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INVERSE SCATTERING ON GRAPHEN — VERTEX MODEL AND EDGE MODEL

HIROSHI ISOZAKI

1. Introduction

1.1. **Brief summary.** The problem we addrees here is the spectral theory and inverse scattering associated with Schrödinger operators on perturbed periodic lattices. Among many periodic structures appearing in material science, we are interested in the hexagonal lattice because of its generality in carbonic materials in physical side and also in the geometry of lattice problem in mathematical side. A well-known example is the graphen, whose simplest model is the hexagonal lattice with Hamiltonian defined by a difference operator between vertices of the nearest neighbors. We call it a *vertex model.* As perturbations, one can consider potentials or defects, which means to deform the lattice structure by removing or adding edges. The scattering theory developed for the continuous model for Schrödinger operators is also extended to this discrete model. Our main concern is the inverse problem. Our results are:

- *A compactly supported scalar potential is uniquely reconstructed from the S-matrix of one fixed energy.*
- *The S-matrix determines the structure of the planar graph in a finite part.*
- *The convex hull of the defects of the form of convex polygon is determined by the S-matrix of one fixed energy.*

There is another model for graphen, in which we take into account of effects of edges. We consider $-(d/dz)^2 + q_{\mathbf{e}}(z)$ on each edge $\mathbf{e}$ with Kirchhoff conditions on vertices. We call it an *edge model,* although it is usually called a metric graph. The study of spectral properties for the edge model is reduced to that of the vertex model. We can then obtain the following result.

- *Assume that $q_{\mathbf{e}}(z) \in L^2(0,1)$ and real-valued, symmetric, i.e. $q_{\mathbf{e}}(z) = q_{\mathbf{e}}(1-z)$, moreover $q_{\mathbf{e}}(z) = 0$ except for a finite number of edges $\mathbf{e}$. Then, the $q_{\mathbf{e}}(z)$'s are determined by the S-matrix for all energies.*

Our theory, in particular the forward problem of scattering, can be extended to more general lattices. However, for the simplicity of explanation, we restrict ourselves here to the hexagonal lattice.

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2. Hexagonal lattice and its Hamiltonian

Figure 1 represents a hexagonal lattice. We can find two lattices : the one consisting of white dots, and the other black dots. Letting

$$\mathcal{L}_0 = \{\mathbf{v}(n)\,;\, n = (n_1, n_2) \in \mathbf{Z}^2\},$$

$$\mathbf{v}(n) = n_1\mathbf{v}_1 + n_2\mathbf{v}_2,$$

$$\mathbf{v}_1 = 1 + \omega, \quad \mathbf{v}_2 = \omega(1+\omega), \quad \omega = e^{\pi i/3},$$

we define the *vertex set* $\mathcal{L}_0$ by

$$\mathcal{V}_0 = \Big(p_1 + \mathcal{L}_0\Big) \cup \Big(p_2 + \mathcal{L}_0\Big).$$

Consequently, the wave function has two components in $\ell^2(\mathbf{Z})$. Denoting it by $\widehat{u}(n) = (\widehat{u}_1(n), \widehat{u}_2(n))$, we define the *vertex Laplacian* by

$$(\widehat{\Delta}_{\mathcal{V}}\widehat{u})(n) = \frac{1}{3}\begin{pmatrix} \displaystyle\sum_{|\mathbf{v}(n')-\mathbf{v}(n)|=1} \widehat{u}_2(n') \\ \displaystyle\sum_{|\mathbf{v}(n')-\mathbf{v}(n)|=1} \widehat{u}_1(n') \end{pmatrix}.$$

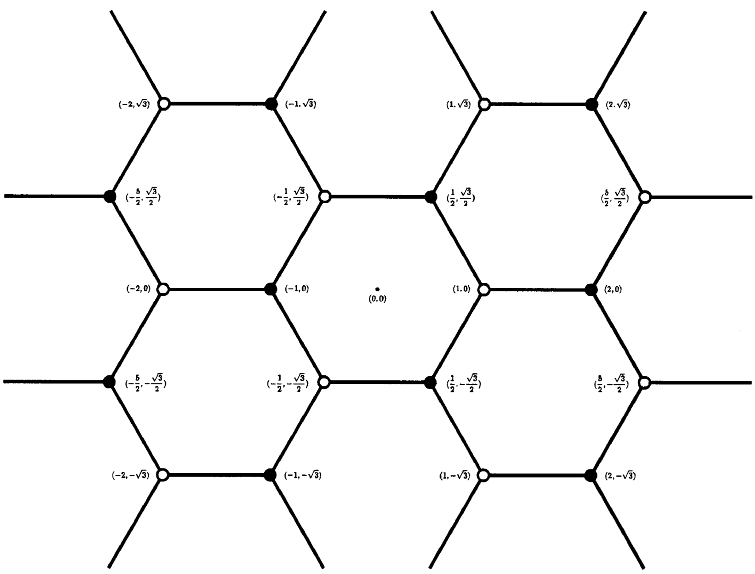

Figure 1. Hexagonal lattice

To study the wave propagation on the lattice, let us first recall the case of continuous model, in which the free Schrödinger equation is

$$(-\Delta - \lambda)u = 0.$$

Passing to the Fourier transform, it becomes $(|\xi|^2-\lambda)\widetilde{u}(\xi)=0$ [1]. The physical solution is the L^2-density on the sphere, hence has the asymptotic expansion

$$\begin{aligned} u(x) &= C(\lambda)\int_{S^{n-1}} e^{i\sqrt{\lambda}\omega\cdot x}\widetilde{u}(\sqrt{\lambda}\omega)d\omega \\ &\simeq C_+\frac{e^{i\sqrt{\lambda}r}}{r^{(n-1)/2}}\widehat{u}(\sqrt{\lambda}\theta)+C_-\frac{e^{-i\sqrt{\lambda}r}}{r^{(n-1)/2}}\widehat{u}(-\sqrt{\lambda}\theta) \end{aligned}$$

with $\theta=x/r$, $r=|x|$. This also holds for the perturbed equation $(-\Delta+V(x)-\lambda)u=0$, where $V(x)$ is compactly supported, i.e.

$$u(x)\simeq C_+\frac{e^{i\sqrt{\lambda}r}}{r^{(n-1)/2}}\varphi_{out}(\theta)+C_-\frac{e^{-i\sqrt{\lambda}r}}{r^{(n-1)/2}}\varphi_{in}(\theta). \tag{2.1}$$

The operator

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

is the S-matrix. Note that the sphere $\sqrt{\lambda}S^{n-1}$ is the characteristic surface of the operator $-\Delta-\lambda$.

The free Schrödinger equation on the hexagonal lattice is

$$(-\widehat{\Delta}_{\mathcal{V}}-\lambda)\widehat{u}=0.$$

Passing to the Fourier series, we have

$$(H_0(x)-\lambda)u(x)=0, \quad \text{on} \quad \mathbf{T}^2=(\mathbf{R}/2\pi\mathbf{Z})^2,$$

$$H_0(x)=-\frac{1}{3}\begin{pmatrix} 0 & 1+e^{-ix_1}+e^{-ix_2} \\ 1+e^{ix_1}+e^{ix_2} & 0\end{pmatrix}.$$

The physical solution is an L^2-density supported in a submanifold on the torus:

$$M_\lambda=\left\{x\in\mathbf{T}^2\,;\,\det(H_0(x)-\lambda)=0\right\},$$

$$\det(H_0(x)-\lambda)=\lambda^2-\frac{1}{9}\left\{3+2(\cos x_1+\cos x_2+\cos(x_1-x_2)\right\}.$$

This is the characteristic surface of the difference operator $-\widehat{\Delta}_{\mathcal{V}}-\lambda$, and is called the Fermi surface. The solution $u(x)$ is then written as

$$u(x)=\frac{\varphi(x)}{p(x,\lambda)-i0}-\frac{\varphi(x)}{p(x,\lambda)+i0},$$

$$\varphi(x)\in L^2(M_\lambda), \quad p(x,\lambda)=\det(H_0(x)-\lambda).$$

This also holds asymptotically (in the sense of singularity) for the perturbed lattice:

$$u(x)\simeq\frac{\varphi_{out}(x)}{p(x,\lambda)-i0}-\frac{\varphi_{in}(x)}{p(x,\lambda)+i0}, \tag{2.2}$$

and the operator

$$S(\lambda): L^2(M_\lambda)\ni\varphi_{in}\to\varphi_{out}\in L^2(M_\lambda)$$

is the S-matrix.

The two terms appearing in the right-hand side of (2.1) are called outgoing and incoming waves. As is seen here, they are distinguished by their spatial behaviors at

[1]In this note, the Fourier trasnsform of a distribution $u(x)$ on $\mathbf{R}^d$ is denoted by $\widetilde{u}(\xi)$, while the Fourier coefficient of a distribution $u(x)$ on the torus $\mathbf{T}^d$ is denoted by $\widehat{u}(n)$

infinity. For the lattice, it does not work well, since the Fermi surface is in general not strictly convex and we encounter difficulties in applying the stationary phase method to the integral on it. Therefore, we pass to the Fourier series and observe the singularities of wave functions on the torus. This leads us to the formulation (2.2).

As a perturbation of the vertex model, we add a scalar potential, or (and) replace its finite part by a general graph. The associated Hamiltonian is denoted by $\widehat{H}_{\mathcal{V}}$. If these perturbations are assumed to be bounded self-adjoint and confined in a compact part, the spectral theory can be developped easily.

We turn to the edge model, which is usually called the metric graph. We consider a hexagonal lattice with vertex set $\mathcal{V}$ and edge set $\mathcal{E}$. Each edge $\mathbf{e} \in \mathcal{E}$ is identified with the interval $[0,1]$. Functios on the edge set $\mathcal{E}$ are denoted by $\widehat{u} = \widehat{u}_{\mathcal{E}} = \{\widehat{u}_{\mathbf{e}}(z)\,;\, \mathbf{e} \in \mathcal{E}\}$. The Hamitonian $\widehat{H}_{\mathcal{E}}$ is defined by

$$\big(\widehat{H}_{\mathcal{E}}\widehat{u}_{\mathcal{E}}\big)_{\mathbf{e}}(z) = \Big(-\frac{d^2}{dz^2} + q_{\mathbf{e}}(z)\Big)\widehat{u}_{\mathbf{e}}(z), \quad \mathbf{e} \in \mathcal{E},$$

assuming the Kirchhoff condition on $\widehat{u}_{\mathcal{E}}$. For $\mathbf{e} \in \mathcal{E}$, denote its end points by $\mathbf{e}(0) = 0$, $\mathbf{e}(1) = 1$. Then, the *Kirchhoff condition* is

(K-1) $\widehat{u}_{\mathcal{E}}(z)$ *is continuous on* $\mathcal{E}$.

(K-2) *For each* $\mathbf{e} \in \mathcal{E}$, $\widehat{u}_{\mathbf{e}} \in C^1([0,1])$, *and*

$$\sum_{\mathbf{e}(0)=v} \widehat{u}'_{\mathbf{e}}(0) = \sum_{\mathbf{e}(1)=v} \widehat{u}'_{\mathbf{e}}(1), \quad \forall v \in \mathcal{V}.$$

The assumption on the potentials are as follows:

(E-1) $q_{\mathbf{e}}(z)$ *is real-valued, and* $q_{\mathbf{e}}(z) \in L^2(0,1)$.

(E-2) $q_{\mathbf{e}}(z) = 0$ *except for a finite number of edges.*

(E-3) $q_{\mathbf{e}}(z) = q_{\mathbf{e}}(1-z)$.

This makes $\widehat{H}_{\mathcal{E}}$ self-adjoint on $L^2(\mathcal{E})$.

There is a simple relation between the vertex Laplacian and the edge Laplacian. On each edge, the solution of the Schrödinger equation

$$\Big(-(d/dz)^2 + q_{\mathbf{e}}(z) - \lambda\Big)\widehat{u}_{\mathbf{e}} = \widehat{f}_{\mathbf{e}}, \quad \text{on} \quad (0,1)$$

is written as

$$c_{\mathbf{e}}(1,\lambda)\frac{\phi_{\mathbf{e}0}(z,\lambda)}{\phi_{\mathbf{e}0}(1,\lambda)} + c_{\mathbf{e}}(0,\lambda)\frac{\phi_{\mathbf{e}1}(z,\lambda)}{\phi_{\mathbf{e}1}(0,\lambda)} + r_{\mathbf{e}}(\lambda)\widehat{f}_{\mathbf{e}},$$

$$r_{\mathbf{e}}(\lambda) = \Big(-(d/dz)^2_D + q_{\mathbf{e}}(z) - \lambda\Big)^{-1},$$

where $\big(d/dz\big)^2_D$ is the Dirichlet Laplacian on $(0,1)$, and $\phi_{\mathbf{e}i}(z,\lambda)$ is the solution to the equation

$$\Big(-(d/dz)^2 + q_{\mathbf{e}}(z) - \lambda\Big)\phi_{\mathbf{e}i}(z,\lambda) = 0, \quad \text{on} \quad (0,1),$$

$$\phi_{\mathbf{e}0}(0,\lambda) = 0, \quad \phi'_{\mathbf{e}0}(0,\lambda) = 1,$$

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

The coefficients $c_{\mathbf{e}}(1,\lambda)$, $c_{\mathbf{e}}(0,\lambda)$ are determined by the Kirchhoff condition. The point is that

$$\text{Kirchhoff condition} = \text{Vertex equation}$$

Namely, the following equation holds:

$$\begin{aligned}
&\sum_{\mathbf{e}(0)=v} \frac{1}{\phi_{\mathbf{e}0}(1,\lambda)} c_{\mathbf{e}}(1,\lambda) + \sum_{\mathbf{e}(1)=v} \frac{1}{\phi_{\mathbf{e}1}(0,\lambda)} c_{\mathbf{e}}(0,\lambda) \\
&+ \sum_{\mathbf{e}(0)=v} \frac{\phi'_{\mathbf{e}1}(0,\lambda)}{\phi_{\mathbf{e}1}(0,\lambda)} c_{\mathbf{e}}(0,\lambda) - \sum_{\mathbf{e}(1)=v} \frac{\phi'_{\mathbf{e}0}(1,\lambda)}{\phi_{\mathbf{e}0}(1,\lambda)} c_{\mathbf{e}}(1,\lambda) \\
&= \sum_{\mathbf{e}(1)=v} \frac{d}{dz} r_{\mathbf{e}}(\lambda) \widehat{f}_{\mathbf{e}}\Big|_{z=1} - \sum_{\mathbf{e}(0)=v} \frac{d}{dz} r_{\mathbf{e}}(\lambda) \widehat{f}_{\mathbf{e}}\Big|_{z=0}.
\end{aligned}$$

Therefore, when $q_{\mathbf{e}}(z) = 0$, we have the following representation:

$$\Big(\big(\widehat{H}^{(0)}_{\mathcal{E}} - \lambda \big)^{-1} \widehat{f} \Big) \Big|_{\mathbf{e}} = c_{\mathbf{e}}(1,\lambda) \frac{\sin \sqrt{\lambda} z}{\sqrt{\lambda}} + c_{\mathbf{e}}(0,\lambda) \frac{\sin \sqrt{\lambda}(1-z)}{\sqrt{\lambda}} + r^{(0)}_{\mathbf{e}}(\lambda) \widehat{f}_{\mathbf{e}},$$

on each edge $\mathbf{e}$, and

$$c_{\mathbf{e}}(1,\lambda) = c_{\mathbf{e}'}(0,\lambda) = \Big(\widehat{R}^{(0)}_{\mathcal{V}}(\lambda) \widehat{F}^{(0)}_{\mathcal{E}}(\lambda) \widehat{f} \Big)(v),$$

for $\mathbf{e}(1) = \mathbf{e}'(0) = v$, where

$$\widehat{R}^{(0)}_{\mathcal{V}}(\lambda) = \frac{\sin \sqrt{\lambda}}{\sqrt{\lambda}} \Big(- \widehat{\Delta}_{\mathcal{V}} + \cos \sqrt{\lambda} \Big)^{-1},$$

$$\Big(\widehat{F}^{(0)}_{\mathcal{E}}(\lambda) \widehat{f} \Big)(v) = -\frac{1}{3} \Big(\sum_{\mathbf{e}(1)=v} \frac{d}{dz} r^{(0)}_{\mathbf{e}}(\lambda) \widehat{f}_{\mathbf{e}}\Big|_{z=1} - \sum_{\mathbf{e}(0)=v} \frac{d}{dz} r^{(0)}_{\mathbf{e}}(\lambda) \widehat{f}_{\mathbf{e}}\Big|_{z=0} \Big).$$

This formula suggests that the properties of the continuous spectrum of the edge Schrödinger operator are inherited from those of the vertex Schrödinger operator.

The spectra of the vertex and edge Schrödinger operators are as follows.

Lemma 2.1. *(1)* $\sigma_e(\widehat{H}_{\mathcal{V}}) = [-1, 1]$.
(2) $\sigma(\widehat{H}_{\mathcal{E}}) = [0,\infty) \cup \sigma_D$, *where* $\sigma_D = \cup_{\mathbf{e}\in\mathcal{E}} \sigma_p(-(d/dz)^2_D + q_{\mathbf{e}}(z))$.

3. Rellich type theorem

To study the continuous model for the Schrödinger operator on $\mathbf{R}^n$, appropriate function spaces are the Besov type spaces $B^*(\mathbf{R}^n)$ and $B^*_0(\mathbf{R}^n)$ defined by

$$B^*(\mathbf{R}^n) \ni f \Longleftrightarrow \sup_{R>1} \frac{1}{R} \int_{|x|<R} |f(x)|^2 dx < \infty,$$

$$B^*_0(\mathbf{R}^n) \ni f \Longleftrightarrow \lim_{R\to\infty} \frac{1}{R} \int_{|x|<R} |f(x)|^2 dx = 0.$$

The following theorem, proven by Rellich and Bekua, is fundamental in studying the continuous spectrum.

Theorem 3.1. *Let $\lambda > 0$. If $u(x) \in B_0^*(\mathbf{R}^n)$ satisfies the Helmholtz equation $(-\Delta - \lambda)u = 0$ on $\{|x| > R\}$ for a constant $R > 0$, then $u(x) = 0$ on $\{|x| > R\}$.*

This theorem implies the non-existence of eigenvalues embedded in the continuous spectrum. It also palys an important role in the inverse scattering theory.

We consider the counter part of this theorem on the lattice. For the periodic lattice $\mathcal{V}$, we define the Besov type speces by

$$B^*(\mathcal{V}) \ni \widehat{v} \Longleftrightarrow \sup_{R>1} \frac{1}{R} \sum_{|n|<R} |\widehat{v}(n)|^2 < \infty,$$

$$B_0^*(\mathcal{V}) \ni \widehat{v} \Longleftrightarrow \lim_{R\to\infty} \frac{1}{R} \sum_{|n|<R} |\widehat{v}(n)|^2 = 0.$$

Passing to the Fourier series, we define

$$B^*(\mathbf{T}^d) \ni v \Longleftrightarrow \widehat{v} \in B^*(\mathcal{V}),$$

$$B_0^*(\mathbf{T}^d) \ni v \Longleftrightarrow \widehat{v} \in B_0^*(\mathcal{V}).$$

Sometimes, it is more convenient to use the Fourier transform. Multiplying a cut-off function (a partition of unity) and passing to the Fourier transform $\widetilde{v}(\xi)$, we can also define

$$B^*(\mathbf{T}^d) \ni v \Longleftrightarrow \sup_{R>1} \frac{1}{R} \int_{|x|<R} |\widetilde{v}(\xi)|^2 d\xi < \infty,$$

$$B_0^*(\mathbf{T}^d) \ni v \Longleftrightarrow \lim_{R\to\infty} \frac{1}{R} \int_{|x|<R} |\widetilde{v}(\xi)|^2 d\xi = 0.$$

For the lattice space, the Rellich type theorem should be rephrased as follows.

Theorem 3.2. *Suppose $\widehat{u} \in B_0^*(\mathcal{V})$ satisfies $(-\widehat{\Delta}_{\mathcal{V}} - \lambda)\widehat{v} = 0$ near infinity of the lattice space. Then, $\widehat{v} = 0$ near infinity.*

Extending $\widehat{u}$ to be 0 in the finite part and passing to the Fourier series, we obtain the equation

$$(H_0(x) - \lambda)u(x) = f(x),$$

where $f(x)$ is a trigonometric polynomial, since its Fourier coefficients are compactly supported. Then, the Rellich type theorem on the lattice is formulated and proved in the following form.

Theorem 3.3. *Let $\lambda \in (-1,1)\backslash\{0, \pm 1/3, \pm 1\}$. Let $u(x) \in B_0^*(\mathbf{T}^2)$ satisfy $(H_0(x) - \lambda)u(x) = f(x)$, where $f(x)$ is a trigonometric polynomial. Then, $u(x)$ is also a trigonometric polynomial.*

The proof relies on the HilbertNullStellenSatz ([18], [2]). Similar theorem also holds for the edge Hamiltonian. In particular, the non-existnece of embedded eigenvalues follows. Put

$$\sigma_{\mathcal{V}} = (-1,1) \setminus \{0, \pm 1/3, \pm 1\},$$

$$\sigma_{\mathcal{E}} = (0,\infty) \setminus \Big(\sigma_D \cup \{\lambda; -\cos\sqrt{\lambda} = 0, \pm 1/3, \pm 1\}\Big).$$

Corollary 3.4. *(1)* $\sigma_p(\widehat{H}_{\mathcal{V}}) \cap \sigma_{\mathcal{E}} = \emptyset$.
(2) $\sigma_p(\widehat{H}_{\mathcal{E}}) \cap \sigma_{\mathcal{E}} = \emptyset$.

For the preceeding results about the spectra of vertex models and edge models, see e.g. [6], [16], [14], [5], [6], [13].

4. Forward problem

For the vertex model, the space $\widehat{B}(\mathcal{V})$ is defined by

$$\widehat{B}(\mathcal{V}) \ni \widehat{f} \Longleftrightarrow \sum_{j=0}^{\infty} r_j^{1/2} \Big(\sum_{r_{j-1} \leq |n| < r_j} |\widehat{f}(n)|^2 \Big)^{1/2} < \infty,$$

where $r_{-1} = 0$, $r_j = 2^j$ $(j \geq 0)$. Then, the spaces $\widehat{B}(\mathcal{V})$, $\widehat{B}^*(\mathcal{V})$ rig the Hilbert space $\ell^2(\mathcal{V})$:

$$\widehat{B}(\mathcal{V}) \subset \ell^2(\mathcal{V}) \subset \widehat{B}^*(\mathcal{V}).$$

For the edge model, the Besov type spaces $\widehat{B}(\mathcal{E})$, $\widehat{B}^*(\mathcal{E})$, $\widehat{B}_0^*(\mathcal{E})$ are defined similarly, e.g.

$$\widehat{B}^*(\mathcal{E}) \ni \widehat{f} \Longleftrightarrow \sup_{R>1} \frac{1}{R} \sum_{\mathbf{e} \subset B_R} \|\widehat{f}_{\mathbf{e}}\|^2_{L^2(0,1)} < \infty,$$

where $B_R = \{x \in \mathbf{R}^2\,;\, |x| < R\}$. Their counter parts on the torus are defined by

$$\begin{aligned} B(\mathbf{T}^2 \times I_{\mathcal{E}}) \ni f &\Longleftrightarrow \widehat{f} \in \widehat{B}(\mathcal{E}), \\ B^*(\mathbf{T}^2 \times I_{\mathcal{E}}) \ni f &\Longleftrightarrow \widehat{f} \in \widehat{B}^*(\mathcal{E}), \\ B_0^*(\mathbf{T}^2 \times I_{\mathcal{E}}) \ni f &\Longleftrightarrow \widehat{f} \in \widehat{B}_0^*(\mathcal{E}), \end{aligned}$$

where $I_{\mathcal{E}} = (0,1)$, and $\widehat{f}$ denotes the Fourier coefficient of $f(x,z)$ with respect to x (with a suitable cut-off function).

Let $\widehat{R}_{\mathcal{V}}(z) = (\widehat{H}_{\mathcal{V}} - z)^{-1}$ and $\widehat{R}_{\mathcal{E}}(z) = (\widehat{H}_{\mathcal{E}} - z)^{-1}$. Then, the following weak $*$-limits exist.

Theorem 4.1. *For* $\lambda \in \sigma_{\mathcal{V}}$, $\widehat{R}_{\mathcal{V}}(\lambda \pm i0) \in \mathbf{B}(\widehat{B}(\mathcal{V}); \widehat{B}^*(\mathcal{V}))$.

Theorem 4.2. *For* $\lambda \in \sigma_{\mathcal{E}}$, $\widehat{R}_{\mathcal{E}}(\lambda \pm i0) \in \mathbf{B}(\widehat{B}(\mathcal{E}); \widehat{B}^*(\mathcal{E}))$.

Once we have proven this limiting absorption principle, one can follow the stationary theory of scattering developed by Kato-Kuroda [12], Ikebe [10], Agmon [1] without any difficulty, namely, existence and completeness of time-dependent wave operators, eigenfunction expansion theory, unitarity of the S-matrix and its representation by generalized eigenfunctions.

In some energy region, one can define the S-matrix by using the asymptotic behavior of wave functions at the infinity of the lattice space. However, for both of the vertex model and the edge model, it is more convenient to obeserve the behavior of singularities of wave functions on the torus, since there is no restricton of energy. For the vertex model, it is stated as follows. Recall that $H_0(x)$ has two eigenvalues $\lambda_j(x)$ and the eigenprojections $P_j(x)$, $j = 1, 2$. Define

$$M_{\lambda,j} = \{x \in \mathbf{T}^2\,;\, \lambda_j(x) = \lambda\},$$

$$M_\lambda = M_{\lambda,1} \cup M_{\lambda,2}.$$

Theorem 4.3. *Let $\lambda \in \sigma_{\mathcal{V}}$. For any $\varphi^{in} \in L^2(M_\lambda)$, there exist a unique $\varphi^{out} \in L^2(M_\lambda)$ and $\widehat{u} \in B^*(\mathcal{V})$ such that*

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

$$\begin{aligned} u \simeq & \frac{1}{2\pi i}\sum_{j=1,2} \frac{1}{\lambda_j(x) - \lambda \mp i0} \otimes P_j(x)\varphi^{out} \\ & - \frac{1}{2\pi i}\sum_{j=1,2} \frac{1}{\lambda_j(x) + \lambda \mp i0} \otimes P_j(x)\varphi^{in}, \end{aligned}$$

where $f \simeq g$ means $f - g \in B_0^*(\mathbf{T}^2)$. The unitary operator

$$S(\lambda) : L^2(M_\lambda) \ni \varphi^{in} \to \varphi^{out} \in L^2(M_\lambda)$$

is the S-matrix.

For the edge model, the above theorem is stated as follows.

Theorem 4.4. *Let $\lambda \in \sigma_{\mathcal{E}}$. For any incoimg data $\phi^{in} \in L^2(M_{-\cos\sqrt{\lambda}})$, there exist a unique solution $\widehat{u} \in \widehat{B}^*(\mathcal{E})$ of the equation*

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

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

$$\begin{aligned} u \simeq & B(\lambda)\sum_{j=1,2} \frac{1}{\lambda_j(x) + \cos\sqrt{\lambda} - i\epsilon(\lambda)} \otimes P_j(x)\varphi^{out} \\ & - B(\lambda)\sum_{j=1,2} \frac{1}{\lambda_j(x) + \cos\sqrt{\lambda} + i\epsilon(\lambda)} \otimes P_j(x)\varphi^{in}, \end{aligned}$$

where $f \simeq g$ means $f - g \in B_0^*(\mathbf{T}^2 \times I_{\mathcal{E}})$. The unitary operator

$$S(\lambda) : L^2(M_{-\cos\sqrt{\lambda}}) \in \varphi^{in} \to \varphi^{out} \in L^2(M_{-\cos\sqrt{\lambda}})$$

is the S-matrix.

Here $B(\lambda) \in \mathbf{B}(B^*(\mathbf{T}^2 \times I_{\mathcal{E}}); B^*(\mathbf{T}^2 \times I_{\mathcal{E}}))$ and $\epsilon(\lambda) = \pm 1$, however we omit the precise definition.

5. From S-matrix to D-N map

As in the case of continuous model, the inverse scattering on the whole space is reduced to an inverse boundary value problem in a bounded domain. Take a sufficiently large bounded set containing all perturbations. Then, the equation in the whole space is split into three parts: the exterior boundary value problem, the interior boundary value problem and the (integral) equation on the boundary.

We follow the same approach for the vertex model and edge model. Take a bounded domain Ω_{int} enclosing all perturbations, and let Ω_{ext} be the exterior domain so that

$$\Omega_{ext} \cup \Omega_{int} = \mathcal{V}, \qquad \partial\Omega_{ext} = \partial\Omega_{int}.$$

Consider the Dirichlet problem

$$\begin{cases} (-\widehat{\Delta}_{\mathcal{V}} - \lambda)\widehat{u} = 0, & \text{in} \quad \Omega_{int}, \\ \widehat{u} = \widehat{f}, & \text{on} \quad \partial\Omega_{int}. \end{cases}$$

The Neumann derivative is defined by

$$\partial_\nu \widehat{u} = -\widehat{\Delta}_{\mathcal{V}}\widehat{u}\Big|_{\partial\Omega_{int}}.$$

Then, the D-N map, Dirichlet-to-Neumann map, is defined by

$$\Lambda_{int}(\lambda) : \widehat{f} \to \partial_\nu \widehat{u}.$$

The S-matrix is defined in the whole space and in the exterior domain as well. We denote them $S(\lambda)$ and $S_{ext}(\lambda)$, and define the scattering amplitudes

$$S(\lambda) = I - 2\pi i A(\lambda), \quad S_{ext}(\lambda) = I - 2\pi i A_{ext}(\lambda).$$

Then, the following formula holds:

$$A_{ext}(\lambda) - A(\lambda) = \widehat{\mathcal{I}}^{(+)}(\lambda) B_\Sigma(\lambda)^{-1} \big(\widehat{\mathcal{I}}^{(-)}(\lambda)\big)^*, \tag{5.1}$$

$$B_\Sigma(\lambda) = \Lambda_{int}(\lambda) - \Lambda_{ext}(\lambda) - \lambda\chi_\Sigma.$$

Here, $\Sigma = \partial\Omega_{int} = \partial\Omega_{ext}$, $\widehat{\mathcal{I}}^{(\pm)}(\lambda) : L^2(M_\lambda) \to \ell^2(\Sigma)$ are some injective operators, $\Lambda_{ext}(\lambda)$ is the D-N map in the exterior domain, and χ_Σ is the characterisitic function of Σ. Since all perturbations are confined to Ω_{int}, we know $\widehat{\mathcal{I}}^{(\pm)}(\lambda)$ and $\Lambda_{ext}(\lambda)$. Therefore, (5.1) means that $S(\lambda)$ and $\Lambda_{int}(\lambda)$ determine each other.

The edge model can be dealt with similarly.

6. Inverse scattering

6.1. **Vertex model - reconstruction of the potential.** In the inverse boundary value problem for the continuous case, the exponentially growing solution for the Schrödinger equation plays an important role. It solves the Schrödinger equation $(-\Delta + V(x) - \lambda)u = 0$ in $\mathbf{R}^n$, and is exponentially growing in a half-space, and exponentially decaying in the opposite half-space. There is a counter part of this solution in the discrete model. In [11], we used a solution to the discrete Schrödinger equation on the square lattice, which vanishes in a half-space and non-zero in the opposite half-space, to recontsruct the scalar potential from the S-matrix. A similar idea works well for the hexaogonal lattice.

Theorem 6.1. *Consider the vertex Schrödinger operator on the hexagonal lattice with a compactly supported scalar potential. Then, the potential is uniquely reconstructed from the S-matrix $S(\lambda)$ for an arbitrarily given fixed energy $\lambda \in \sigma_{\mathcal{V}}$.*

6.2. **Vertex model-recovery as a planar graph.** Another central issue in the inverse boundary value problem for the continuous model is the reconstruction of the Riemannian metric from the D-N map with 0 energy. This is an interpretation of the inverse problem of electrical impedance tomography. We expect that the metric is determined by the D-N map up to a diffeomorphism which leaves the boundary of the domain invariant. It is proved in 2-dimensions in the general setting, and for the real analytic case with dimension $n \geq 3$.

The counter part of the Riemannian manifold in the discrete model is the planar graph. By the works of Colin de Verdière [7], [8] and Curtis-Morrow [9], it is known that the D-N map determines the planar graph up to elementary transformations. In the case of hexagonal lattice, the D-N map for the planar graph corresponds to the S-matrix with energy at the bottom of the continuous spectrum. Therefore, we obtain the following theorem.

Theorem 6.2. *For a sequence of energies $\lambda_n \in \sigma_{\mathcal{V}}$ such that $\lambda_n \to -1$, the S-matrices $S(\lambda_n)$ determine the perturbed finite part of the hexagonal lattice up to elementary transformations.*

The equivalence of the S-matrix and the D-N map can be proven for a wide class of lattices, e.g. those introduced in [2]. Therefore, Theorem 6.2 holds for such class of vertex models.

6.3. **Vertex model - proving defects.** A physically important example of the perturbation as a graph is the defect of the lattice. We consider the case where the defects are bounded. By virtue of Theorem 6.2, one can reconstruct the perturbed graph *topologically*. However, it does not give the information of the location of defects. To study it, we utilize the above mentioned analogue of exponentially growing solution to the Schrödinger equation on the hexagonal lattice. Take a straight line L in the lattice and construct the solution to the free Schrödinger equation which vanishes below L but does not vanish above L. Suppose that the all defects are lying below L. If we take it as an input of the D-N map, the output is the same as that of the unperturbed case. Let us move the line L downwards. Then, it will touch the defects. At this moment, the output of the D-N map changes, and we conclude that there is a defect on the line L. Therefore, we can enclose the defects from above. Changing the dierction of the line L, we get the following theorem.

Theorem 6.3. *Assume that the defects consist of finite convex polygons. Then, from the S-matrix $S(\lambda)$ with an arbitrarily fixed energy $\lambda \in \sigma_{\mathcal{V}}$, one can determine the convex hull of the defects.*

Theorems 6.1 ,6.2, 6.3 will appear in [3].

6.4. **Edge model - reconstuction of the potential.** One can use the same idea for the edge model. By the above procedure, one can compute the coefficients for the perturbed vertex Laplacian from the D-N map. It consists of $\phi_{\mathbf{e}0}(0,\lambda)$, where $\phi_{\mathbf{e}0}(z)$ is the solution to the Schrödinger equation $(-(d/dz)^2+q_{\mathbf{e}}(z)-\lambda)\phi_{\mathbf{e}0}(z,\lambda)=0$ with initial data $\phi_{\mathbf{e}0}(0,\lambda)=0$. Then, the zeros of $\phi_{\mathbf{e}(0)}(0,\lambda)$ are the Dirichlet eigenvalues of the operator $-(d/dz)^2+q_{\mathbf{e}}(z)-\lambda$. Recall Borg's theorem [4], which is the starting point of the inverse spectral theory : A symmetric potential on $(0,1)$ is determined by its Dirichlet eigenvalues. We have thus arrived at the following theorem.

Theorem 6.4. *Let I be an open interval in $\sigma_{\mathcal{E}}$. Then, the potential is determined from the S-matrix $S(\lambda)$ for all energies $\lambda \in I$.*

One can also deal with non-zero back ground potentials.

Theorem 6.5. *Let $q_0(z) \in L^2(0,1)$ be real and symmetric. Suppose that the edge potentials $q_{\mathbf{e}}(z)$ coincide with $q_0(z)$ except for a finite number of edges. Let I be an open interval in $\sigma_{\mathcal{E}}$. Then, the potential $q_{\mathcal{E}}$ is determined from the S-matrix $S(\lambda)$ for all energies $\lambda \in I$.*

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HIROSHI ISOZAKI

Professor Emeritus, University of Tsukuba, Tsukuba, 305-8571, Japan