which is shown as the gray area in Fig.1 of the hexagonal lattice.

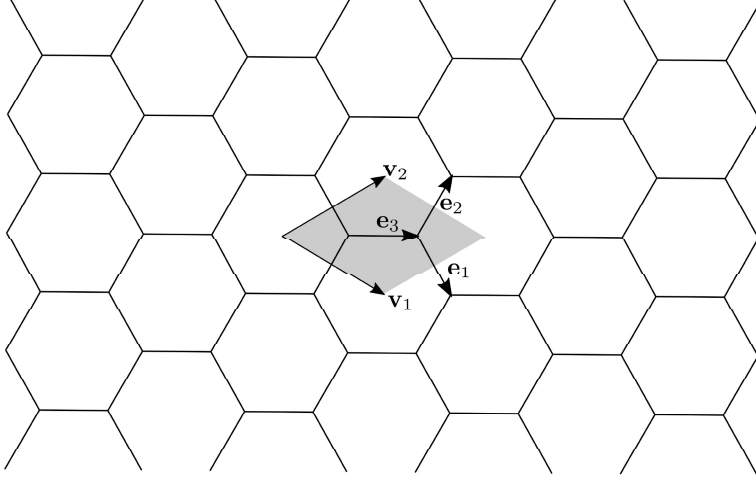


Figure 1: The hexagonal lattice and its fundamental domain

2.2 Fourier Transform

Denote the flat torus by $\mathbb{T}^2 = \mathbb{R}^2/2\pi\mathbb{Z}^2$. We define the fundamental graph $\Gamma_* = (\mathcal{V}_*, \mathcal{E}_*)$ of the hexagonal lattice Γ , whose vertex set is $\mathcal{V}_* = \{p_*^{(1)}, p_*^{(2)}\}$ and the edge set is $\mathcal{E}_* = \{e_{1*}, e_{2*}, e_{3*}\}$, see Fig.2.

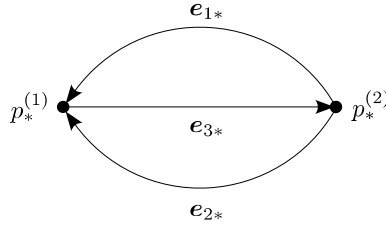


Figure 2: The fundamental graph of the hexagonal lattice

We define the unitary operator $\mathcal{U}_{\mathcal{E}} = (\mathcal{U}_{\mathcal{E},1}, \mathcal{U}_{\mathcal{E},2}, \mathcal{U}_{\mathcal{E},3}) : L^2(\mathcal{E}) \rightarrow L^2(\mathbb{T}^2 \times \mathcal{E}_*)$ as follows: for $f = \{f_e\}_{e \in \mathcal{E}} = \cup_{j=1}^3 \{f_{e_j+[n]}\}_{n \in \mathbb{Z}^2}$,

$$(\mathcal{U}_{\mathcal{E},j}f)(\xi, x) = \frac{1}{2\pi} \sum_{n \in \mathbb{Z}^2} e^{-in \cdot \xi} f_{e_j+[n]}(x), \quad (\xi, x) \in \mathbb{T}^2 \times [0, 1].$$

The adjoint operator of $\mathcal{U}_{\mathcal{E},j}^*$ is

$$(\mathcal{U}_{\mathcal{E},j}^*g)_{e_j+[n]}(x) = \frac{1}{2\pi} \int_{\mathbb{T}^2} e^{in \cdot \xi} g(\xi, x) d\xi$$

for the function g on $\mathbb{T}^2 \times [0, 1]$.

Let us define the index of the edges as follows:

$$\text{Ind}(\mathbf{e}) = \begin{cases} (1, 0), & \text{if } \mathbf{e} = \mathbf{e}_{1*}, \\ (0, 1), & \text{if } \mathbf{e} = \mathbf{e}_{2*}, \\ (0, 0), & \text{if } \mathbf{e} = \mathbf{e}_{3*}. \end{cases}$$

We also define

$$\delta_j(v) = \begin{cases} 1, & \text{if } v = \mathbf{e}_{j*}(1), \\ 0, & \text{if } v = \mathbf{e}_{j*}(0). \end{cases}$$

Put $\hat{H}_{\mathcal{E}_*}^{(0)} = \mathcal{U}_{\mathcal{E}} H_{\mathcal{E}}^{(0)} \mathcal{U}_{\mathcal{E}}^*$ with domain $\text{Dom}(\hat{H}_{\mathcal{E}_*}^{(0)}) = \mathcal{U}_{\mathcal{E}} \text{Dom}(H_{\mathcal{E}}^{(0)})$ on $L^2(\mathbb{T}^2 \times \mathcal{E}_*)$. By the Floquet-Bloch theory, $\hat{H}_{\mathcal{E}_*}^{(0)}$ has the direct integral decomposition (cf. [3]):

$$\hat{H}_{\mathcal{E}_*}^{(0)} = \int_{\mathbb{T}^2}^{\oplus} \hat{H}_{\mathcal{E}_*}^{(0)}(\xi) d\xi,$$

where for $\hat{u} = \mathcal{U}_{\mathcal{E}} u = \{\hat{u}_{\mathbf{e}_{j*}}(\xi, x)\}_{j=1}^3$, $(\xi, x) \in \mathbb{T}^2 \times [0, 1]$,

$$(\hat{H}_{\mathcal{E}_*}^{(0)} \hat{u})_{\mathbf{e}_{j*}}(\xi, x) = -\hat{u}_{\mathbf{e}_{j*}}''(\xi, x), \quad \hat{u}_{\mathbf{e}_{j*}}'' = \frac{\partial^2 \hat{u}_{\mathbf{e}_{j*}}}{\partial x^2}(\xi, x).$$

For $\hat{u} = \{\hat{u}_{\mathbf{e}_{j*}}(\xi, x)\}_{j=1}^3$, the Kirchhoff condition (K-1) and (K-2) are transferred as

$$e^{-i\delta_j v \text{Ind}(\mathbf{e}_{j*}) \cdot \xi} \hat{u}_{\mathbf{e}_{j*}}(\xi, \delta_j(v)) = e^{-i\delta_k(v) \text{Ind}(\mathbf{e}_{k*}) \cdot \xi} \hat{u}_{\mathbf{e}_{k*}}(\xi, \delta_k(v)),$$

for a common end point $v \in \mathcal{V}_*$ of \mathbf{e}_{j*} and \mathbf{e}_{k*} , and

$$\sum_{j=1}^3 (-1)^{\delta_j(v)} e^{-i\delta_j(v) \text{Ind}(\mathbf{e}_{j*}) \cdot \xi} \hat{u}_{\mathbf{e}_{j*}}'(\xi, \delta_j(v)) = 0, \quad \hat{u}_{\mathbf{e}_{j*}}'(\xi, x) = \frac{\partial \hat{u}_{\mathbf{e}_{j*}}}{\partial x}(x, x),$$

for $v \in \mathcal{V}_*$.

2.3 Spectrum of Metric Laplacian

Let us define the twisted discrete Laplacian $\Delta_{\mathcal{V}_*}(\xi)$ on \mathcal{V}_* as follows:

$$(\Delta_{\mathcal{V}_*}(\xi)\psi)(v) = \frac{1}{3} \sum_{(v, v') \in \mathcal{E}_*} e^{-i(-1)^{\delta_j(v')} \text{Ind}(\mathbf{e}_{j*}) \cdot \xi} \psi(v'), \quad \psi \in \ell^2(\mathcal{V}_*).$$

The eigenvalue problem of $\hat{H}_{\mathcal{E}_*}^{(0)}$ is closely related to that of $-\Delta_{\mathcal{V}_*}(\xi)$ on $\ell^2(\mathcal{V}_*)$. The equation $-\Delta_{\mathcal{V}_*}(\xi)\psi = \mu(\xi)\psi$ holds if and only if

$$\begin{bmatrix} -\mu(\xi) & -p(\xi) \\ -p(\xi) & -\mu(\xi) \end{bmatrix} \begin{bmatrix} \psi(p_*^{(1)}) \\ \psi(p_*^{(2)}) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

where for $\xi = (\xi_1, \xi_2) \in \mathbb{T}^2$,

$$p(\xi) = \frac{1}{3} (1 + e^{-i\xi_1} + e^{i\xi_2}).$$

Then we have

$$\sigma(-\Delta_{\mathcal{V}_*}(\xi)) = \{\pm |p(\xi)|\}.$$

Here we note that

$$|p(\xi)| = \frac{1}{3} \sqrt{3 + 2 \cos \xi_1 + 2 \cos \xi_2 + 2 \cos (\xi_1 - \xi_2)} \in [0, 1].$$

Put $\mu_1(\xi) = -|p(\xi)|$ and $\mu_2(\xi) = |p(\xi)|$. The corresponding normalized eigenfunctions are

$$a_k(\xi) = \frac{1}{\sqrt{2}|p(\xi)|} \begin{bmatrix} (-1)^{k-1} p(\xi) \\ |p(\xi)| \end{bmatrix}, \quad k = 1, 2.$$

The spectrum of $H_{\mathcal{E}_*^{(0)}}(\xi)$ is well-known (cf. [3], [4]). Define

$$z_{j,k}(\xi) = \begin{cases} z_k(\xi) + \pi j, & \text{if } j \text{ is even,} \\ (\pi - z_k(\xi)) + \pi j, & \text{if } j \text{ is odd,} \end{cases}$$

where

$$z_k(\xi) = \arccos(-\mu_k(\xi)) \in [0, \pi], \quad k = 1, 2.$$

Then, we have

$$\begin{aligned} \hat{H}_{\mathcal{E}_*^{(0)}}(\xi) &= \hat{H}_{\mathcal{E}_*^{(0)}}^D(\xi) \oplus \hat{H}_{\mathcal{E}_*^{(0)}}^V(\xi), \\ \hat{H}_{\mathcal{E}_*^{(0)}}^D(\xi) &= \sum_{j \geq 0} (\pi j)^2 \hat{P}_j^D(\xi), \quad \hat{H}_{\mathcal{E}_*^{(0)}}^V(\xi) = \sum_{j \geq 0, k \in \{1,2\}} z_{j,k}(\xi)^2 \hat{P}_{j,k}^V(\xi), \end{aligned}$$

where $\hat{P}_{j,k}^D(\xi)$ and $\hat{P}_{j,k}^V(\xi)$ are projections to eigenvalues $(\pi j)^2$ and $z_{j,k}(\xi)^2$. Therefore, we have

$$\sigma_{\text{ac}}(H_{\mathcal{E}}^{(0)}) = \sigma_{\text{ac}}(H_{\mathcal{E}}) = \cup_{j \geq 0, k \in \{1,2\}} [\lambda_{j,k}^-, \lambda_{j,k}^+] = \cup [0, \infty),$$

where

$$\lambda_{j,k}^{\pm} = \begin{cases} (z_k^{\pm} + \pi j)^2, & \text{if } j \text{ is even,} \\ (\pi - z_k^{\mp} + \pi j)^2, & \text{if } j \text{ is odd.} \end{cases}$$

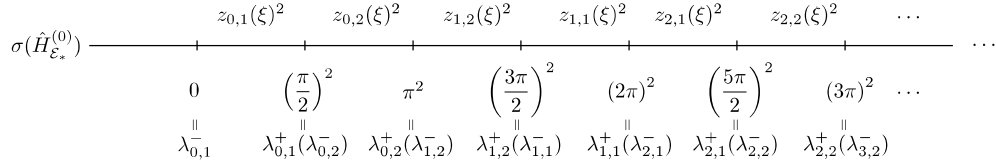
Moreover, we have the eigenvalues of infinite multiplicities:

$$\sigma_{\text{fb}}(H_{\mathcal{E}}^{(0)}) = \left\{ (\pi j)^2; j = 1, 2, \dots \right\}.$$

The spectrum of $H_{\mathcal{E}}^{(0)}$ is shown in Fig.3.

For $\lambda_{j,k}^- < \lambda < \lambda_{j,k}^+$, it holds that $0 < (\cos \sqrt{\lambda})^2 < 1$. We define the Fermi surface

$$M(\cos \sqrt{\lambda}) = \left\{ \xi \in \mathbb{T}^2; |p(\xi)|^2 = (\cos \sqrt{\lambda})^2 \right\},$$

Figure 3: The spectrum of $H_{\mathcal{E}}^{(0)}$.

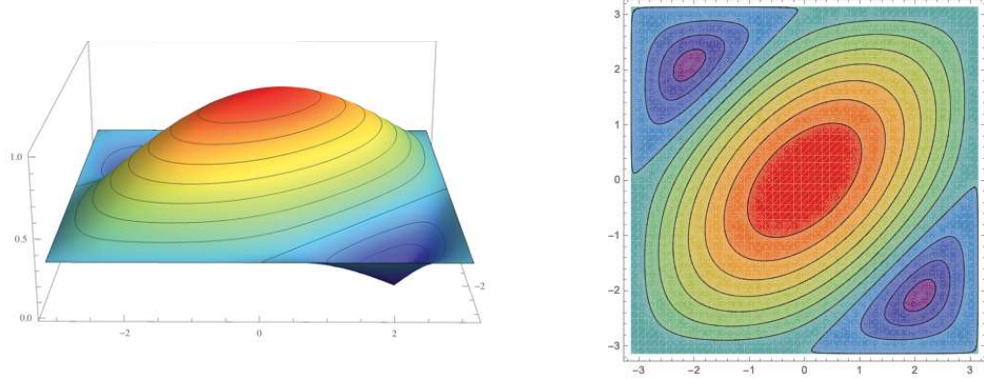
and

$$M_k(\cos \sqrt{\lambda}) = \left\{ \xi \in \mathbb{T}^2; \mu_k(\xi) = \cos \sqrt{\lambda} \right\}, \quad k = 1, 2.$$

Let $\mathcal{T}^{(0)} = \sigma_{\text{fb}}(H_{\mathcal{E}}^{(0)}) \cup \left\{ \lambda > 0; \cos \sqrt{\lambda} = 0, \pm 1/3 \right\}$. Then,

$$\nabla_{\xi} (|p(\xi)|) = \frac{1}{9} \begin{bmatrix} -\sin \xi_1 - \sin(\xi_1 - \xi_2) \\ -\sin \xi_2 + \sin(\xi_1 - \xi_2) \end{bmatrix} \neq 0$$

for $\xi = (\xi_1, \xi_2) \in M(\cos \sqrt{\lambda})$. Therefore, for $\lambda \in [\lambda_{j,k}^-, \lambda_{j,k}^+] \setminus \mathcal{T}^{(0)}$, $M(\cos \sqrt{\lambda})$ is one dimensional real analytic submanifold of \mathbb{T}^2 . See Fig.4.

Figure 4: The Fermi surface $M(\cos \sqrt{\lambda})$ is the level set of $|p(\xi)|^2$.

3 Scattering Theory

We define the weighted L^2 -norm on \mathcal{E} for $f = \cup_{j=1}^3 \{f_{\mathbf{e}_j+[n]}\}_{n \in \mathbb{Z}^2}$:

$$\|f\|_{L^{2,s}(\mathcal{E})}^2 = \sum_{l=1}^3 \sum_{n \in \mathbb{Z}^2} (1 + |n|)^s \|f_{\mathbf{e}_l+[n]}\|_{L^2(0,1)}^2, \quad s \in \mathbb{R}.$$

Then the weighted L^2 -space is

$$L^{2,s}(\mathcal{E}) = \left\{ f = \cup_{j=1}^3 \{f_{\mathbf{e}_j+[n]}\}_{n \in \mathbb{Z}^2}; \|f\|_{L^{2,s}(\mathcal{E})} < \infty \right\}.$$

We also define the Agmon-Hörmander spaces $\mathcal{B}(\mathcal{E})$ and $\mathcal{B}^*(\mathcal{E})$ by the following norms:

$$\|f\|_{\mathcal{B}(\mathcal{E})} = \sum_{l=1}^3 \sum_{j=0}^{\infty} r_j^{1/2} \left(\sum_{r_{j-1} \leq |n| < r_j} \|f_{e_l+[n]}\|_{L^2(0,1)}^2 \right)^{1/2}, \quad r_{-1} = 0, r_j = 2^j, j \geq 1,$$

$$\|u\|_{\mathcal{B}^*(\mathcal{E})}^2 = \sup_{\rho > 1} \frac{1}{\rho} \sum_{l=1}^3 \sum_{|n| < \rho} \|u_{e_l+[n]}\|_{L^2(0,1)}^2.$$

We note that for $s > 1/2$,

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

We define $\mathcal{B}_0^*(\mathcal{E})$ by the totality of $u \in \mathcal{B}^*(\mathcal{E})$ such that

$$\lim_{\rho \rightarrow \infty} \frac{1}{\rho} \sum_{l=1}^3 \sum_{|n| < \rho} \|u_{e_l+[n]}\|_{L^2(0,1)}^2 = 0.$$

The corresponding function spaces on $\mathbb{T}^2 \times \mathcal{E}^*$ is defined by passing them to $\mathcal{U}_{\mathcal{E}}$.

Let $R_{\mathcal{E}}^{(0)}(\kappa) = (H_{\mathcal{E}}^{(0)} - \kappa)^{-1}$ for $\kappa \in \mathbb{C} \setminus [0, \infty)$. Then the weak* limits $R_{\mathcal{E}}^{(0)}(\lambda \pm i0) = \lim_{\epsilon \downarrow 0} R_{\mathcal{E}}^{(0)}(\lambda \pm i\epsilon)$ exists in $\mathcal{B}(\mathcal{B}(\mathcal{E}), \mathcal{B}^*(\mathcal{E}))$ for $\lambda \in (0, \infty) \setminus \mathcal{T}^{(0)}$. $u_{\pm}^{(0)} = R_{\mathcal{E}}^{(0)}(\lambda \pm i0)f$ is said to be outgoing (+) and incoming (-) in view of the singularity expansion on the Fermi surface (cf. [1]).

Let $h_e = -d^2/dx^2 + q_e$ with the Dirichlet boundary condition at $e(0)$ and $e(1)$ for $e \in \mathcal{E}$. Put $\mathcal{T} = \mathcal{T}^{(0)} \cup (\cup_{e \in \mathcal{E}} \sigma(h_e))$.

Let $R_{\mathcal{E}}(\kappa) = (H_{\mathcal{E}} - \kappa)^{-1}$ for $\kappa \in \mathbb{C} \setminus \mathbf{R}$. By the resolvent equation, we have $R_{\mathcal{E}}(\kappa) = R_{\mathcal{E}}^{(0)}(\kappa)(1 - qR_{\mathcal{E}}^{(0)}(\kappa))$. We put $Q_{\mathcal{E}}(\kappa) = 1 - qR_{\mathcal{E}}(\kappa)$. Then the limiting absorption principle holds, i.e., $R_{\mathcal{E}}(\lambda \pm i0) \in \mathcal{B}(\mathcal{B}(\mathcal{E}), \mathcal{B}^*(\mathcal{E}))$ for $\lambda \in (0, \infty) \setminus \mathcal{T}$. We also call $u_{\pm} = R_{\mathcal{E}}^{(0)}(\lambda \pm i0)f$ outgoing (+) and incoming (-).

Then we can prove the following theorem. For the proof, see [2].

Theorem 3.1 (Rellich Type Theorem) *Let $\lambda \in (0, \infty) \setminus \mathcal{T}$. Suppose that $u \in \mathcal{B}(\mathcal{E})$ satisfies $(H_{\mathcal{E}} - \lambda)u = 0$ and u is outgoing (or incoming). Then $u = 0$.*

3.1 Scattering Amplitude

We define the Hilbert spaces $\mathbf{h}_k(\lambda)$, $k = 1, 2$:

$$\mathbf{h}_k = \begin{cases} L^2(M_k(\cos \sqrt{\lambda}) \times \mathcal{E}_*), & \text{if } \lambda \in (\lambda_{j,k}^-, \lambda_{j,k}^+), j \geq 0, \\ \{0\}, & \text{otherwise.} \end{cases}$$

We put $\mathbf{h}(\lambda) = \mathbf{h}_1(\lambda)a_1(\xi) \oplus \mathbf{h}_2(\lambda)a_2(\xi)$, where $a_k(\xi)$, $k = 1, 2$, are the normalized eigenfunctions of the twisted Laplacian $-\Delta_{\mathcal{V}_*}(\xi)$. The distorted Fourier

transformation $\mathcal{F}^{(0)}(\lambda) = (\mathcal{F}_1^{(0)}(\lambda), \mathcal{F}_2^{(0)}(\lambda)) \in \mathbf{B}(\mathcal{B}(\mathcal{E}), \mathbf{h}(\lambda))$ associated with $H_{\mathcal{E}}^{(0)}$ is defined by

$$\mathcal{F}_k^{(0)} f = \begin{cases} \hat{P}_{j,k}^V(\lambda) \hat{f}|_{M_k(\cos \sqrt{\lambda})}, & \text{if } \lambda \in (\lambda_{j,k}^-, \lambda_{j,k}^+), j \geq 0, \\ \{0\}, & \text{otherwise.} \end{cases}$$

We note that $\mathcal{F}^{(0)}(\lambda)^* \in \mathbf{B}(\mathbf{h}(\lambda), \mathcal{B}^*(\mathcal{E}))$. Then we have the following lemma. For the proof, see [2].

Lemma 3.1 *For $\lambda \in (0, \infty) \setminus \mathcal{T}^{(0)}$, we have*

- $\mathcal{F}^{(0)}(\lambda)$ diagonalizes $H_{\mathcal{E}}^{(0)}$, i.e., $\mathcal{F}^{(0)}(\lambda)(H_{\mathcal{E}}^{(0)} - \lambda) = 0$,
- $\mathcal{F}^{(0)}(\lambda)^* \phi$ for any $\phi \in \mathbf{h}(\lambda)$ is a generalized eigenfunction of $H_{\mathcal{E}}^{(0)}$.

The distorted Fourier transformation $\mathcal{F}^{(\pm)}(\lambda) = (\mathcal{F}_1^{(\pm)}(\lambda), \mathcal{F}_2^{(\pm)}(\lambda))$ associated with $H_{\mathcal{E}}$ is defined by

$$\mathcal{F}_k^{(\pm)}(\lambda) = \mathcal{F}_k^{(0)}(\lambda) Q_{\mathcal{E}}(\lambda \pm i0), \quad k = 1, 2.$$

Then we have the following lemma. For the proof, see [2].

Lemma 3.2 *For $\lambda \in (0, \infty) \setminus \mathcal{T}$, we have*

- $\mathcal{F}^{(\pm)}(\lambda)$ diagonalizes $H_{\mathcal{E}}^{(0)}$, i.e., $\mathcal{F}^{(\pm)}(\lambda)(H_{\mathcal{E}} - \lambda) = 0$,
- $\mathcal{F}^{(\pm)}(\lambda)^* \phi$ for any $\phi \in \mathbf{h}(\lambda)$ is a generalized eigenfunction of $H_{\mathcal{E}}$ in $\mathcal{B}^*(\mathcal{E})$.

Define the scattering amplitude $A(\lambda)$ by

$$A(\lambda) = \mathcal{F}^{(+)} q \mathcal{F}^{(0)}(\lambda)^*, \quad \lambda \in (0, \infty) \setminus \mathcal{T}.$$

Let $P_{\text{ac}}(H_{\mathcal{E}}^{(0)})$ be the projection on the absolutely continuous space of $H_{\mathcal{E}}^{(0)}$. It is well-known that the scattering matrix $S(\lambda)$ associated with the wave operator

$$W_{\pm} = \text{s-lim}_{t \rightarrow \pm\infty} e^{itH_{\mathcal{E}}} e^{-itH_{\mathcal{E}}^{(0)}} P_{\text{ac}}(H_{\mathcal{E}}^{(0)})$$

is written by $S(\lambda) = 1 - 2\pi i A(\lambda)$.

4 Boundary Value Problem

We take the bounded domain $\Omega^i = (\overline{\mathcal{V}^i}, \mathcal{E}^i)$, $\overline{\mathcal{V}^i} = \mathcal{V}^i \cup \partial\mathcal{V}^i$, as Fig.5:

- \mathcal{V}^i is “the internal points” of Ω^i ,
- $\partial\mathcal{V}^i$ is “the boundary points” of Ω^i

Here we impose the additional assumption on the potential $q = \{q_{\mathbf{e}}\}_{\mathbf{e} \in \mathcal{E}}$:

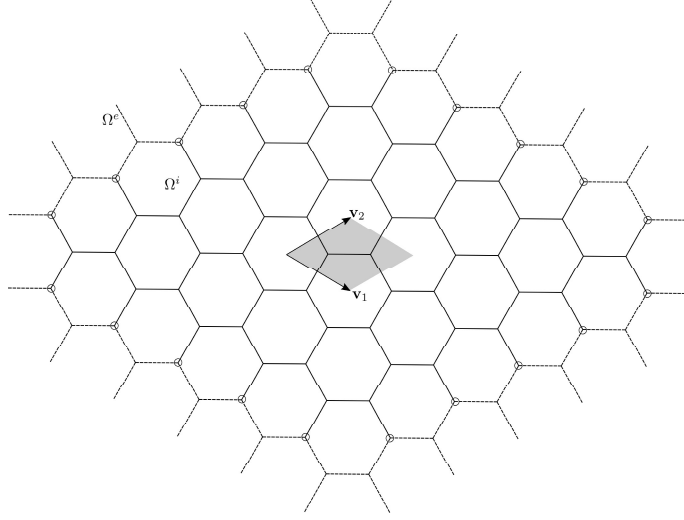


Figure 5: Bounded Domain in the Hexagonal Lattice.

(Q-4) $\text{supp}(q) \subset \{\mathbf{e} \in \mathcal{E}^i; \mathbf{e}(0), \mathbf{e}(1) \in \mathcal{V}^i\}$.

Let us consider the Dirichlet boundary problem on \mathcal{E}^i . We define the differential operator $-\Delta_{\mathcal{E}}^i + q$ on Ω^i by

$$(-\Delta_{\mathcal{E}}^i + q)u = \{-u''_{\mathbf{e}} + q_{\mathbf{e}}u_{\mathbf{e}}\}_{\mathbf{e} \in \mathcal{E}^i},$$

with

$$\text{Dom}(-\Delta_{\mathcal{E}}^i + q) = \{u \in H^2(\mathcal{E}^i); u \text{ satisfies (K-1) and (K-2), } u|_{\partial\mathcal{V}^i} = 0\}.$$

Let $\sigma_D(-d^2/dx^2 + q_{\mathbf{e}})$ be the Dirichlet eigenvalues of $-d^2/dx^2 + q_{\mathbf{e}}$ on \mathbf{e} . We put

$$\mathcal{T} = \cup_{\mathbf{e} \in \mathcal{E}^i} \sigma_D(-d^2/dx^2 + q_{\mathbf{e}}).$$

We note that \mathcal{T} is a discrete set. We also note that there may exist Dirichlet eigenfunctions of $H_{\mathcal{E}} = -\Delta_{\mathcal{E}}^i + q$ supported on cycles of edges (ex. the eigenfunctions associated with flat band spectrum $\sigma_{\text{fb}}(H_{\mathcal{E}}^{(0)})$). These Dirichlet eigenvalues of $H_{\mathcal{E}}$ are embedded in the continuous spectrum $\sigma_{\text{cont}}(H_{\mathcal{E}}) = [0, \infty)$.

For $\lambda \in \mathbb{C} \setminus \sigma_D(-\Delta_{\mathcal{E}}^i + q)$ and $f \in \ell^2(\partial\mathcal{V}^i)$, there exists a unique solution $u = \{u_{\mathbf{e}}\}_{\mathbf{e} \in \mathcal{E}^i}$ of the following boundary value problem:

$$(-\Delta_{\mathcal{E}}^i + q)u = 0 \text{ in } \mathcal{E}^i, \quad u = f \text{ on } \partial\mathcal{V}^i.$$

We define the Dirichlet-Neumann (D-N) map $\Lambda_{\mathcal{E}}^i(\lambda)$ as follows: for $f \in \ell^2(\partial\mathcal{V}^i)$,

$$(\Lambda_{\mathcal{E}}^i(\lambda)f)(p) = -\partial_{\mathbf{e}}u(p), \quad p \in \partial\mathcal{V}^i, \quad \mathbf{e} \in \mathcal{E}_p \cap \mathcal{E}^i,$$

where u is the solution of the above boundary value problem.

Taking into account of the Kirchhoff conditions at $v \in \mathcal{V}^i$, one can obtain the Green's formula by integration by parts:

$$\begin{aligned} & \sum_{e \in \mathcal{E}^i} \int_0^1 \left((\Delta_{\mathcal{E}}^i u)_e \cdot \overline{u_e} - u_e \cdot \overline{(\Delta_{\mathcal{E}}^i u)_e} \right) dx \\ &= \sum_{p \in \partial \mathcal{V}^i} \left((\Lambda_{\mathcal{E}}^i(\lambda) f) \cdot \overline{f(p)} - f(p) \cdot \overline{(\Lambda_{\mathcal{E}}^i(\lambda) f)(p)} \right). \end{aligned}$$

We remark that $\Lambda_{\mathcal{E}}^i(\lambda) f$ is regarded as the outer normal derivative in this sense.

By using the D-N map $\Lambda_{\mathcal{E}}^i(\lambda)$, one can construct the outgoing solution u to $(H_{\mathcal{E}} - \lambda)u = 0$. If the scattering amplitudes $A^{q_1}(\lambda)$ and $A^{q_2}(\lambda)$ for q_1 and q_2 coincide, the outgoing solutions satisfy $u^{q_1} - u^{q_2} \in \mathcal{B}_0^*(\mathcal{E})$. By using the Rellich type uniqueness theorem, we have $u^{q_1} = u^{q_2}$. Then the D-N map for q_1 and q_2 coincide. Therefore we have

Lemma 4.1 *Suppose that q_1 and q_2 satisfies (Q-1) - (Q-4). Then $A^{q_1} = A^{q_2}$ if and only if $\Lambda_{\mathcal{E}}^{q_1, i}(\lambda) = \Lambda_{\mathcal{E}}^{q_2, i}(\lambda)$.*

For the proof of the lemma, see [2].

Then we have the following main theorem.

Theorem 4.1 *Suppose that we know the scattering amplitude $A(\lambda)$ associated with the Schrödinger operator $H_{\mathcal{E}}$ for $\lambda \in I$, where I is an open interval in $(0, \infty) \setminus \mathcal{T}$. Then we can determine the potential $q = \{q_e\}_{e \in \mathcal{E}}$ uniquely.*

In view of the Lemma 4.1, we only have to derive a reconstruction from $\Lambda_{\mathcal{E}}^i(\lambda)$ to determine $q = \{q_e\}_{e \in \mathcal{E}^i}$.

Inverse Boundary Value Problem: Given $\Lambda_{\mathcal{E}}^i(\lambda)$ for $\lambda \in \mathbb{C} \setminus \sigma_D(-\Delta_{\mathcal{E}}^i + q)$, can we determine the potential $q = \{q_e\}_{\mathcal{E}^i}$?

4.1 Inverse Spectral Problem on Finite Interval

Let us consider the Dirichlet problem on $[0, 1]$:

$$-y'' + qy = \kappa y \text{ in } (0, 1), \quad y(0) = y(1) = 0. \quad (2)$$

Let $\kappa(q) = \{\kappa_1, \kappa_2, \dots\}$ be all the Dirichlet eigenvalues of (2). If q is real-valued and symmetric, then $\kappa(q)$ and q is one-to-one by the Borg's theorem (cf. [5]).

Theorem 4.2 *(Borg's theorem) Let $E = \{q \in L^2(0, 1); q(1-x) = q(x)\}$. Then $E : q \mapsto \kappa(q)$ is one-to-one.*

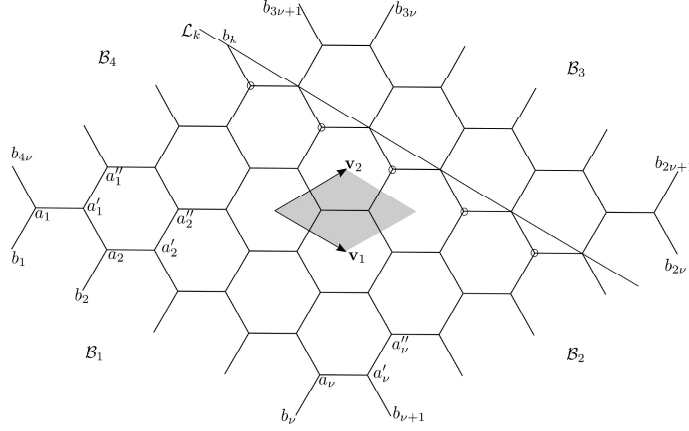


Figure 6: Labeling of the boundary $\partial\mathcal{V}^i = \cup_{j=1}^4 \mathcal{B}_j$

4.2 Special Solution of Cauchy Problem on Ω

Split the boundary of Ω^i into parts $\partial\mathcal{V}^i = \mathcal{B}_1 \cup \mathcal{B}_2 \cup \mathcal{B}_3 \cup \mathcal{B}_4$, where

$$\mathcal{B}_1 = \{b_1, \dots, b_\nu\}, \quad \mathcal{B}_2 = \{b_{\nu+1}, \dots, b_{2\nu}\},$$

$$\mathcal{B}_3 = \{b_{2\nu+1}, \dots, b_{3\nu}\}, \quad \mathcal{B}_4 = \{b_{3\nu+1}, \dots, b_{4\nu}\}.$$

See Fig.6. We can construct a special solution of the Cauchy problem by the D-N map, which grows to a particular direction.

We identify $f \in \ell^2(\partial\mathcal{V}^i)$ with $f = [f(b_1), \dots, f(b_{4\nu})]^T \in \mathbb{C}^{4\nu}$. So we can regard the D-N map $\Lambda_{\mathcal{E}}^i(\lambda)$ as $4\nu \times 4\nu$ matrix. We write $f(\mathcal{B}_j) = [f(b_{(j-1)\nu+1}), \dots, f(b_{j\nu})]^T$. Let $\Lambda(\lambda; \mathcal{B}_j, \mathcal{B}_k)$ be a $\nu \times \nu$ submatrix of the D-N map such that $\Lambda(\lambda; \mathcal{B}_j, \mathcal{B}_k) f(\mathcal{B}_k) \in \ell^2(\mathcal{B}_j)$. Then we split $\Lambda_{\mathcal{E}}^i(\lambda)$ into block matrix expression:

$$\Lambda_{\mathcal{E}}^i(\lambda) = \begin{bmatrix} \Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_1) & \Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_2) & \cdots & \Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_4) \\ \Lambda(\lambda; \mathcal{B}_2, \mathcal{B}_1) & \Lambda(\lambda; \mathcal{B}_2, \mathcal{B}_2) & \cdots & \Lambda(\lambda; \mathcal{B}_2, \mathcal{B}_4) \\ \vdots & \vdots & \ddots & \vdots \\ \Lambda(\lambda; \mathcal{B}_4, \mathcal{B}_1) & \Lambda(\lambda; \mathcal{B}_4, \mathcal{B}_2) & \cdots & \Lambda(\lambda; \mathcal{B}_4, \mathcal{B}_4) \end{bmatrix}.$$

Suppose $f(\mathcal{B}_j) = 0$, $j = 1, 2, 4$ and $(\Lambda_{\mathcal{E}}^i(\lambda) f)(\mathcal{B}_1) = 0$. Then we can construct the solutions on all the edges $e \in \mathcal{E}$ uniquely as $u_e = 0$ from \mathcal{B}_1 to \mathcal{B}_3 . See Fig.7. We note that $\lambda \notin \cup_{e \in \mathcal{E}} \sigma_D(-d^2/dx^2 + q_e)$. Thus we proved the following lemma. For the details, see [2].

Lemma 4.2 *If $\Lambda \in \mathcal{C} \setminus (\sigma_D(-\Delta_{\mathcal{E}}^i + q) \cup \mathcal{T})$, then the matrices $\Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_3)$ and $\Lambda(\lambda; \mathcal{B}_2, \mathcal{B}_4)$ are regular.*

As a consequence of the Lemma 4.2, we have the following fact.

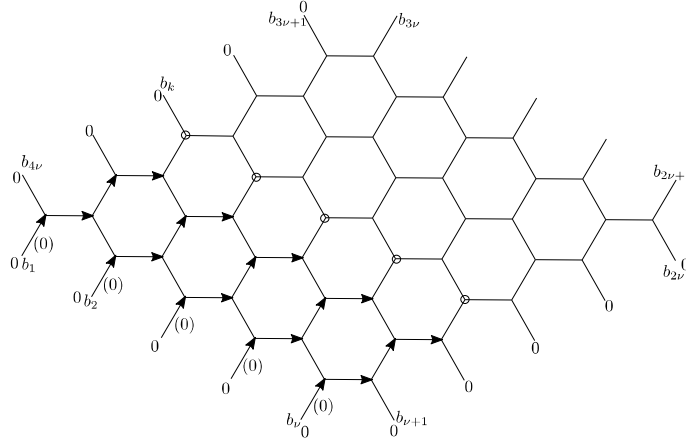


Figure 7: Construction of the solutions for the Cauchy problem.

Corollary 4.1 *Let $\lambda \in \mathbb{C} \setminus (\sigma_D(-\Delta_{\mathcal{E}}^i + q) \cup \mathcal{T})$. If $g(\mathcal{B}_1) \in \mathbb{C}^\nu$ and $f(\mathcal{B}_j) \in \mathbb{C}^\nu$, $j = 1, 2, 4$, are given, then there exists a unique $f(\mathcal{B}_3) \in \mathbb{C}^\nu$ such that*

$$(\Lambda_{\mathcal{E}}^i(\lambda)f)(\mathcal{B}_1) = g(\mathcal{B}_1).$$

Moreover, we have

$$f(\mathcal{B}_3) = \Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_3)^{-1} \left(g(\mathcal{B}_1) - \sum_{j=1,2,4} \Lambda(\lambda; \mathcal{B}_1, \mathcal{B}_j) f(\mathcal{B}_j) \right). \quad (3)$$

In view of the corollary, $f(\mathcal{B}_3)$ is determined by the D-N matrix $\Lambda_{\mathcal{E}}^i(\lambda)$ and the given vectors $g(\mathcal{B}_1)$ and $f(\mathcal{B}_j)$, $j = 1, 2, 4$. See Fig.8

In the same way, if $g(\mathcal{B}_2) \in \mathbb{C}^\nu$ and $f(\mathcal{B}_j) \in \mathbb{C}^\nu$, $j = 1, 2, 3$, are given, then there exists a unique $f(\mathcal{B}_4) \in \mathbb{C}^\nu$ such that

$$f(\mathcal{B}_4) = \Lambda(\lambda; \mathcal{B}_4, \mathcal{B}_2)^{-1} \left(g(\mathcal{B}_2) - \sum_{j=1,2,3} \Lambda(\lambda; \mathcal{B}_2, \mathcal{B}_j) f(\mathcal{B}_j) \right), \quad (4)$$

which means that $f(\mathcal{B}_4)$ is determined by the D-N matrix $\Lambda_{\mathcal{E}}^i(\lambda)$ and the given vectors $g(\mathcal{B}_2)$ and $f(\mathcal{B}_j)$, $j = 1, 2, 3$.

Then we have the following theorem.

Theorem 4.3 *Let $I \subset (0, \infty) \setminus (\sigma_D(-\Delta_{\mathcal{E}}^i + q) \cup \mathcal{T})$ be an open interval. If the D-N map $\Lambda_{\mathcal{E}}^i(\lambda)$ is given for any $\lambda \in I$, then the potential $q = \{q_{\mathbf{e}}\}_{\mathbf{e} \in \mathcal{E}^i}$ is determined uniquely.*

The reconstruction procedure consists of several steps. At Step 1, we put the Cauchy data $f(\mathcal{B}_j)$, $j = 1, 2, 3$, and $g(\mathcal{B}_2)$ as in Fig.9. Then, using the formula (4), we get $f(\mathcal{B}_3)$. Moreover, we have the following:

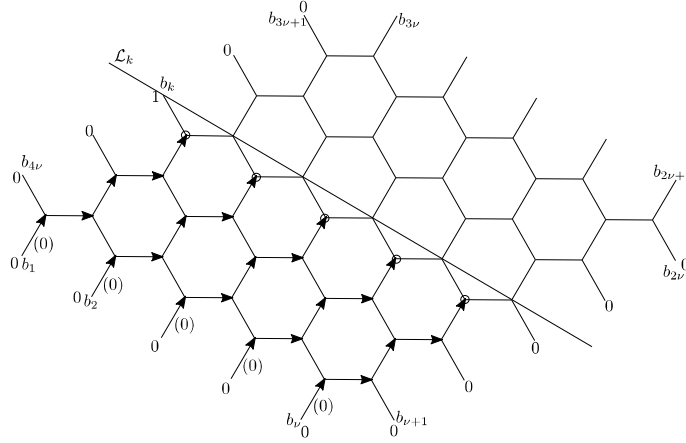


Figure 8: the unique special solution of the Cauchy problem.

- Since the D-N map is given, we can compute the value $u(\diamond)$ at $\diamond \in \mathcal{V}^i$.
- $u(\circ) = 0$ by the special solution of the Cauchy problem.
- Consider $-u_e'' + q_e u_e = \lambda u_e$ on the edge \otimes . Put $e(0) = \circ$. Then we obtain the fundamental solution $u_e(x, \lambda)$, satisfying $u_e(0, \lambda) = 0$, $u_e'(0, \lambda) = 1$.
- By the analytic continuation of $\Lambda_{\mathcal{E}}^i(\lambda)$ with respect to $\lambda \in \mathbb{C}$, we know all the zeros of $u_e(1, \lambda)$ (i.e., all the Dirichlet eigenvalues on e).
- By the Borg's theorem, we can determine q_e on \otimes .

To be more specific, there are two types of edges e of $\otimes 1$ and $\otimes 2$ in Fig.9 whose reconstruction procedures slightly differ.

Step 1 on e of $\otimes 1$:

Let $e = \otimes 1$, and $e(0) = \circ$, $e(1) = \diamond$. Then u_e is the solution of

$$-u_e'' + q_e u_e = \lambda u_e \text{ in } (0, 1), \quad u_e(0) = 0, \quad u_e'(0) = f_1(\lambda), \quad u_e(1) = g_1(\lambda),$$

where $f_1(\lambda)$ and $g_1(\lambda)$ are analytic for λ . Put $\psi_e = u_e/f_1(\lambda)$. Then ψ_e is the solution of

$$-\psi_e'' + q_e \psi_e = \lambda \psi_e \text{ in } (0, 1), \quad \psi_e(0) = 0, \quad \psi_e'(0) = 1, \quad \psi_e(1) = \frac{g_1(\lambda)}{f_1(\lambda)}.$$

By the analytic continuation of $f_1(\lambda)/g_1(\lambda)$, we know all the zeros of $\psi_e(1)$ which are Dirichlet eigenvalues on e of $\otimes 1$. By the Borg's theorem, we can determine q_e on e of type $\otimes 1$.

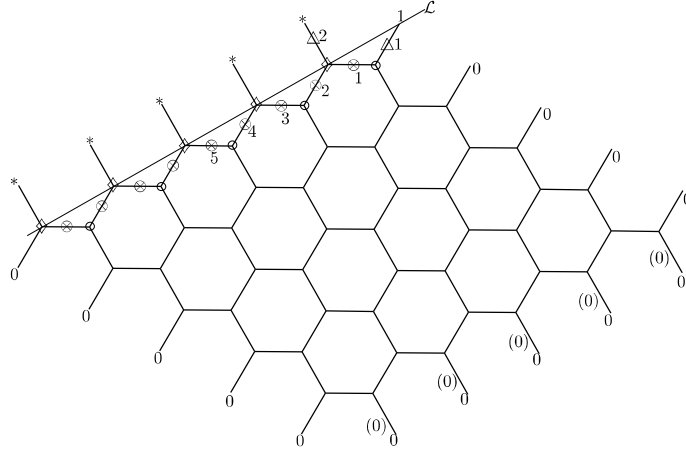


Figure 9: The reconstruction procedure of Step 1.

Step 1 on e of $\otimes 2$:

Let $e = \otimes 1$, and $e(0) = \circ$, $e(1) = \diamond$. Then u_e is the solution of

$$-u_e'' + q_e u_e = \lambda u_e \text{ in } (0, 1), \quad u_e(0) = 0, \quad u_e(1) = g_2(\lambda), \quad u_e'(1) = f_2(\lambda),$$

where $f_2(\lambda)$ and $g_2(\lambda)$ are analytic for λ . Put $\psi_e = u_e/f_2(\lambda)$. Then ψ_e is the solution of

$$-\psi_e'' + q_e \psi_e = \lambda \psi_e \text{ in } (0, 1), \quad \psi_e(0) = 0, \quad \psi_e(1) = \frac{g_2(\lambda)}{f_2(\lambda)}, \quad \psi_e'(1) = 1.$$

By the analytic continuation of $f_2(\lambda)/g_2(\lambda)$, we know all the zeros of $\psi_e(1)$ which are Dirichlet eigenvalues on e of $\otimes 2$. By the Borg's theorem, we can determine q_e on e of type $\otimes 2$.

We can repeat the above procedures for e of $\otimes j$, $j = 3, 4, \dots$, right below the line \mathcal{L} in Fig.9.

At Step 2, using the formula (3), we follow the same procedure as Step 1. See Fig.10. Then we can reconstruct the potentials q_e for $e = \otimes$ right below the line \mathcal{L}' in Fig.10.

At Step 3, we already know the potential q_e for $e = \times$ in Fig.11. Then, using the formula (4) as Step 1, we can reconstruct the potential q_e for $e = \otimes$ in Fig.11. Repeating this procedure, we can reconstruct the potential q_e for $e = \times$ in Fig.12 right above the line \mathcal{L}' before Step 4.

At Step 4, using the formula (3) as Step 2, we can reconstruct the potential q_e for $e = \otimes$ in Fig.12. Repeating this procedure, we can reconstruct the potential q_e for $e = \times$ in Fig.13 right above the line \mathcal{L} .

So far, we arrive at one size smaller unknown region where the potential q_e 's are unknown. Then we can restart Step 1 to Step 5 in the smaller region.

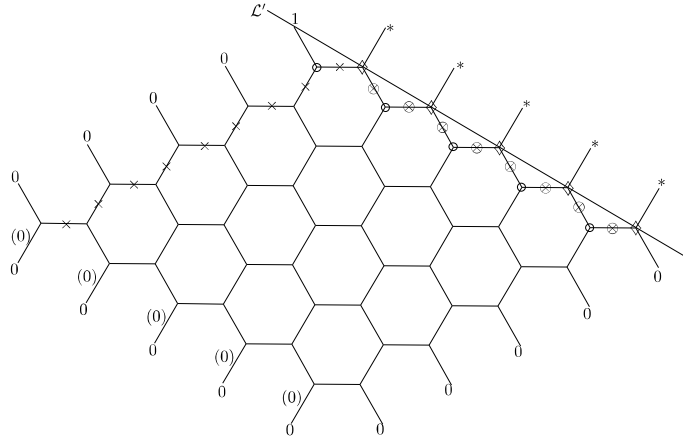


Figure 10: The reconstruction procedure of Step 2.

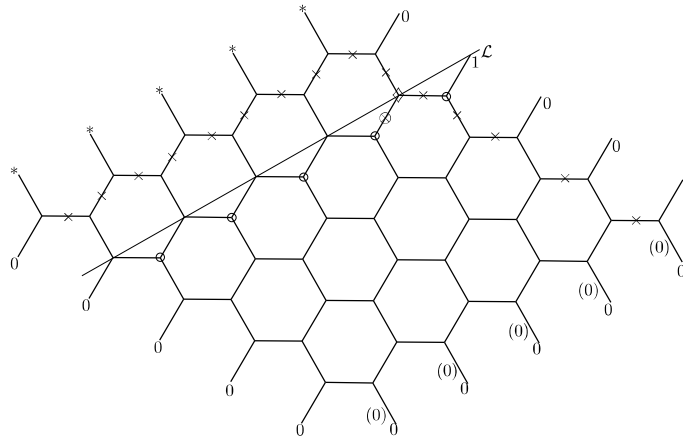


Figure 11: The reconstruction procedure of Step 3.

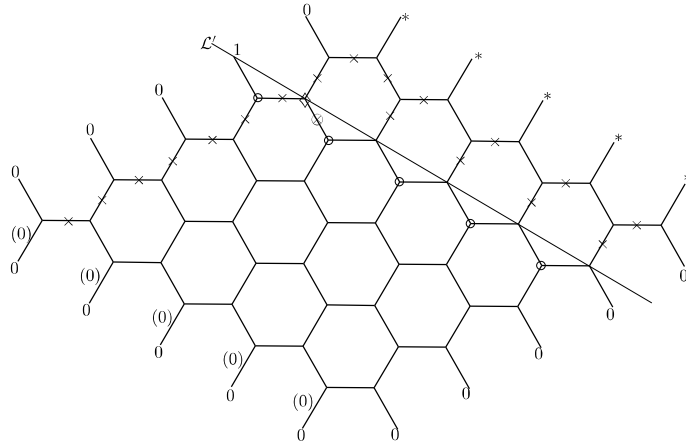


Figure 12: The reconstruction procedure of Step 4.

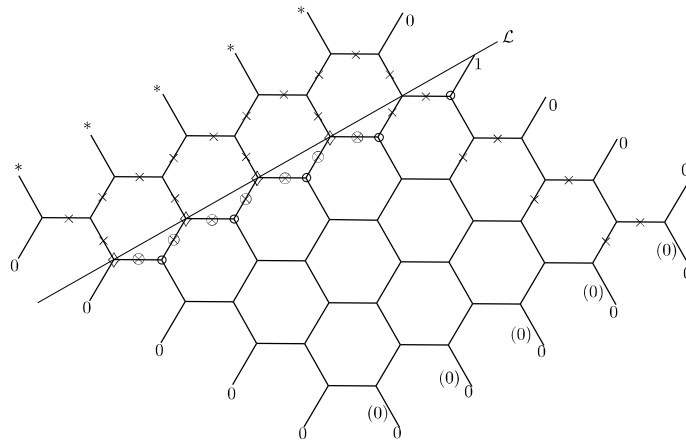


Figure 13: The reconstruction procedure of Step 5.

Finally, we can reconstruct all the potential q_e , $e \in \mathcal{E}^i$. For the details of the reconstruction procedure, see [2].

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