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On the boundary part spectrum of the discrete Schrödinger operator

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1. Introduction

Let $\{V\}$ be a family of the ν-dimensional cubes in the ν-dimensional integer lattice $\mathbb{Z}^\nu$, centered at $0 \in \mathbb{Z}^\nu$ increasing to $\mathbb{Z}^\nu$, i.e., $V \uparrow \mathbb{Z}^\nu$. Let us consider the following Hamiltonian in $L^2(V)$:

$$H_V := \varkappa\Delta_V + \xi_V, \tag{1}$$

where Δ_V is the discrete Laplacian on V with zero Dirichlet boundary conditions (the restriction of the operator $\Delta\varphi(x) := \sum_{|y-x|=1} \varphi(y)$, $x \in \mathbb{Z}^\nu$, to V); $|x| := |x^1| + \dots + |x^\nu|$; $\xi_V := \{\xi(x)\}_{x\in V}$ is a real function (a potential); $\varkappa$ is a positive constant. Let $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_{|V|}$ be eigenvalues and $\psi_1(x), \psi_2(x), \ldots, \psi_{|V|}(x)$ $(x \in V)$ the corresponding (normed) eigenfunctions of the operator (1); $|V|$ stands for the number of points in V.

The purpose of the paper is to investigate the structure of the eigenpairs $\lambda_i, \psi_i(\cdot)$ for each $1 \leqslant i \leqslant K$ and each V, provided extreme values of the sample ξ_V possess a strongly pronounced geometric structure described by conditions (2)–(6) below; cf. also Theorem.

The main idea of investigation (related to the theory of "rare scatterers") is based on the cluster expansion method for resolvents. This method was particularly used in [4] to study the spectral properties of Hamiltonians on the whole of $\mathbb{Z}^\nu$ with an infinite sequence of (widely spaced) potential peaks. The physical analysis of the "rare scatterers" model was carried out in the monograph [5]. The main feature of the subject is that the interaction between potential peaks can be neglected and the eigenpairs associated with a block of potential peaks can be determined by the eigenpairs of the separate peaks.

To formulate the main result of the paper, let us introduce the following notation. Fix a constant $L > 0$, and define the subset $\widetilde{\Pi} \subset V$ by $\widetilde{\Pi} = \widetilde{\Pi}(V, L) := \{x \in V : \xi(x) \geqslant L\}$. Throughout we assume that $\widetilde{\Pi} \neq \varnothing$. Write $\widetilde{\xi}(x) := \xi(x)$ if $x \in V\backslash\widetilde{\Pi}$, and $\widetilde{\xi}(x) := 0$ if $x \in \widetilde{\Pi}$. Let $r(\widetilde{\Pi}) := \min\left\{|x-y| : x \in \widetilde{\Pi},\ y \in \widetilde{\Pi}, x \neq y\right\}$ if $|\widetilde{\Pi}| \geqslant 2$, and $r(\widetilde{\Pi}) := |V|^{1/\nu}$ if $|\widetilde{\Pi}| = 1$. For any $u \in \widetilde{\Pi}$, let $\widetilde{\lambda}(u)$ be the maximal eigenvalue of the "single peak" Hamiltonian $h_V^{(u)} := \varkappa\Delta_V + \widetilde{\xi}_V + \xi(u)\delta_u$, where $\delta_u := \{\delta_u(x)\}_{x\in V}$ denotes the Kronecker symbol, i.e., $\delta_u(x) := 1$ if $x = u$, and $\delta_u(x) := 0$ if $x \neq u$. We note that

$\lambda := \widetilde{\lambda}(u)$ is the maximal solution of the equation $g_\lambda(u,u) = 1/\xi(u)$, where $g_\lambda(\cdot\,,\cdot)$ stands for Green's function of the Hamiltonian $\varkappa\Delta_V + \widetilde{\xi}_V$.

For $\varrho > 0$, write $\Pi = \Pi(V, L, \varrho) := \{u \in \widetilde{\Pi} : \widetilde{\lambda}(u) \geqslant L + 2\nu\varkappa + \varrho\}$. If $\Pi \neq \varnothing$, let $\widetilde{\lambda}_1 \geqslant \widetilde{\lambda}_2 \geqslant \ldots \geqslant \widetilde{\lambda}_{|\Pi|}$ be the variational series of the sample $\widetilde{\lambda}(x)$, $x \in \Pi$, and write $\widetilde{\lambda}_{|\Pi|+1} := L + 2\nu\varkappa + \varrho$. Define $A(\lambda)$ by

$$A(\lambda) := \log\frac{\lambda - L}{2\nu\varkappa} \quad \text{for } \lambda \geqslant L + 2\nu\varkappa + \varrho.$$

In the trivial case where $\widetilde{\Pi} = \Pi = \{\widetilde{z}\}$ (i.e., H_V is the "single peak" Hamiltonian $H_V = \varkappa\Delta_V + \widetilde{\xi}_V + \xi(\widetilde{z})\delta_{\widetilde{z}}$), we have that $\lambda_1 = \widetilde{\lambda}_1$ and

$$|\psi_1(x)| \leqslant c_1(\varrho)\exp\{-A(\lambda_1)\,|x - \widetilde{z}|\}, \quad x \in V,$$

with $c_1(\varrho) := (2\nu\varkappa + \varrho)/\varrho$.

For $\left|\widetilde{\Pi}\right| \geqslant 2$, $K \in \mathbb{N} := \{1, 2, \ldots\}$ and $\delta > 0$, we introduce the following conditions on the sample ξ_V:

$$|\Pi| \geqslant K, \tag{2}$$

$$\min_{u \in V\setminus\Pi}\left(\widetilde{\lambda}_{K+1} - \xi(u)\right) \geqslant \frac{2\nu\varkappa^2}{\varrho}, \tag{3}$$

$$16c_1(\varrho)\sum_{x\in V\setminus\{0\}} \exp\left\{-2(1-\delta)A(\widetilde{\lambda}_{K+1})|x|\right\} < 1, \tag{4}$$

$$\min_{1\leqslant k\leqslant K}\left(\widetilde{\lambda}_k - \widetilde{\lambda}_{k+1}\right) \geqslant \exp\left\{-\frac{\delta}{2}c_2(\varrho)r(\widetilde{\Pi})\right\} \tag{5}$$

and, finally,

$$r(\widetilde{\Pi}) \geqslant c_3(\varrho)\log\left|\widetilde{\Pi}\right| + c_4(\varrho) \tag{6}$$

with $c_2(\varrho) := \log\frac{2\nu\varkappa+\varrho}{2\nu\varkappa}$, $c_3(\varrho) := \frac{2}{\delta c_2(\varrho)}$ and $c_4(\varrho) := c_3(\varrho)(2c_2(\varrho) + \log(24\nu c_1(\varrho)) + |\log\varkappa| + 4c_1(\varrho)/c_2(\varrho))$.

We now define the sites $\widetilde{z}_k \in \Pi$ by $\widetilde{\lambda}(\widetilde{z}_k) := \widetilde{\lambda}_k$; $1 \leqslant k \leqslant K$.

Theorem. *Fix V, and assume that ξ_V satisfies* (2)–(6) *with constants $L > 0$, $1 \leqslant K \leqslant |V| - 1$, $\varrho > 0$ and $0 < \delta < 1/2$ (which all may depend on V). Then for any $1 \leqslant k \leqslant K$,*

$$\left|\lambda_k - \widetilde{\lambda}_k\right| \leqslant \exp\left\{-2(1-\delta)A(\widetilde{\lambda}_k)r(\widetilde{\Pi})\right\} \tag{7}$$

and

$$|\psi_k(x)| \leqslant 4c_1(\varrho)\exp\{-(1-\delta)A(\lambda_k)\,|x - \widetilde{z}_k|\}, \quad x \in V. \tag{8}$$

REMARK 1. Assumptions (5) and (6) are to avoid the interaction among single high peaks of ξ_V in the model (1). Assumptions (3)and (4) ensure that the interaction between a single peak and a multiple (double, triple, etc.) one is negligible.

REMARK 2. Let $\xi(x)$, $x \in \mathbb{Z}^\nu$, be independent identically distributed random variables (a random potential) with a common distribution function $F(t) = P(\xi(0) \leqslant t)$, $-\infty < t < \infty$. Let $f(s)$, $s \geqslant 0$, stand for the inverse function of $\log(1 - F(\cdot\,))$. Assume that there exists a distribution density $p(\cdot\,) := F'(\cdot\,) \leqslant \text{const}$ and that $f(s) - f(s\delta) \to \infty$, as $s \to \infty$ for each $0 < \delta < 1$. Fix constants $0 < \varepsilon' < \varepsilon < 1/2$. Then, with probability 1, ξ_V satisfies conditions (2)–(6) with $L = L_{V,\varepsilon} := f((1-\varepsilon)\log|V|)$, $\varrho = \varrho_{V,\varepsilon,\varepsilon'} := L_{V,\varepsilon'} - L_{V,\varepsilon}$ and $K = K_V := \frac{1}{2}|V|^{\varepsilon'}$, for each $0 < \delta < 1/2$ and for each V large enough. See [1] for the proofs.

REMARK 3. A detailed analysis of the boundary part spectrum for the deterministic (random as well) Hamiltonian $H_V(1)$ under various conditions on ξ_V is carried out in our forthcoming paper [2] (which includes Theorem of the present article). See also an announcement [3] on the results of [2].

2. Proof of Theorem

We shall treat the case $K \geqslant 2$. If $K = 1$, the proof is similar.

Let $G_\lambda^{(z)}(x,y)$, $g_\lambda(x,y)$ and $g_\lambda^{(z)}(x,y)$ ($x \in V, y \in V$) be Green's functions of the Hamiltonians $H_V^{(z)} := \varkappa\Delta_V + (1-\delta_z)\xi_V$, $h_V := \varkappa\Delta_V + \widetilde{\xi}_V$ and $h_V^{(z)} := h_V + \xi(z)\delta_z$. Write $\tau := \exp\left\{-\frac{\delta}{2}c_2(\varrho)r(\widetilde{\Pi})\right\}$ and $\lambda_0 := \widetilde{\lambda}_K - \tau/3$. For fixed $z \in \widetilde{\Pi}$, we introduce the following (close) subset $\Lambda(z) \subset [\lambda_0, \infty)$ by

$$\Lambda(z) := \left\{\lambda \geqslant \lambda_0 : \min_{u \in \widetilde{\Pi}\setminus\{z\}} \left|\frac{1}{\xi(u)} - g_\lambda(u,u)\right| \lambda^2 \geqslant \frac{2(\lambda - L)^2 \left|\widetilde{\Pi}\right|}{\lambda - L - 2\nu\varkappa} \mathrm{e}^{-\delta A(\lambda) r(\widetilde{\Pi})}\right\}. \quad (9)$$

Note that for each $\lambda \in \Lambda(z)$, Green's functions $g_\lambda(\cdot\,,\cdot\,)$ and $g_\lambda^{(u)}(\cdot\,,\cdot\,)$, $u \in \widetilde{\Pi}\setminus\{z\}$, exist and, moreover,

$$\begin{aligned} |g_\lambda(x,u)| &\leqslant \frac{(\lambda - L)^2}{\lambda(\lambda - L - 2\nu\varkappa)(\lambda - \widetilde{\xi}(x))} \mathrm{e}^{-A(\lambda)|x-u|}, \\ \left|g_\lambda^{(u)}(x,u)\right| &= \left|\frac{g_\lambda(x,u)}{1 - \xi(u) g_\lambda(u,u)}\right|, \quad x \in V, \end{aligned} \quad (10)$$

by expanding $g_\lambda(\cdot\,,\cdot\,)$ over $\varkappa\Delta_V$ as in [2] and taking into account the resolvent identity $g_\lambda^{(u)}(x,u) = g_\lambda(x,u) + g_\lambda^{(u)}(x,u)\xi(u)g_\lambda(u,u)$, $x \in V$, $u \in \widetilde{\Pi}\setminus\{z\}$.

Lemma 1. (i) *For each $\lambda \in \Lambda(z)$, Green's function $G_\lambda^{(z)}(\cdot,\cdot)$ exists and, moreover,*

$$\left|G_\lambda^{(z)}(x,z)\right| \leqslant \frac{2(\lambda-L)}{\lambda(\lambda-L-2\nu\varkappa)} e^{-(1-\delta)A(\lambda)|x-z|}, \quad x \in V, \tag{11}$$

and

$$\left|G_\lambda^{(z)}(z,z) - g_\lambda(z,z)\right| \leqslant \frac{(\lambda-L)^2}{\lambda^2(\lambda-L-2\nu\varkappa)} e^{-(2-\delta)A(\lambda)r(\widetilde{\Pi})}. \tag{12}$$

(ii) $\lambda \in \Lambda(z)$ *is an eigenvalue of H_V if and only if λ is a solution of the equation*

$$G_\lambda^{(z)}(z,z) = \frac{1}{\xi(z)}. \tag{13}$$

In this case, the corresponding (normed) eigenfunction has the form

$$\psi(x) = G_\lambda^{(z)}(x,z)\Bigl(\sum_{y\in V}\Bigl(G_\lambda^{(z)}(y,z)\Bigr)^2\Bigr)^{-1/2}, \quad x \in V. \tag{14}$$

Proof. (i) Fix $y \in V$ and $\lambda \in \Lambda(z)$, and consider the equation

$$\left(\lambda - H_V^{(z)}\right)\omega(\cdot) = \sum_{u\in\widetilde{\Pi}\setminus\{z\}} \delta_u(\cdot)\xi(u)g_\lambda(u,y). \tag{15}$$

Applying the resolvent operator $g_\lambda := (\lambda - h_V)^{-1}$ to the both sides of (15), we rewrite (15) in the following form:

$$\omega(\cdot) - \sum_{u\in\widetilde{\Pi}\setminus\{z\}} g_\lambda(\cdot,u)\xi(u)\omega(u) = \sum_{u\in\widetilde{\Pi}\setminus\{z\}} g_\lambda(\cdot,u)\xi(u)g_\lambda(u,y).$$

Since $\lambda \in \Lambda(z)$, Gerzhgorin's theorem implies that this equation has an unique solution $\omega(\cdot)$. Now, applying the operator $\lambda - H_V^{(z)}$ to $q(\cdot) := g_\lambda(\cdot,y) + \omega(\cdot)$, we get that $q(\cdot) \equiv G_\lambda^{(z)}(\cdot,y)$. Since y is chosen arbitrarily, this implies that $\lambda \notin \operatorname{Spect}(H_V^{(z)})$.

Estimates (11) and (12) follow by applying (10) to the following cluster expansion for $G_\lambda^{(z)}(\cdot,z)$:

Lemma 2 [2]. *For all $x \in V$, all $y \in V$,*

$$G_\lambda^{(z)}(x,y) = g_\lambda(x,y) + \sum_{k\geqslant 1}\sum_{\Gamma:u_1\to u_2\to\cdots\to u_k} g_\lambda^{(u_1)}(x,u_1)\xi(u_1)\Bigl(\prod_{l=2}^{k} g_\lambda^{(u_l)}(u_{l-1},u_l)\xi(u_l)\Bigr)g_\lambda(u_k,y);$$

here the sum $\sum_\Gamma$ is taken over non-stopping paths $\Gamma : u_1 \to u_2 \to \cdots \to u_k$ of the length $k-1$ which are constrained to lie in $\widetilde{\Pi}\setminus\{z\}$.

(ii) Let $\lambda \in \Lambda(z)$ satisfy the equation $H_V\psi(\cdot) = \lambda\psi(\cdot)$ for some $\psi(\cdot) \not\equiv 0$. Rewrite the equation in the form $(\lambda - H_V^{(z)})\psi(\cdot) = \xi(z)\psi(z)\delta_z(\cdot)$ and then apply the resolvent operator $G_\lambda^{(z)} := (\lambda - H_V^{(z)})^{-1}$. We easily obtain from this that λ satisfies (13) and $\psi(\cdot)$ has the form (14). The converse follows by the same arguments.

Introduce the following intervals: $I := [\lambda_0, \infty)$, $I_k := [\widetilde{\lambda}_k - \tau/3, \widetilde{\lambda}_k + \tau/3]$. Clearly $I_k \subset I$ and $I_k \cap I_l = \varnothing$ for $1 \leqslant k < l \leqslant K$, according to (5) and the definitions.

Lemma 3. *Under the conditions* (2)–(6),
(i) $I_k \subset \Lambda(\widetilde{z}_k)$ *for each* $1 \leqslant k \leqslant K$,
(ii) $I \setminus \bigcup_{k=1}^{K} I_k \subset \bigcap_{k=1}^{K} \Lambda(\widetilde{z}_k)$,
and, finally,
(iii) *for fixed* $1 \leqslant k \leqslant K$, *if* $\lambda \in \Lambda(\widetilde{z}_k)$ *satisfies the equation* (13), *then*

$$\left|\lambda - \widetilde{\lambda}_k\right| \leqslant \exp\{-2(1-\delta)A(\widetilde{\lambda}_k)r(\widetilde{\Pi})\}$$

and, consequently, $\lambda \in I_k$.

Proof. (i)–(ii) In view of (6), the right-hand side of inequality in (9) does not exceed $\tau/6$ for all $\lambda \geqslant \lambda_0$. Let us consider the minimum in (9). First, according to the definition of $\widetilde{\lambda}(u)$ and (6), for each $\lambda \geqslant \lambda_0$ and each $u \in \Pi$,

$$\left|\frac{1}{\xi(u)} - g_\lambda(u,u)\right|\lambda^2 = \left|g_{\widetilde{\lambda}(u)}(u,u) - g_\lambda(u,u)\right|\lambda^2 \geqslant \begin{cases} |\lambda - \widetilde{\lambda}(u)|/2, & \text{if } \lambda \geqslant \widetilde{\lambda}(u)/2, \\ \lambda/2, & \text{otherwise.} \end{cases}$$

Second, by expanding g_λ over $\varkappa\Delta_V$, we obtain from (3) and (6) that for each $\lambda \geqslant \lambda_0$ and each $u \in \widetilde{\Pi}\setminus\Pi$,

$$\left(\frac{1}{\xi(u)} - g_\lambda(u,u)\right)\lambda^2 \geqslant \frac{1}{g_\lambda(u,u)} - \xi(u) \geqslant \tau.$$

Summarizing these estimates, we arrive at the claimed assertions.

(iii) We now fix $z := z_k$ and $\lambda \in \Lambda(z)$ satisfying the conditions of Lemma 3(iii). By (13) and the definition of $\widetilde{\lambda}(z)$,

$$\left|G_\lambda^{(z)}(z,z) - g_\lambda(z,z)\right| = \left|g_{\widetilde{\lambda}(z)}(z,z) - g_\lambda(z,z)\right| \geqslant \begin{cases} \frac{1}{2}\left|\widetilde{\lambda}(z) - \lambda\right|\lambda^{-2}, & \text{if } \lambda \geqslant \frac{1}{2}\widetilde{\lambda}(z), \\ \frac{1}{2}\lambda^{-1}, & \text{otherwise.} \end{cases} \tag{16}$$

On the other hand, we have from (12) that the left-hand side of (16) does not exceed $2\nu\varkappa c_1(\varrho)\lambda^{-2}\exp\{-A(\lambda)((2-\delta)r(\widetilde{\Pi}) - 1)\}$. From these estimates combined with (6), it follows the claimed assertions of (iii).

We now finish the proof of Theorem by using Lemmas 1 and 3. If $\lambda \in I \setminus \cup_{k=1}^{K} I_k$, then a combination of Lemma 3(ii)–(iii) and Lemma 1(ii) shows that $\lambda \notin \text{Spect}\,(H_V)$.

For $1 \leqslant k \leqslant K$, we learn from the estimation (12) and condition (6) that there exists in $I_k \subset \Lambda(\widetilde{z}_k)$ a solution of (13) with $z := \widetilde{z}_k$ which we denote by λ_k. Now, again by Lemmas 1(ii) and 3(iii), we obtain the estimate (7) for λ_k, and by Lemma 1(i), we obtain the estimate (8) for $\psi_k(\cdot\,)$ (14), as claimed. Finally, the uniqueness of the solution λ_k in I_k is readily shown by applying (11) and (4) to the resolvent identity:

$$G_{\lambda}^{(z)}(z,z) - G_{\lambda'}^{(z)}(z,z) = (\lambda' - \lambda) \sum_{x \in V} G_{\lambda'}^{(z)}(x,z) G_{\lambda}^{(z)}(x,z) \quad \text{with} \quad z := \widetilde{z}_k,$$

where $\lambda, \lambda' \in I_k$ satisfy (13) with $z := \widetilde{z}_k$. Theorem is proven.

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Apie diskrečiojo Šriodingerio operatoriaus viršutinį spektrą

A. Astrauskas

Nagrinėjama diskrečiojo Šriodingerio operatoriaus baigtinėse srityse ekstremaliųjų tikrinių reikšmių struktūra ekstremaliai retų potencialo pikų atveju. Naudojamas rezolvenčių skleidimo klasteriais metodas.