Note on the spectrum of discrete Schrödinger operators

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Abstract

The spectrum of discrete Schrödinger operator $L + V$ on the $d$-dimensional lattice is considered, where $L$ denotes the discrete Laplacian and $V$ a delta function with mass at a single point. Eigenvalues of $L + V$ are specified and the absence of singular continuous spectrum is proven. In particular it is shown that an embedded eigenvalue does appear for $d \geq 5$ but does not for $1 \leq d \leq 4$.

1 Introduction

In this paper we are concerned with the spectrum of $d$-dimensional discrete Schrödinger operators on square lattices. Let $\ell^2(\mathbb{Z}^d)$ be the set of $\ell^2$ sequences on the $d$-dimensional lattice $\mathbb{Z}^d$. We consider the spectral property of a bounded self-adjoint operator defined on $\ell^2(\mathbb{Z}^d)$:

$$L + V;$$

(1.1)
where the $d$-dimensional discrete Laplacian $L$ is defined by

$$L\psi(x) = \frac{1}{2d} \sum_{|x-y|=1} \psi(y)$$

(1.2)

and the interaction $V$ by

$$V\psi(x) = v\delta_0(x)\psi(x).$$

(1.3)

Here $v > 0$ is a non-negative coupling constant and $\delta_0(x)$ denotes the delta function with mass at $0 \in \mathbb{Z}^d$, i.e., $\delta_0(x) = \begin{cases} 1, & x = 0 \\ 0, & x \neq 0. \end{cases}$ To study the spectrum of $L + V$ we form $L + V$ by the Fourier transformation. Let $\mathbb{T}^d = [-\pi, \pi]^d$ be the $d$-dimensional torus, and $F : \ell^2(\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$ be the Fourier transformation defined by

$$(F\psi)(\theta) = \sum_{x \in \mathbb{Z}^d} \psi(n)e^{-ix\cdot\theta},$$

where $\theta = (\theta_1, \ldots, \theta_d) \in \mathbb{T}^d$. The inverse Fourier transformation is then given by

$$(F^{-1}\psi)(x) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \psi(\theta)e^{ix\cdot\theta}d\theta.$$

Hence $L + V$ is transformed to a self-adjoint operator on $L^2(\mathbb{T}^d)$:

$$F(L + V)F^{-1}\psi(\theta) = \left(\frac{1}{d} \sum_{j=1}^d \cos \theta_j \right) \psi(\theta) + \frac{v}{(2\pi)^d} \int_{\mathbb{T}^d} \psi(\theta)d\theta.$$ 

(1.4)

In what follows we denote the right-hand side of (1.4) by $H = H(v)$, and we set $H(0) = H_0$. Thus

$$H = g + v(\varphi, \cdot)_{L^2(\mathbb{T}^d)} \varphi, \quad \varphi = (2\pi)^{-d/2} \mathbb{1},$$

(1.5)

where $(\cdot, \cdot)_{L^2(\mathbb{T}^d)}$ denotes the scalar product on $L^2(\mathbb{T}^d)$, which is linear in the right-component and anti-linear in the left-component, and $g$ is the multiplication by the real-valued function:

$$g(\theta) = \frac{1}{d} \sum_{j=1}^d \cos \theta_j.$$ 

(1.6)

Hence $H$ can be realized as a rank-one perturbation of the discrete Laplacian $g$. We study the spectrum of $H$. We denote the spectrum (resp. point spectrum, discrete spectrum, absolutely continuous spectrum, singular continuous spectrum, essential spectrum) of self-adjoint operator $T$ by $\sigma(T)$ (resp. $\sigma_p(T), \sigma_d(T), \sigma_{ac}(T), \sigma_{sc}(T), \sigma_{ess}(T)$).
2 Results

In the continuous case the Schrödinger operator is defined by $H_S = -\Delta + \sigma V$ in $L^2(\mathbb{R}^d)$. Let $V \geq 0$ and $V \in L^1_{\text{loc}}(\mathbb{R}^d)$. Let $N$ denote the number of strictly negative eigenvalues of $H_S$. It is known that $N \geq 1$ for all values of $v > 0$ for $d = 1, 2$ \cite{Sim05}. However in the case of $d \geq 3$, by the Lieb-Thirring bound \cite{Lie76} $N \leq a \int |vV(x)|^{d/2} dx$ follows with some constant $a$ independent of $V$.

In particular for sufficiently small $v$, it follows that $N = 0$. For the discrete case similar results to those of the continuous version may be expected. We summarize the result obtained in this paper below.

**Theorem 2.1** The spectrum of $H$ is as follows:

$(\sigma_{ac}(H) \text{ and } \sigma_{ess}(H))$  
$\sigma_{ac}(H) = \sigma_{ess}(H) = [-1, 1]$ for all $v \geq 0$ and $d \geq 1$.

$(\sigma_{sc}(H))$  
$\sigma_{sc}(H) = \emptyset$ for all $v \geq 0$ and $d \geq 1$.

$(\sigma_p(H))$

$(d = 1, 2)$ For each $v > 0$, there exists $E > 1$ such that $\sigma_p(H) = \sigma_d(H) = \{E\}$. In particular $E = \sqrt{1 + v^2}$ in the case of $d = 1$.

$(d = 3, 4)$

$(v > v_c)$ There exists $E > 1$ such that $\sigma_p(H) = \sigma_d(H) = \{E\}$.

$(v \leq v_c)$ $\sigma_p(H) = \emptyset$.

$(d \geq 5)$

$(v > v_c)$ There exists $E > 1$ such that $\sigma_p(H) = \sigma_d(H) = \{E\}$.

$(v = v_c)$ $\sigma_p(H) = \{1\}$.

$(v < v_c)$ $\sigma_p(H) = \emptyset$.

We give the proof of Theorem 2.1 in Section 3 below. The absolutely continuous spectrum $\sigma_{ac}(H)$ and essential spectrum $\sigma_{ess}(H)$ are discussed in Section 3.1 eigenvalues $\sigma_p(H)$ in Theorem 3.1 and Theorem 3.2 and singular continuous spectrum $\sigma_{sc}(H)$ in Theorem 3.6.

3 Spectrum

3.1 Absolutely continuous spectrum and essential spectrum

It is known and fundamental to show that $\sigma_{ac}(H) = \sigma_{ess}(H) = [-1, 1]$. Note that $\sigma(H_0) = \sigma_{ac}(H_0) = \sigma_{ess}(H) = [-1, 1]$ is purely absolutely continuous spectrum and purely essential spectrum. Since the perturbation $v(\varphi, \cdot)\varphi$ is a rank-one operator, the essential spectrum leaves invariant. Then $\sigma_{ess}(H) = [-1, 1]$. Let $\mathcal{H}_{ac}$ denote the absolutely continuous part of $H$. The self-adjoint operator $H$ is a rank-one perturbation of $g$. Then the wave operator $W_{\pm} = \lim_{t \to \pm \infty} e^{itH(v)} e^{-itH_0}$ exists and is complete, which implies that $H_0$ and $H(v)\mathcal{H}_{ac}$ are unitarily equivalent by $W_{\pm}^{-1}H_0 W_{\pm} = H(v)\mathcal{H}_{ac}$. In particular $\sigma_{ac}(H) = \sigma_{ac}(H_0) = [-1, 1]$ follows.
3.2 Eigenvalues

3.2.1 Absence of embedded eigenvalues in \([-1, 1]\)

In this section we discuss eigenvalues of \(H\). Namely we study the eigenvalue problem \(H\psi = E\psi\), i.e.,

\[
v(\varphi, \psi)\varphi = (E - g)\psi.
\]

(3.1)

The key lemma is as follows.

**Lemma 3.1** \(E \in \sigma_p(H)\) if and only if

\[
\frac{1}{E - g} \in L^2(\mathbb{T}^d) \quad \text{and} \quad v = (2\pi)^d \left( \int_{\mathbb{T}^d} \frac{1}{E - g(\theta)} d\theta \right)^{-1}.
\]

(3.2)

Furthermore when \(E \in \sigma_p(H)\), it follows that

\[
H \frac{1}{E - g} = E \frac{1}{E - g},
\]

i.e., \(\frac{1}{E - g}\) is the eigenvector associated with \(E\). In particular every eigenvalue is simple.

**Proof:** Suppose that \(E \in \sigma_p(H)\). Then \((E - g)\psi = v(\varphi, \psi)\varphi\). Since \(\psi \in L^2(\mathbb{T}^d)\) and \((E - g)\psi\) is a constant, \(E - g \neq 0\) almost everywhere and \(\psi = v(\varphi, \psi)\varphi/(E - g)\) follows. Thus \((E - g)^{-1} \in L^2(\mathbb{T}^d)\). Inserting \(\psi = c(E - g)^{-1}\) with some constant \(c\) on both sides of \((E - g)\psi = v(\varphi, \psi)\varphi\), we obtain the second identity in (3.2) and then the necessity part follows. The sufficiency part can be easily seen. We state the absence of embedded eigenvalues in the interval \([-1, 1]\). This can be derived from (3.2). We summarize it in the theorem below:

**Theorem 3.2** \(\sigma_p(H) \cap [-1, 1] = \emptyset\).

Suppose that \(-1 \in \sigma_p(H)\). Then there exists a non-zero vector \(\psi\) such that \((\psi, (g + 1)\psi) + v(\varphi, \psi)^2 = 0\). Thus \((\psi, (g + 1)\psi) = 0\) and \(|(\varphi, \psi)|^2 = 0\) follow. However we see that \((\psi, (g + 1)\psi) \neq 0\), since \(g\) has no eigenvalues (has purely absolutely continuous spectrum). Then it is enough to show \(\sigma_p(H) \cap (-1, 1) = \emptyset\).

We shall check that \(\frac{1}{E - g} \notin L^2(\mathbb{T}^d)\) for \(-1 < E < 1\). By a direct computation we have

\[
\int_{\mathbb{T}^d} \frac{1}{(E - g(\theta))^2} d\theta = \int_{[-1-E,1-E]^d} \frac{1}{(\sum_{j=1}^d X_j)^2} \prod_{j=1}^d \frac{1}{\sqrt{1 - (X_j + E)^2}} dX.
\]

Changing variables by \(X_1 = Z_1, \ldots, X_{d-1} = Z_{d-1}\) and \(\sum_{j=1}^d X_j = Z\). Then we have

\[
\int_{\mathbb{T}^d} \frac{1}{(E - g(\theta))^2} d\theta = \int_{\mathbb{T}^{d-1}} \frac{1}{(Z - Z_1 - \cdots - Z_{d-1} + E)^2} \prod_{j=1}^{d-1} \frac{1}{\sqrt{1 - (Z_j + E)^2}} J dZ \prod_{j=1}^{d-1} dZ_j,
\]

where \(J = \prod_{j=1}^{d-1} \sqrt{1 - (Z_j + E)^2}\).
where \( J = | \det \left( \frac{\partial (Z_1, \ldots, Z_{d-1})}{\partial (X_1, \ldots, X_d)} \right) | = 1 \) is a Jacobian and \( \Delta \) denotes the inside of a \( d \)-dimensional convex polygon including the origin, since \(-1 < E < 1\), and \( \bar{\Delta} \) is the closure of \( \Delta \). Then we can take a rectangle such that \([-\delta, \delta]^d \subset \Delta\) for sufficiently small \( 0 < \delta \). We have the lower bound
\[
\int_{T^d} \frac{1}{(E - g(\theta))^2} d\theta \geq \text{const} \times \int_{-\delta}^{\delta} \frac{1}{Z^2} dZ
\]
and the right-hand side diverges. Then the theorem follows from (3.2). \( \text{qed} \)

3.2.2 Eigenvalues in \([1, \infty)\)

Operator \( H \) is bounded by the bound \( \| H \| \leq 1 + v/(2\pi)^d \). Then by Theorem 3.2 and \( v > 0 \), eigenvalues are included in the interval \([1, (2\pi)^dv + 1]\) whenever they exist. We define the critical value \( v_c \) by
\[
v_c = (2\pi)^d \left( \int_{T^d} \frac{1}{1 - g(\theta)} d\theta \right)^{-1} \in [0, \infty)
\] (3.3)
with convention \( \frac{1}{\infty} = 0 \).

Lemma 3.3 (1) The function \([1, \infty) \ni E \mapsto \int_{T^d} \frac{1}{E - g(\theta)} d\theta \) is continuously decreasing.

(2) \( v_c = 0 \) for \( d = 1, 2 \) and \( v_c > 0 \) for \( d \geq 3 \).

(3) \((E - g)^{-1} \in L^2(T^d)\) for all \( d \geq 1 \) and \( E > 1 \).

(4) \((1 - g)^{-1} \in L^2(T^d)\) for \( d \geq 5 \) and \((1 - g)^{-1} \notin L^2(T^d)\) for \( 1 \leq d \leq 4 \).

Proof: (1) and (3) are straightforward. In order to show (2) it is enough to consider a neighborhood \( U \) of points where the denominator \( 1 - g(\theta) \) vanishes. On \( U \), approximately
\[
1 - g(\theta) \approx \frac{1}{2d} \sum_{j=1}^{d} \theta_j^2.
\] (3.4)

Then
\[
\int_{U} \frac{1}{1 - g(\theta)} d\theta \approx \int_{U} \frac{1}{2d} \sum_{j=1}^{d} \theta_j^2 d\theta \approx \text{const} \times \int_{U'} \frac{r^{d-1}}{r^2} dr.
\]
We have \( \int_{U} \frac{1}{2d} \sum_{j=1}^{d} \theta_j^2 d\theta < \infty \) for \( d \geq 3 \) and \( \int_{U} \frac{1}{2d} \sum_{j=1}^{d} \theta_j^2 d\theta = \infty \) for \( d = 1, 2 \).

Then (2) follows. (4) can be proven in a similar manner to (2). Since
\[
\int_{U} \frac{1}{(1 - g(\theta))^2} d\theta \approx \int_{U} \frac{1}{(2d) \sum_{j=1}^{d} \theta_j^2)^2} d\theta \approx \text{const} \times \int_{U'} \frac{r^{d-1}}{r^4} dr,
\]
we have \((1 - g)^{-1} \in L^2(T^d)\) for \( d \geq 5 \) and \((1 - g)^{-1} \notin L^2(T^d)\) for \( d = 1, 2, 3, 4 \).

From this lemma we can immediately obtain results on eigenvalue problem of
\[
v(\varphi, \psi) = (E - g)\psi.
\] (3.5)
Theorem 3.4 \(d = 1, 2\) \([3.2]\) has a unique solution \(\psi = \frac{1}{E-g}\) up to a multiplicative constant and \(E > 1\) for each \(v > 0\). In particular \(E = \sqrt{1 + v^2}\) for \(d = 1\).

\((d = 3, 4)\) \([3.2]\) has the unique solution \(\psi = \frac{1}{E-g}\) up to a multiplicative constant and \(E > 1\) for \(v > v_c\) and no non-zero solution for \(v \leq v_c\). In particular \(1\) is not eigenvalue for \(H(v_c)\).

\((d \geq 5)\) \([3.2]\) has the unique solution \(\psi = \frac{1}{E-g}\) up to a multiplicative constant and \(E \geq 1\) for \(v \geq v_c\) and no non-zero solution for \(v < v_c\). In particular \(E = 1\) is eigenvalue for \(H(v_c)\).

Proof: In the case of \(d = 1, 2\), \([3.2]\) is fulfilled for all \(v > 0\), and \(\frac{1}{\pi} \int_{\mathbb{T}} \frac{1}{E-g(\theta)} = 1\) follows from \(H \frac{1}{E-g} = \frac{E}{E-g}\). Thus \(E = \sqrt{1 + v^2}\) for \(d = 1\). In the case of \(d = 3, 4\), \([3.2]\) is fulfilled for \(v > v_c\), but not for \(v = v_c\). In the case of \(d \geq 5\), \([3.2]\) is fulfilled for \(v \geq v_c\).

3.3 Absence of singular continuous spectrum

Let \(\langle T \rangle_\varphi = \langle \varphi, T \varphi \rangle\) be the expectation of \(T\) with respect to \(\varphi\). We introduce three subsets in \(\mathbb{R}\). Let

\[
X = \left\{ x \in \mathbb{R} | \text{Im} \langle (H_0 - (x + i0))^{-1} \rangle_{\varphi} > 0 \right\}
\]

\[
Y = \left\{ x \in \mathbb{R} | \langle (H_0 - x)^{-2} \rangle_{\varphi}^{-1} > 0 \right\}
\]

\[
Z = \mathbb{R} \setminus (X \cup Y).
\]

Note that \(\text{Im} \langle (H_0 - (x + i\epsilon))^{-1} \rangle_{\varphi} \leq \epsilon \langle (H_0 - x)^{-2} \rangle_{\varphi}\). Then \(X, Y, Z\) are mutually disjoint. Let \(\mu_{v}^{\text{ac}}\) (resp. \(\mu_{v}^{\text{sc}}\) and \(\mu_{v}^{\text{pp}}\)) be the spectral measure of the absolutely continuous spectral part of \(H(v)\) (resp. singular continuous part, point spectral part). A key ingredient to prove the absence of singular continuous spectrum of a self-adjoint operator with rank-one perturbation is the result of [SW86, Theorem 1(b) and Theorem 3] and [Aro57]. We say that a measure \(\eta\) is supported on \(A\) if \(\eta(\mathbb{R} \setminus A) = 0\).

Proposition 3.5 For any \(v \neq 0\), \(\mu_{v}^{\text{ac}}\) is supported on \(X\), \(\mu_{v}^{\text{pp}}\) is supported on \(Y\) and \(\mu_{v}^{\text{sc}}\) is supported on \(Z\). In particular when \(\mathbb{R} \setminus X \cup Y\) is countable, \(\sigma_{\text{sc}}(H) = \emptyset\) follows.

Proof: The former result is due to [SW86, Theorem 1(b) and Theorem 3]. Since any countable sets have \(\mu_{v}^{\text{ac}}\)-zero measure, the latter statement also follows.

Theorem 3.6 \(\sigma_{\text{sc}}(H) = \emptyset\).

Proof: We shall show that \(\mathbb{R} \setminus X \cup Y\) is countable. Let \(E \in \sigma_{p}(H)\). Then it is shown in \([3.2]\) that \(\langle (H_0 - E)^{-2} \rangle_{\varphi} = \int_{\mathbb{T}} \frac{1}{g(\theta) - E^2} d\theta < \infty\). Then \(E \in Y\). Let \(x \in (-\infty, -1) \cup (1, \infty)\). It is clear that \(\langle (H_0 - E)^{-2} \rangle_{\varphi} < \infty\). Then

\[
\sigma_{p}(H) \cup (-\infty, -1) \cup (1, \infty) \subset Y.
\]
Let \( x \in (-1, 1) \). Then \((x - g)^{-1} \not\in L^2(\mathbb{R}^d)\) follows from the proof of Theorem 3.2.

We have

\[
\text{Im} \left\langle (H_0 - (x + i\epsilon))^{-1} \right\rangle \phi = \int_{\mathbb{T}^d} \frac{\epsilon}{(g(\theta) - x)^2 + \epsilon^2} d\theta.
\]

We can compute the right-hand side above in the same way as in the proof of Theorem 3.2:

\[
\int_{\mathbb{T}^d} \frac{\epsilon}{(g(\theta) - x)^2 + \epsilon^2} d\theta \geq (2\delta)^{d-1}d^2 \int_{-\delta}^{\delta} \frac{\epsilon}{Z^2 + \epsilon^2} d\epsilon.
\]

Then the right-hand side above converges to \((2\delta)^{d-1}d^2\pi > 0\) as \(\epsilon \downarrow 0\). Then

\[ (-1, 1) \subset X. \tag{3.7} \]

By (3.6) and (3.7), \( \mathbb{R} \setminus X \cup Y \subset \{-1, 1\} \), the theorem follows from Proposition 3.5.

4 Concluding remarks

Our next issue will be to consider the spectral properties of discrete Schrödinger operators with the sum (possibly infinite sum) of delta functions:

\[
L + v \sum_{j=1}^{n} \delta_{a_j} \quad 1 < n \leq \infty. \tag{4.1}
\]

This is transformed to

\[
H = g + v \sum_{j=1}^{n} (\varphi_j, \cdot) \varphi_j \tag{4.2}
\]

by the Fourier transformation, where \( \varphi_j = (2\pi)^{-d/2} e^{-i\theta a_j} \). Note that

\[
(\varphi_i, \varphi_j) = (2\pi)^{-d} \int_{\mathbb{T}^d} e^{i(a_i - a_j)\theta} d\theta = \delta_{ij}.
\]

When \( n < \infty \), \( H \) is a finite rank perturbation of \( g \). Then the absolutely continuous spectrum and the essential spectrum of \( H \) are \([-1, 1]\). In this case the discrete spectrum is studied in e.g., [HMO11] for \( d = 1 \). See also [DKS05]. The absence of singular continuous spectrum of \( H \) may be shown by an application of the Mourre estimate [Mou80]. In order to study eigenvalues we may need further effort.

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