September 24, 2012 Université de Sud Toulon-Var

Spectrum of Discrete Schrödinger Operator and Discrete Laplacian

Department of Mathematics, Faculty of Engineering, Shinshu University

Akito Suzuki

Motivation

Let us consider \mathbb{Z}^d as a (idealized) crystal lattice. Then :

- A vertex of $\mathbb{Z}^d \to \text{atom}$ (or ion) that forms the crystal.
- An **edge** connecting two vertices \rightarrow a chemical bond of two atoms.
- The **spectrum** of $-\Delta_{\mathbb{Z}^d} \to$ the energy of an electron in the crystal.

Part I: We consider $H = -\Delta_{\mathbb{Z}^d} + \delta(x)$ describing an electron interacting with an impurity.

Part II: We deform \mathbb{Z}^d by adding another vertex periodically. Then the resulting graph describes a deformed crystal by adding another atom.

We are interested in how the spectrum changes in the presence of an impurity and in deforming the lattice.

PART I: Discrete Schrödinger operator

Joint work with F. Hiroshima, I. Sasaki and T. Shirai

1 Definition of Laplacian on a graph

Let G = (V(G), E(G)) be a graph:

- $\bullet \ V(G)$: the set of vertices
- $\bullet \ E(G)$: the set of edges

If there is an edge connecting two vertices x and y, then we denote the edge by $\{x, y\}$, say that x is adjacent to y, and write $x \sim y$.

• deg $x = #\{y \in V(G) \mid y \sim x\}$

Example:

• \mathbb{Z}^d is a graph.

 $V(\mathbb{Z}^d) = \mathbb{Z}^d, \ E(\mathbb{Z}^d) = \{\{x, y\} \mid |x - y| = 1\}$

For example, in the case of d = 1, $x \in \mathbb{Z}$ is adjacent to $y = x \pm 1$. In general, for $x \in \mathbb{Z}^d$, we have $\deg x = 2d$. Define the Laplacian $-\Delta_G$ on G as follows:

$$(-\Delta_G \psi)(x) = \frac{1}{\deg x} \sum_{y \sim x} \{\psi(x) - \psi(y)\}, \quad \psi \in \ell^2(V(G))$$

• $\ell^2(V(G)) = \{\psi : V(G) \to \mathbb{C} \mid \sum_{x \in V(G)} (\deg x) | \psi(x) |^2 < \infty\}$

• $\langle \psi, \varphi \rangle = \sum_{x \in V(G)} (\deg x) \overline{\psi(x)} \varphi(x)$

Then $-\Delta_G$ is bounded self-adjoint on $\ell^2(V(G))$.

Example : the Laplacian on $\mathbb Z$

• $\forall x \in \mathbb{Z}$ is adjacent to $x \pm 1$ and $\deg x = 2$.

$$ullet$$
 $-\Delta_{\mathbb{Z}}$ is

$$(-\Delta_{\mathbb{Z}}\psi)(x) = \frac{1}{2}\{(\psi(x) - \psi(x+1)) + (\psi(x) - \psi(x-1))\}$$
$$= \psi(x) - \frac{1}{2}(\psi(x+1) + \psi(x-1))$$

What is the Laplacian on \mathbb{Z} ?

Let
$$\psi(x) = \phi(hx)$$
. Then
 $\psi(x+1) = \psi(x) + h\psi'(x) + \frac{h^2}{2}\psi''(x) + O(h^3)$
 $\psi(x-1) = \psi(x) - h\psi'(x) + \frac{h^2}{2}\psi''(x) + O(h^3)$
 $\therefore -\psi''(x) = \frac{1}{h^2}(-\Delta_{\mathbb{Z}}\psi)(x) + O(h)$

Warm up: Let \mathcal{F} be the discrete Fourier transformation:

$$(\mathcal{F}\psi)(k) = \sum_{x \in \mathbb{Z}} e^{-ik \cdot x} \psi(x), \quad k \in [-\pi, \pi].$$

Then $\mathcal{F}\psi(\cdot\pm 1)(k) = e^{\pm ik}(\mathcal{F}\psi)(k)$ and

$$\mathcal{F}(-\Delta_{\mathbb{Z}})\mathcal{F}^{-1} = 1 - \cos k.$$
$$\therefore \sigma(-\Delta_{\mathbb{Z}}) = [0, 2].$$

2 Problem

The spectrum of the Schrödinger operator with a delta potential: Let $H(v) = -\Delta_{\mathbb{Z}^d} - v\delta_0(x)$ ($v \ge 0$). $\delta_0(x) = \begin{cases} 0, & x \neq 0\\ 1, & x = 0 \end{cases}$

In the case of v = 0:

$$\sigma(H(0)) = \sigma_{\text{ess}}(H(0)) = \sigma(-\Delta_{\mathbb{Z}^d}) = [0, 2]$$

Since $\delta_0(x)$ is a finite rank operator, we have

$$\sigma_{\rm ess}(H(v)) = [0, 2], \quad v \ge 0, d \ge 1.$$

We are interested in

- $\sigma_{\rm p}(H(v))$: the set of eigenvalues
- $\sigma_{\rm d}(H(v))$: the set of discrete eigenvalues

REMARK 1 (embedded eigenvalue). In general, $\sigma_d(H(v)) \subset \sigma_p(H(v))$. For example, it is possible that

 $E \in \sigma_{p}(H(v)) \setminus \sigma_{d}(H(v))$ is an embedded eigenvalue.

REMARK 2 (continuous analog). Let

$$H_{\mathcal{S}}(v) = -\Delta_{\mathbb{R}^d} - vW(x)$$

be the Schrödinger operator on $L^2(\mathbb{R}^d)$ and suppose that

 $W \ge 0, \quad W \in C_0^\infty(\mathbb{R}^d).$

Then $\sigma_{\rm ess}(H_{\rm S}(v)) = [0,\infty)$ for all $d \ge 1$ and $v \ge 0$ and

- $d = 1, 2 \Longrightarrow H_{S}(v)$ has an eigenvalue E(v) < 0 for all v > 0.
- $d \ge 3 \Longrightarrow \exists v_0 > 0$ such that
 - i) $H_{\rm S}(v)$ has no negative eigenvalue for $v < v_0$
 - ii) $H_{\rm S}(v)$ has an eigenvalue E(v) < 0 for $v > v_0$

3 The spectrum of $H(v) = -\Delta_{\mathbb{Z}^d} - v\delta_0(x)$

Let

$$g_d(k) = \frac{1}{d} \sum_{j=1}^d \cos k_j$$

with $k = (k_1, \cdots, k_d) \in [-\pi, \pi]^d$. Note that

$$\mathcal{F}(-\Delta_{\mathbb{Z}^d})\mathcal{F}^{-1} = 1 - g_d$$

and hence $\sigma(-\Delta_{\mathbb{Z}^d}) = [0,2].$ Similarly, we have

$$\mathcal{F}H(v)\mathcal{F}^{-1} = 1 - g_d - vP, \quad L^2([-\pi,\pi]^d).$$

where

$$(Pf)(k) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} f(k) dk, \quad f \in L^2([-\pi,\pi]^d).$$

Let $\varphi \equiv (2\pi)^{-d/2} \in L^2([-\pi,\pi]^d)$. Then $Pf = \langle \varphi, f \rangle_{L^2([-\pi,\pi]^d)} \varphi$, so the dimension of the range of P is one and P is a finite rank operator.

THEOREM 1.

(1) $d = 1, 2: \forall v > 0, \exists E(v) < 0$ such that $\sigma_{\rm d}(H(v)) = \sigma_{\rm p}(H(v)) = \{E(v)\}.$ In particular, if d = 1, then $E(v) = 1 - \sqrt{1 + v^2}$. (2) $d = 3, 4: \exists v_c > 0$ such that i) $v \leq v_{\rm c} \Rightarrow \sigma_{\rm p}(H(v)) = \emptyset$. ii) $v > v_{c} \Rightarrow \sigma_{d}(H(v)) = \sigma_{p}(H(v)) = \{E(v)\}$ with some E(v) < 0. (3) $d \geq 5$: $\exists v_c > 0$ such that i) $v < v_{\rm c} \Rightarrow \sigma_{\rm p}(H(v)) = \emptyset$. ii) $v = v_{\rm c} \Rightarrow \sigma_{\rm p}(H(v)) = \{0\}.$ iii) $v > v_{c} \Rightarrow \sigma_{d}(H(v)) = \sigma_{p}(H(v)) = \{E(v)\}$ with some E(v) < 0. **REMARK 3.** For d = 1, 2, we set $v_c = 0$. Then

- $0 \le v \le v_{c} \Rightarrow \sigma(H(v)) = \sigma(-\Delta_{\mathbb{Z}^{d}}) = [0, 2].$
- For $1 \le d \le 4$, $E(v) \in \sigma_p(H(v))$ iff. $v > v_c$.
- For $d \ge 5$, $E(v) \in \sigma_p(H(v))$ iff. $v \ge v_c$.
- It is easy to see, for d = 1, E(v) is monotonically decreasing in $v \ge v_c$ and $\lim_{v \to v_c} E(v) = 0$. This is the case for $d \ge 2$.
- In particular, $E(v_c) = 0$ is an embedded eigenvalue for $d \ge 5$.



4 Proof of Theorem 1

Let $h(v) = g_d + vP$. Then $\mathcal{F}H(v)\mathcal{F}^{-1} = 1 - h(v)$ and hence $\lambda \in \sigma_p(h(v)) \iff 1 - \lambda \in \sigma_p(H(v)).$ $\ker(h(v) - \lambda) = \ker(H(v) - E), \quad E = 1 - \lambda.$

We will consider $\sigma_{\mathbf{p}}(h(v))$:

LEMMA 1. $\lambda \in \sigma_{p}(h(v))$ is equivalent to:

$$\frac{1}{\lambda - g_d} \in L^2([-\pi, \pi]^d) \quad \text{and} \quad v = (2\pi)^d \left(\int_{[-\pi, \pi]^d} \frac{dk}{\lambda - g_d(k)} \right)^{-1}$$

Moreover, if ψ is an eigenvector of $\lambda \in \sigma(h(\lambda))$, then

$$\psi(k) = rac{c}{\lambda - g_d(k)}$$
 with some $c \in \mathbb{C}$.

In particular, $\lambda \in \sigma_p(h(\lambda))$ is simple.

Proof of LEMMA 1: Let ψ be an eigenvector of $\lambda \in \sigma_p(h(\lambda))$. Then

$$g_d(k)\psi(k) + \frac{v}{(2\pi)^d} \int_{[-\pi,\pi]^d} \psi(k)dk = \lambda\psi(k)$$

$$\therefore \psi(k) = \frac{c}{\lambda - g_d(k)} \in L^2([-\pi,\pi]^d), \qquad (1)$$

where

$$c = \frac{v}{(2\pi)^d} \int_{[-\pi,\pi]^d} \psi(k) dk.$$
 (2)

Substituting (1) into (2), we have

$$1 = \frac{v}{(2\pi)^d} \int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} dk$$
$$\therefore v = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} \right)^{-1}$$

Condition:
$$v = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} dk \right)^{-1}$$

Note that

$$\lambda \in (-1,1) \iff \frac{1}{\lambda - g_d} \not\in L^1([-\pi,\pi]^d)$$

and hence $\sigma_{\mathbf{p}}(h(v)) \cap (-1,1) = \emptyset$. Since

$$\lambda \in (-\infty, -1] \Longleftrightarrow \int_{[-\pi, \pi]^d} \frac{1}{\lambda - g_d(k)} dk \le 0,$$

we see that $\sigma_{\mathbf{p}}(h(v)) \subset [1, \infty)$.

LEMMA 2. The function

$$[1,\infty) \ni \lambda \mapsto (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} dk \right)^{-1} \in [v_c,\infty)$$

is a continuous (strictly) increasing function, where

$$v_{\rm c} = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{1 - g_d(k)} dk \right)^{-1} \in [0,\infty).$$

From LEMMA 2, we observe that

$$v \in [v_{\rm c}, \infty) \iff \exists \lambda = \lambda(v) \quad \text{s.t.} \quad v = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} dk \right)^{-1}$$

Let us calculate the value of $v_{\rm c}$. Note that

$$1 - g_d(k) \approx \frac{|k|^2}{2d}, \quad |k| \approx 0$$
$$\int_{[-\pi,\pi]^d} \frac{1}{1 - g_d(k)} dk \ge c \int_{[-\epsilon,\epsilon]^d} \frac{1}{|k|^2} dk = +\infty, \quad d = 1, 2$$
$$\therefore v_{\rm c} = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{1 - g_d(k)} dk \right)^{-1} \quad \begin{cases} = 0, \quad d = 1, 2\\ > 0, \quad d \ge 3. \end{cases}$$

Hence, we have $\sigma_{\rm p}(h(v)) = \emptyset$ if $d \ge 3$ and $v \in [0, v_{\rm c})$.

Condition: $\frac{1}{\lambda - g_d} \in L^2([-\pi, \pi]^d)$

Note that if $v \in (v_c, \infty)$, then $\exists \lambda = \lambda(v) \in (1, \infty)$ such that λ satisfies $v = (2\pi)^d \left(\int_{[-\pi,\pi]^d} \frac{1}{\lambda - g_d(k)} dk \right)^{-1}$. If $\lambda(v) > 1$, then $\inf_{k \in [-\pi,\pi]^d} |\lambda(v) - g_d(k)| > 0$ and hence $\frac{1}{\lambda(v) - g_d} \in L^2([-\pi,\pi]^d)$.

 $\therefore \lambda(v) \in \sigma_{\mathbf{p}}(h(v)), \quad v > v_{\mathbf{c}}.$

$$\begin{array}{ll} \displaystyle \frac{\ln \ \text{the case of }v=v_{\rm c}\text{:}}{\lambda(v_{\rm c})=1 \ \text{and}}\\ & \displaystyle \frac{1}{|1-g_d(k)|^2}\approx \frac{4d^2}{|k|^4}, \quad \text{near} \ k=0. \end{array}$$
 Hence

$$\frac{1}{1-g_d} \in L^2([-\pi,\pi]^d) \iff d \ge 5.$$

PART II: Discrete Laplacian on a graph

5 Models

DEFINITION 1.

(1) A vertex of degree one is called an end vertex. (2) An edge incident to an end vertex is called a pendant edge. (3) Let G be a graph obtained from \mathbb{Z}^d by adding pendant edges periodically. Then we say that $G \in \mathscr{G}^d$.

We consider the spectrum of $-\Delta_G$ on $G \in \mathscr{G}^d$ with d = 1, 2.

REMARK 4. In the case of the crystal lattice:

Adding a pendant edge to $\mathbb{Z}^d \longrightarrow adding another atom to the crystal$ $<math>\rightarrow deformation of the crystal.$

We are interested in how the spectrum changes in deforming the crystal.

Example 1. Let $G_{1,1} \in \mathscr{G}^1$ be a graph obtained from \mathbb{Z} by adding a pendant edge at each vertex of \mathbb{Z} . Then we identify $V(G_{1,1,})$ with $\mathbb{Z} \times \{0,1\}$ as follows:

- A vertex $n \in \mathbb{Z}$ is identified with $(n, 0) \in \mathbb{Z} \times \{0, 1\}$.
- An end vertex adjacent to $n \in \mathbb{Z}$ is identified with $(n, 1) \in \mathbb{Z} \times \{0, 1\}$.



Let us calculate the spectrum of $-\Delta_{G_{1,1}}$:

• The Laplacian $-\Delta_{G_{1,1}}$ on $\ell^2(\mathbb{Z} \times \{0,1\})$ is given as follows. The vertex $(n,0) \in \mathbb{Z} \times \{0,1\}$ has degree 3 and

$$(-\Delta_{G_{1,1}}\psi)(n,0) = \frac{1}{3} \{ (\psi(n,0) - \psi(n+1,0)) + (\psi(n,0) - \psi(n,1)) \} + (\psi(n,0) - \psi(n,0)) + (\psi(n,0) - \psi(n,1)) \}.$$

The vertex $x = (n, 1) \in \mathbb{Z} \times \{0, 1\}$ has degree 1 and

$$(-\Delta_{G_{1,1}}\psi)(n,1) = \psi(n,1) - \psi(n,0)$$

• Let $\mathcal{J}: \ell^2(\mathbb{Z} \times \{0,1\}) \longrightarrow L^2([-\pi,\pi]^d; \mathbb{C}^2)$ be a unitary operator defined by

$$(\mathcal{J}\psi)(k) = \begin{pmatrix} \hat{\psi}(k,0)\\ \hat{\psi}(k,1) \end{pmatrix}, \quad \psi \in \ell^2(\mathbb{Z} \times \{0,1\}),$$

where $\hat{\psi}(k,s) = (2\pi)^{-1/2} \sum_{n \in \mathbb{Z}} e^{-ikn} \psi(n,s)$, $(k,s) \in [-\pi,\pi] \times \{0,1\}$.

• Using \mathcal{J} , we have

$$\mathcal{J}(-\Delta_{G_{1,1}})\mathcal{J}^{-1} = \begin{pmatrix} 1 - \frac{2}{3}\cos k & -\frac{1}{3} \\ -1 & 1 \end{pmatrix} \quad \text{on } L^2([-\pi, \pi]^d; \mathbb{C}^2).$$

• The eigenvalues of this matrix are

$$\lambda_{\pm}(k) = 1 - \frac{1}{3}\cos k \pm \frac{1}{3}\sqrt{\cos^2 k + 3}$$

and hece

$$\sigma(-\Delta_{G_{1,1}}) = \{\lambda_{-}(k) \mid k \in [-\pi, \pi]\} \cup \{\lambda_{+}(k) \mid k \in [-\pi, \pi]\}$$
$$= \left[0, \frac{2}{3}\right] \cup \left[\frac{4}{3}, 2\right]$$

• In particular, $-\Delta_{G_{1,1}}$ has a spectral gap!

Example 2. Let $G_{2,1} \in \mathscr{G}^1$ be a graph obtained from \mathbb{Z} by adding a pendant edge to \mathbb{Z} alternately. We still consider $V(G_{2,1}) \subset \mathbb{Z} \times \{0,1\}$. Graph $G_{2,1}$



$$\mathcal{J}(-\Delta_{G_{2,1}})\mathcal{J}^{-1} = \begin{pmatrix} 1 & -\frac{1+e}{3} & -\frac{1}{3} \\ -\frac{1+e^{ik}}{2} & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

• The eigenvalues of the matrix is $\lambda_0(k) \equiv 1$ and

$$\lambda_{\pm}(k) = 1 \pm \sqrt{\frac{2 + \cos k}{3}}$$

and

$$\sigma(-\Delta_{G_{2,1}}) = \left[0, \ 1 - \frac{1}{\sqrt{3}}\right] \cup \{1\} \cup \left[1 + \frac{1}{\sqrt{3}}, \ 2\right]$$

• In particular, $\sigma_p(-\Delta_{G_{2,1}}) = \{1\}$ and $-\Delta_{G_{2,1}}$ has a spectral gap!

REMARK 5. The periodicity of pendant edges of $G \in \mathscr{G}^1$ means that:

 $\exists r \in \mathbb{N}$ such that

$$(n,1) \in V(G) \iff (n+r,1) \in V(G).$$

Example: For $G_{1,1}$ and $G_{2,1}$, we see that r = 1 and r = 2, respectively.

Let $G \in \mathscr{G}^1$ with a period $r \in \mathbb{N}$. Then we define

$$s := \#\{(n,1) \in V(G) \mid n = 1, \cdots r\}$$

Example: For $G_{1,1}$ and $G_{2,1}$, we see that s = 1.

THEOREM 2. Let G and r be as above. Suppose that $s \ge 1$. Then: (1) $-\Delta_G$ has a spectral gap around one, i.e.,

 $\sigma(-\Delta_G) \cap (1-\epsilon, 1+\epsilon) = \emptyset$ with some $\epsilon > 0$.

(2) $-\Delta_G$ has no eigenvalue except for one, i.e.,

 $\sigma_{\mathbf{p}}(-\Delta_G) \setminus \{1\} = \emptyset.$

(3) $1 \in \sigma_p(-\Delta_G)$ iff. there is a series of vertices of degree two satisfying the following: (i) these vertices are adjacent to each other and adjacent to vertices of dgree three at the both ends; (ii) the number of these vertices in this series is odd.

Example: We consider the following graph $G_{4,1} \in \mathscr{G}^1$ with a period r = 4 and s = 1.



(n,0) (n+1,0)(n+2,0) (n+3,0)(n+4,0)Then (n+1,0), (n+2,0), (n+3,0) are a series of vertices of degree two satisfying (i) and (ii):

(i) (n + 1, 0), (n + 2, 0), (n + 3, 0) are adjacent to each other and (n + 1, 0) and (n + 3, 0) adjacent to vertices of degree three.

(ii) The number of these vertices of degree two is three, so it is odd. Hence we have $1 \in \sigma_p(-\Delta_{G_{4,1}})$. **Example:** In the case of $G_{2,1}$, (n + 1, 0) is a vertex of degree two satisfying (i) and (ii) in the following sense:

Graph $G_{2,1}$



Example: We consider the following graph $G_{3,1} \in \mathscr{G}^1$ with a period r = 3 and s = 1.



Then (n + 1, 0), (n + 2, 0) are a series of vertices of degree two, which are adjacent to each other and adjacent to vetices of degree three at both ends.

However, the number of these vetices are two.

Hence $\sigma_{\mathbf{p}}(-\Delta_{G_{3,1}}) = \emptyset$.

6 Idea of the proof of Theorem 2 (3)

In the case of $-\Delta_{G_{2,1}}$, we have

$$\mathcal{J}(-\Delta_{G_{2,1}})\mathcal{J}^{-1} = \begin{pmatrix} 1 & -\frac{1+e^{-ik}}{3} & -\frac{1}{3} \\ -\frac{1+e^{ik}}{2} & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \equiv L(k).$$

The eigenvalue λ of L(k) satisfy

$$\begin{aligned} |\lambda - L(k)| &= \begin{vmatrix} \lambda - 1 & \frac{1 + e^{-ik}}{3} & \frac{1}{3} \\ \frac{1 + e^{ik}}{2} & \lambda - 1 & 0 \\ 1 & 0 & \lambda - 1 \end{vmatrix} \equiv \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \\ &= a_{11}a_{22}a_{33} - a_{13}a_{31}a_{22} - a_{12}a_{21}a_{33} = 0. \end{aligned}$$

Since $a_{ii} = (\lambda - 1)$, we see that $\lambda = 1$ an eigenvalue of L(k). In order to extend this result, we use a graph theoretic calculation as follows: We consider r + s = 3 vertices in a period such as (n, 0), (n + 1, 0) and (n, 1) and call them 1, 2 and 3. Then the factor $a_{jj} = \lambda - 1$ corresponds to a vertex i; the factor $a_{ij}a_{ji}$ corresponds to an edge connecting i and j.



In the case where (ii) are not satisfied:

For $G_{3,1}$, we consider r + s = 4 vertices in a period such as (n, 0), (n + 1, 0), (n + 2, 0) and (n, 1) and call them 1, 2, 3 and 4.



Since the number of vetices of degree two which are adjacent to each other in a period is two, $(\lambda - 1)^0$ is possible. Hence there is no eigenvalue.

REMARK 6. Higher dimensional cases are more complicated. Indeed, there are graphs $G, G' \in \mathscr{G}^2$ such that $-\Delta_G$ has a spectral gap but $-\Delta_{G'}$ has no spectral gap.

Thank you for your kind attention!