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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 $1 \leq d \leq 4$.

Keywords. discrete Schrodinger operator, rank-one perturbation

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 ℓ^2 sequences on the d-dimensional lattice $\mathbb{Z}^d$. We consider the spectral property of a bounded self-adjoint operator defined on $\ell^2(\mathbb{Z}^d)$:

$$L+V,$$

where the d-dimensional discrete Laplacian L is defined by

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

and the interaction V by

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

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.,

$$\delta_0(x) = \left\{ \begin{array}{ll} 1, & x = 0 \\ 0, & x \neq 0. \end{array}\right.$$

To study the spectrum of $L+V$ we transform $L+V$ by the Fourier transformation. Let $\mathbb{T}^d = [-\pi,\pi]^d$ be the d-dimensional torus, and $F\colon \ell^2(\mathbb{Z}^d) \to L^2(\mathbb{T}^d)$ 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 $L^2(\mathbb{T}^d)$:

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

In what follows we denote the right-hand side of (1) by $H = H(v)$, and we set $H(0) = H_0$. Thus

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

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:

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

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. $\sigma_{\rm p}(T), \sigma_{\rm d}(T), \sigma_{\rm ac}(T), \sigma_{\rm sc}(T), \sigma_{\rm ess}(H)$).

2. Results

In the continuous case the d-dimensional Schrödinger operator with an external potential vW is defined by the self-adjoint operator $H_S = -\Delta + vW$ in $L^2(\mathbb{R}^d)$. Let $W \leq 0$, not identically zero and $W \in L^1_{\rm loc}(\mathbb{R}^d)$. 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 $d = 1,2$ [Sim05, Proposition 7.4]. However in the case of $d \geq 3$, by the

Lieb-Thirring bound [Lie76] $N \leq a_d \int |vW(x)|^{d/2}dx$ follows with some constant a_d independent of W and v. In particular for sufficiently small $v > 0$, 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 1. *The spectrum of H is as follows:*

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

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

($\sigma_{\rm p}(H)$) *Let the critical value v_c be defined by* (3).

($d = 1, 2$) *For each $v > 0$, there exists $E > 1$ such that $\sigma_{\rm p}(H) = \sigma_{\rm d}(H) = \{E\}$. 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*

$$\sigma_{\rm p}(H) = \sigma_{\rm d}(H) = \{E\}.$$

($v \leq v_c$) $\sigma_{\rm p}(H) = \emptyset$.

($d \geq 5$)

($v > v_c$) *There exists $E > 1$ such that*

$$\sigma_{\rm p}(H) = \sigma_{\rm d}(H) = \{E\}.$$

($v = v_c$) $\sigma_{\rm p}(H) = \{1\}$.
($v < v_c$) $\sigma_{\rm p}(H) = \emptyset$.

We give the proof of Theorem 1 in Section 3 below. The absolutely continuous spectrum $\sigma_{\rm ac}(H)$ and essential spectrum $\sigma_{\rm ess}(H)$ are discussed in Section 3.1, eigenvalues $\sigma_{\rm p}(H)$ in Theorem 3 and Theorem 2, and singular continuous spectrum $\sigma_{\rm sc}(H)$ in Theorem 4.

3. Spectrum

3.1. Absolutely continuous spectrum and essential spectrum

It is known and fundamental to show that $\sigma_{\rm ac}(H) = \sigma_{\rm ess}(H) = [-1, 1]$. Note that $\sigma(H_0) = \sigma_{\rm ac}(H_0) = \sigma_{\rm ess}(H) = [-1, 1]$ 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 $\sigma_{\rm ess}(H) = [-1, 1]$. Let $\mathscr{H}_{\rm ac}$ 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 $H(v)\lceil_{\mathscr{H}_{\rm ac}}$ are unitarily equivalent by $W_\pm^{-1}H_0W_\pm = H(v)\lceil_{\mathscr{H}_{\rm ac}}$. In particular $\sigma_{\rm ac}(H) = \sigma_{\rm ac}(H_0) = [-1, 1]$ 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.,

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

The key lemma is as follows.

Lemma 1. *$E \in \sigma_{\rm p}(H)$ if and only if*

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

Furthermore when $E \in \sigma_{\rm p}(H)$, 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 $E \in \sigma_{\rm p}(H)$. 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 (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 (2).

Theorem 2. $\sigma_{\rm p}(H) \cap [-1, 1) = \emptyset$.

Proof. Suppose that $-1 \in \sigma_{\rm p}(H)$. Then there exists a non-zero vector ψ 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 $\sigma_{\rm p}(H) \cap (-1, 1) = \emptyset$. We shall check that $\frac{1}{E-g} \notin L^2(\mathbb{T}^d)$ for $-1 < E < 1$. By a direct computation we have

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

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

$$\int_{\mathbb{T}^d} \frac{1}{(E - g(\theta))^2}d\theta = \int_\Delta \frac{1}{\frac{1}{d^2}Z^2} \frac{1}{\sqrt{1 - (Z - Z_1 - \cdots - Z_{d-1} + E)^2}} \times \left(\prod_{j=1}^{d-1} \frac{1}{\sqrt{1 - (Z_j + E)^2}}\right) JdZ \prod_{j=1}^{d-1} dZ_j,$$

where $J = \left|\det \frac{\partial(Z_1,\ldots,Z_{d-1},Z)}{\partial(X_1,\ldots,X_d)}\right| = 1$ is a Jacobian and Δ denotes the inside of a d-dimensional convex polygon including the origin, since $-1 < E < 1$, and $\overline{\Delta}$ is the closure of Δ. Then we can take a rectangle $[-\delta,\delta]^d$ such that $[-\delta,\delta]^d \subset \Delta$ for sufficiently small $0<\delta$. We have the lower bound

$$\int_{\mathbb{T}^d} \frac{1}{(E-g(\theta))^2} d\theta \geq \text{const} \times (2\delta)^{d-1} d^2 \int_{-\delta}^{\delta} \frac{1}{Z^2} dZ$$

and the right-hand side diverges. Then the theorem follows from (2). □

3.2.2. Eigenvalues in $[1,\infty)$

Operator H is bounded by the bound $\|H\| \leq 1 + v/(2\pi)^d$. Then by Theorem 2 and $v>0$, eigenvalues are included in the interval $[1,(2\pi)^d v + 1]$ whenever they exist. We define the critical value v_c by

$$v_c = (2\pi)^d \left(\int_{\mathbb{T}^d} \frac{1}{1-g(\theta)} d\theta \right)^{-1} \in [0,\infty) \tag{3}$$

with convention $\frac{1}{\infty} = 0$.

Lemma 2. (1) *The function* $[1,\infty) \ni E \mapsto \int_{\mathbb{T}^d} \frac{1}{E-g(\theta)} d\theta$ *is continuously decreasing.*

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

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

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

$$1 - g(\theta) \approx \frac{1}{2d} \sum_{j=1}^{d} \theta_j^2. \tag{4}$$

Then

$$\int_U \frac{1}{1-g(\theta)} d\theta \approx \int_U \frac{1}{\frac{1}{2d}\sum_{j=1}^d \theta_j^2} d\theta \approx \text{const} \times \int_{U'} \frac{r^{d-1}}{r^2} dr.$$

We have $\int_U \frac{1}{\frac{1}{2d}\sum_{j=1}^d \theta_j^2} d\theta < \infty$ for $d \geq 3$ and $\int_U \frac{1}{\frac{1}{2d}\sum_{j=1}^d \theta_j^2} d\theta = \infty$ for $d = 1,2$. Then (2) follows. (4) can be proven in a similar manner to (2). Since

$$\int_U \frac{1}{(1-g(\theta))^2} d\theta \approx \int_U \frac{1}{(\frac{1}{2d}\sum_{j=1}^d \theta_j^2)^2} d\theta \approx \text{const} \times \int_{U'} \frac{r^{d-1}}{r^4} dr,$$

we have $(1-g)^{-1} \in L^2(\mathbb{T}^d)$ for $d \geq 5$ and $(1-g)^{-1} \notin L^2(\mathbb{T}^d)$ for $d = 1,2,3,4$. □

From this lemma we can immediately obtain results on eigenvalue problem of

$$v(\varphi,\psi)\varphi = (E-g)\psi. \tag{5}$$

Theorem 3. $(d=1,2)$ (5) *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* $d=1$.

$(d=3,4)$ (5) *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* $H(v_c)$.

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

3.3. Absence of singular continuous spectrum

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

$$X = \left\{ x \in \mathbb{R} \,\middle|\, \text{Im}\left\langle (H_0 - (x+i0))^{-1}\right\rangle_\varphi > 0 \right\}$$
$$Y = \left\{ x \in \mathbb{R} \,\middle|\, \left\langle (H_0 - x)^{-2}\right\rangle_\varphi^{-1} > 0 \right\}$$
$$Z = \mathbb{R} \setminus (X \cup Y).$$

Note that $\text{Im}\left\langle (H_0-(x+i\epsilon))^{-1}\right\rangle_\varphi \leq \epsilon\left\langle (H_0-x)^{-2}\right\rangle_\varphi$. Then X, Y and Z are mutually disjoint. Let μ_v^{ac} (resp. μ_v^{sc} and μ_v^{pp}) be the spectral mesure 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 η is supported on A if $\eta(\mathbb{R}\setminus A) = 0$.

Proposition 1. *For any* $v \neq 0$, μ_v^{ac} *is supported on* X, μ_v^{pp} *is supported on* Y *and* μ_v^{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 μ_v^{sc}-zero measure, the latter statement also follows. □

Theorem 4. $\sigma_{\text{sc}}(H) = \emptyset$.

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

$$\sigma_{\text{p}}(H) \cup (-\infty,-1) \cup (1,\infty) \subset Y. \tag{6}$$

Let $x \in (-1,1)$. Then $(x-g)^{-1} \notin L^2(\mathbb{T}^d)$ follows from the proof of Theorem 2. We have

$$\mathrm{Im}\left\langle (H_0 - (x+i\epsilon))^{-1}\right\rangle_\varphi = \int_{\mathbb{T}^d} \frac{\epsilon}{(g(\theta)-x)^2+\epsilon^2} d\theta.$$

We can compute the the right-hand side above in the same way as in the proof of Theorem 2:

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

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

$$(-1,1) \subset X. \tag{7}$$

By (6) and (7), $\mathbb{R} \setminus X \cup Y \subset \{-1,1\}$, the theorem follows from Proposition 1. □

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:

$$L + v\sum_{j=1}^{n} \delta_{a_j} \quad 1 < n \leq \infty. \tag{8}$$

This is transformed to

$$H = g + v\sum_{j=1}^{n} (\varphi_j, \cdot)\varphi_j \tag{9}$$

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.

Note added in proof: After the completion of this paper J. Bellissard and H. Schulz-Baldes send us [BS12] to our attention.

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References

[Aro57] N. Aronszajn, On a problem of Weyl in the theory of singular Strum-Liouville equations, *Am. J. Math.* **79** (1957), 597–610.

[BS12] J. Bellissard and H. Schulz-Baldes, Scattering theory for lattice operators in dimension $d \geq 3$, arXiv:1109.5459v2, preprint 2012.

[DKS05] D. Damanik, R. Killip and B. Simon, Schrödinger operators with few bound states, *Commun. Math. Phys.* **258** (2005), 741–750.

[HMO11] Y. Higuchi, T. Matsumoto and O. Ogurisu, On the spectrum of a discrete Laplacian on $\mathbb{Z}$ with finitely supported potential, *Linear and Multilinear Algebra*, **8** (2011), 917–927.

[Lie76] E.H. Lieb, Bounds on the eigenvalues of the Laplacian and Schrödinger operators, *Bull. AMS* **82** (1976), 751–753

[Mou80] E. Mourre, Absence of singular continuous spectrum for certain self-adjoint operators. *Commun. Math. Phys.* **78** (1981), 391–408.

[Sim05] B. Simon, *Trace Ideals and Their Applications, 2nd ed.* AMS 2005

[SW86] B. Simon and T. Wolff, Singular continuous spectrum under rank one perturbations and localization for random Hamiltonians, *Commun. Pure, App. Math.* **39** (1986), 75–90.

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