

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}^ν , centered at $0 \in \mathbb{Z}^\nu$ increasing to \mathbb{Z}^ν , i.e., $V \uparrow \mathbb{Z}^\nu$. Let us consider the following Hamiltonian in $L^2(V)$:

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

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); κ is a positive constant. Let $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{|V|}$ be eigenvalues and $\psi_1(x), \psi_2(x), \dots, \psi_{|V|}(x)$ ($x \in V$) 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 $1 \leq i \leq K$ 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}^ν 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 $\tilde{\Pi} \subset V$ by $\tilde{\Pi} = \tilde{\Pi}(V, L) := \{x \in V : \xi(x) \geq L\}$. Throughout we assume that $\tilde{\Pi} \neq \emptyset$. Write $\tilde{\xi}(x) := \xi(x)$ if $x \in V \setminus \tilde{\Pi}$, and $\tilde{\xi}(x) := 0$ if $x \in \tilde{\Pi}$. Let $r(\tilde{\Pi}) := \min \{|x - y| : x \in \tilde{\Pi}, y \in \tilde{\Pi}, x \neq y\}$ if $|\tilde{\Pi}| \geq 2$, and $r(\tilde{\Pi}) := |V|^{1/\nu}$ if $|\tilde{\Pi}| = 1$. For any $u \in \tilde{\Pi}$, let $\tilde{\lambda}(u)$ be the maximal eigenvalue of the “single peak” Hamiltonian $h_V^{(u)} := \kappa \Delta_V + \tilde{\xi}_V + \xi(u)\delta_u$, 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

$\lambda := \tilde{\lambda}(u)$ 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 $\varkappa\Delta_V + \tilde{\xi}_V$.

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

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

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

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

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

For $|\tilde{\Pi}| \geq 2$, $K \in \mathbb{N} := \{1, 2, \dots\}$ and $\delta > 0$, we introduce the following conditions on the sample ξ_V :

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

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

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

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

and, finally,

$$r(\tilde{\Pi}) \geq c_3(\varrho) \log |\tilde{\Pi}| + c_4(\varrho) \tag{6}$$

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 $\tilde{z}_k \in \Pi$ by $\tilde{\lambda}(\tilde{z}_k) := \tilde{\lambda}_k$; $1 \leq k \leq K$.

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

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

and

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

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 $F(t) = P(\xi(0) \leq t), -\infty < t < \infty$. Let $f(s), s \geq 0$, stand for the inverse function of $\log(1 - F(\cdot))$. Assume that there exists a distribution density $p(\cdot) := F'(\cdot) \leq \text{const}$ and that $f(s) - f(s\delta) \rightarrow \infty$, as $s \rightarrow \infty$ 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 $K \geq 2$. 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 $H_V^{(z)} := \kappa \Delta_V + (1 - \delta_z) \xi_V, h_V := \kappa \Delta_V + \tilde{\xi}_V$ and $h_V^{(z)} := h_V + \xi(z) \delta_z$. Write $\tau := \exp \left\{ -\frac{\delta}{2} c_2(\varrho) r(\tilde{\Pi}) \right\}$ and $\lambda_0 := \tilde{\lambda}_K - \tau/3$. For fixed $z \in \tilde{\Pi}$, we introduce the following (close) subset $\Lambda(z) \subset [\lambda_0, \infty)$ by

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

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

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

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

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

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

and

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

(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

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

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

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

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

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

Since $\lambda \in \Lambda(z)$, Gerzghorin'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 $\lambda \notin \text{Spect}(H_V^{(z)})$.

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 $y \in V$,

$$G_\lambda^{(z)}(x, y) = g_\lambda(x, y) + \sum_{k \geq 1} \sum_{\Gamma: u_1 \rightarrow u_2 \rightarrow \dots \rightarrow u_k} g_\lambda^{(u_1)}(x, u_1) \xi(u_1) \left(\prod_{l=2}^k g_\lambda^{(u_l)}(u_{l-1}, u_l) \xi(u_l) \right) g_\lambda(u_k, y);$$

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

(ii) Let $\lambda \in \Lambda(z)$ satisfy the equation $H_V \psi(\cdot) = \lambda \psi(\cdot)$ for some $\psi(\cdot) \neq 0$. 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: $I := [\lambda_0, \infty)$, $I_k := [\tilde{\lambda}_k - \tau/3, \tilde{\lambda}_k + \tau/3]$. Clearly $I_k \subset I$ and $I_k \cap I_l = \emptyset$ for $1 \leq k < l \leq K$, according to (5) and the definitions.

Lemma 3. *Under the conditions (2)–(6),*

(i) $I_k \subset \Lambda(\tilde{z}_k)$ for each $1 \leq k \leq K$,

(ii) $I \setminus \bigcup_{k=1}^K I_k \subset \bigcap_{k=1}^K \Lambda(\tilde{z}_k)$,

and, finally,

(iii) for fixed $1 \leq k \leq K$, if $\lambda \in \Lambda(\tilde{z}_k)$ satisfies the equation (13), then

$$|\lambda - \tilde{\lambda}_k| \leq \exp\{-2(1 - \delta)A(\tilde{\lambda}_k)r(\tilde{\Pi})\}$$

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 $\lambda \geq \lambda_0$. Let us consider the minimum in (9). First, according to the definition of $\tilde{\lambda}(u)$ and (6), for each $\lambda \geq \lambda_0$ and each $u \in \Pi$,

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

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

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

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 $\tilde{\lambda}(z)$,

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

On the other hand, we have from (12) that the left-hand side of (16) does not exceed $2\nu\kappa c_1(\varrho)\lambda^{-2} \exp\{-A(\lambda)((2 - \delta)r(\tilde{\Pi}) - 1)\}$. 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 $\lambda \in I \setminus \bigcup_{k=1}^K I_k$, then a combination of Lemma 3(ii)–(iii) and Lemma 1(ii) shows that $\lambda \notin \text{Spect}(H_V)$.

For $1 \leq k \leq K$, we learn from the estimation (12) and condition (6) that there exists in $I_k \subset \Lambda(\tilde{z}_k)$ a solution of (13) with $z := \tilde{z}_k$ 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:

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

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

References

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Apie diskrečiojo Šriodingerio operatoriaus viršutini spektra

A. Austraškas

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