ANALYSIS OF THE NEGATIVE EIGENVALUES OF THE THREE-DIMENSIONAL DISCRETE SCHRÖDINGER OPERATOR

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Abstract

Eigenvalue behaviour of a family of discrete Schrödinger operators $H_{\lambda\mu}$ *depending on parameters* $\lambda, \mu \in \mathrm{R}$ *is studied on the three-dimensional lattice* Z^3. *The non-local potential is described by the Kronecker delta function and the shift operator. The existence of eigenvalues below the essential spectrum and their dependence on the parameters are explicitely proven. We also show that the essential spectrum absorbes the threshold eigenvalue and there exists a particular parabola, on whose left intercept the threshold becomes an embedded eigenvalue and the threshold resonance at its other points.*

Аннотация

Исследуется поведение собственных значений семейства дискретных операторов Шредингера $H_{\lambda\mu}$ *в зависимости от параметров* $\lambda, \mu \in \mathrm{R}$ *на трехмерной решетке* Z^3. *Нелокальный потенциал описывается дельта-функцией Кронекера и оператором сдвига. Существование собственных значений ниже существенного спектра и их зависимость от параметров доказаны в явном виде. Мы также показываем, что существенный спектр поглощает пороговое собственное значение, и существует особая парабола, на левом пересечении которой порог становится вложенным собственным значением, а порог становится резонансом в других своих точках*

Keywords

Discrete Schrödinger operators, threshold resonance, eigenvalues, lattice..

Ключевые слова

дискретные операторы Шрёдингера, пороговый резонанс, собственные значения, решетка.

Introduction

Studying spectral properties of the Schrödinger operators have been and still is one of the most intensive research areas within mathematical physics and operator theory (for recent summaries see [1,2,3,4,5,6,7] and the references therein). It allows us to better understand the physical processes associated to those operators. Particularly, eigenvalue behaviors of the Schrödinger operators on lattices were discussed in many works [8,9,10,11] and were briefly discussed in [11,12,13], provided the potential is the Dirac delta function.

In this paper we aim to investigate the spectrum of a discrete Schrödinger operator with a non-local potential given at the points $x_0, -x_0 \in Z^3$ on the lattice $(-\pi,\pi]^3$. We explicitly show (Theorem 1) the existence of eigenvalues and resonances of the operator and their dependance on the interaction parameters μ, λ, $x_0 \in Z^3$. We show the existence of eigenvalues outside the essential spectrum, threshold eigenvalues and resonances depending on the parameters λ and μ, and the sum of coordinates of the point $x_0 \in Z^3$, which creates the non-local potential. The case of the Schrödinger operator given with the non-local potential at one point $x_0 \in Z^3$ was studied in our work [14]. In [15] thorough description of the discrete spectrum of similar operators was described on lattices Z^d for all dimensions $d \geq 1$.

1. The discrete Schrödinger operator

1.1 The discrete Schrödinger operator in the position representation

For brevity, we use the following notations throughout the paper: Z^3 is the $3-$dimensional lattice and $T^3 = (R/2\pi Z)^3 = (-\pi,\pi]^3$ is the 3-dimensional torus (the first Brillouin zone, i.e., the dual group of Z^3) equipped with the Haar measure.

Let $T(y), y \in Z^3$ be the shift operator

$$(T(y)f)(x) = f(x+y), \quad f \in \ell^2(Z^3),$$

then, the discrete Laplacian Δ on the lattice Z^3 is described by the self-adjoint (bounded) multidimensional Toeplitz-type operator on the Hilbert space $\ell^2(Z^3)$ ([16]) as

$$\Delta = \frac{1}{2}\sum_{\substack{s\in Z^3 \\ |s|=1}}(T(s)-T(0)).$$

Let V_0 be a multiplication operator in $\ell^2(Z^3)$ by the Kronecker delta function $\delta[\cdot,0]$

$$V_0 f(x) = \delta[x,0]f(x).$$

Then, for a given point $x_0 \in Z^3$, we define the non-local potential (see [16]) as

$$V_{x_0} = \lambda V_0 + \mu(V_0 T(x_0) + T^*(x_0)V_0) + \mu(V_0 T(x_0) + T^*(x_0)V_0)^*.$$

The discrete Schrödinger operator $H_{\lambda\mu}$ acting in $\ell^2(Z^3)$, in the position representation, is defined as a bounded self-adjoint perturbation of $-\Delta$ and is of the form

$$H_{\lambda\mu} = -\Delta - V_{x_0}.$$

1.2 Momentum representation of the discrete Schrödinger operator

In the momentum representation, the one-particle Hamiltonian $H_{\lambda\mu}$ can be expressed as

$$H_{\lambda\mu} = H_0 - V_{x_0},$$

where H_0 and V_{x_0} are respectively defined as

$$H_0 = F^*(-\Delta)F \quad \text{and} \quad V_{x_0} = F^*(V_{x_0})F,$$

with $\mathcal{F}$ being the standard Fourier transform $\mathcal{F}: L^2(\mathbb{T}^3) \to \ell^2(\mathbb{Z}^3)$ and $\mathcal{F}^*: \ell^2(\mathbb{Z}^3) \to L^2(\mathbb{T}^3)$ is its inverse. Explicitly, the non-perturbed operator H_0 acts on $L^2(\mathbb{T}^3)$ as a multiplication operator by the function $\varepsilon(\cdot)$:

$$(H_0 f)(p) = \varepsilon(p) f(p), \quad f \in L^2(\mathbb{T}^3),$$

where $\varepsilon(p) = \sum_{j=1}^{3}(1-\cos p_j), \quad p \in \mathbb{T}^3$. The function $\varepsilon(\cdot)$, being a real valued-function on $\mathbb{T}^3$, is referred as the *dispersion relation* of the Laplace operator in the physical literature.

The perturbation V_{x_0} acts on $f \in L^2(\mathbb{T}^3)$ as the two-dimensional integral operator:

$$(V_{x_0} f)(p) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^3} \left(\lambda + \mu\left(e^{\mathrm{i}(x_0,p)} + e^{\mathrm{i}(-x_0,p)} + e^{-\mathrm{i}(x_0,s)} + e^{\mathrm{i}(x_0,s)}\right)\right) f(s)ds,$$

which can be rewritten in a more convenient way as

$$(V_{x_0} f)(p) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^3} \left(\lambda + 2\mu(\cos(x_0,p) + \cos(x_0,s))\right) f(s)ds, \quad f \in L^2(\mathbb{T}^3).$$

To avoid writing the factor of 2 before μ in formulas, we keep the notation μ but we mean 2μ everywhere below.

1.3 The essential spectrum of $H_{\lambda\mu}$

The perturbation V of H_0 is a two dimensional operator, therefore in accordance with the Weyl theorem on the stability of the essential spectrum, the equality $\sigma_{\mathrm{ess}}(H) = \sigma_{\mathrm{ess}}(H_0)$ holds. As H_0 is the multiplication operator by the continuous function $\varepsilon(\cdot)$,

$$\sigma_{\mathrm{ess}}(H_{\lambda\mu}) = [\varepsilon_{\min}, \varepsilon_{\max}] = [0,6].$$

1.4 The Fredholm determinant of $H_{\lambda\mu}$

First, for a complex number $z \in \mathbb{C} \setminus [\varepsilon_{\min}, \varepsilon_{\max}]$, let us introduce the following notations

$$a(z) = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} \frac{1}{\varepsilon(t) - z} dt,$$

$$b(z) = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} \frac{\cos(x_0,t)}{\varepsilon(t) - z} dt,$$

$$c(z) = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} \frac{\cos^2(x_0,t)}{\varepsilon(t) - z} dt.$$

Then, for any $\lambda, \mu \in \mathbb{R}$, the Fredholm determinant associated to the operator $H_{\lambda\mu}$ is defined as a regular function in $z \in \mathbb{C} \setminus [\varepsilon_{\min}, \varepsilon_{\max}]$:

$$\Delta(\lambda, \mu; z) = (1 - \mu b(z))^2 - \mu^2 a(z) c(z) - \lambda a(z).$$

__Lemma 1:__ The number $z \in \mathbb{C} \setminus [\mathcal{E}_{\min}, \mathcal{E}_{\max}]$ *is an eigenvalue of* $H_{\lambda\mu}$ *if and only if* $\Delta(\lambda, \mu; z) = 0$.

Proof. Consider the eigenvalue equation

$$(H_{\lambda\mu} - z) f = 0,$$

which can be rewritten in a more explicit form as

$$[\mathcal{E}(p) - z] f(p) - \frac{\lambda}{(2\pi)^d} \int_{\mathbb{T}^3} f(s) ds - \frac{\mu \cos(x_0, p)}{(2\pi)^d} \int_{\mathbb{T}^3} f(s) ds - \frac{\mu}{(2\pi)^d} \int_{\mathbb{T}^3} \cos(x_0, s) f(s) ds = 0,$$

with $f \in L^2(\mathbb{T}^3)$. Denote

$$C_1 = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} f(t) dt, \quad C_2 = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} \cos(x_0, t) f(t) dt$$

Then, the above equation is equivalent to the system of linear equations with respect to C_1 and C_2

$$\begin{cases} (1 - \mu b(z) - \lambda a(z)) C_1 - \mu a(z) C_2 = 0 \\ (-\lambda b(z) - \mu c(z)) C_1 + (1 - \mu b(z)) C_2 = 0. \end{cases} \tag{1}$$

The solution f and the coefficients C_1, C_2 are related as

$$f(p) = \frac{1}{\mathcal{E}(p) - z} \left((\lambda + \mu \cos(x_0, p)) C_1 + \mu C_2 \right).$$

The Fredholm determinant of the system of linear equations (1) is of the form

$$\Delta(\lambda, \mu; z) = 1 - 2\mu b(z) - \mu^2 d(z) - \lambda a(z), \tag{2}$$

where

$$d(z) = a(z) c(z) - b^2(z).$$

For any $z \in \mathbb{C} \setminus [\mathcal{E}_{\min}, \mathcal{E}_{\max}]$, $a(z)$ is strictly non-zero. Therefore, instead of the equation

$$\Delta(\lambda, \mu; z) = a(z) \left(\frac{1}{a(z)} - \frac{2b(z)}{a(z)} \mu - \frac{d(z)}{a(z)} \mu^2 - \lambda \right) = 0$$

we can study the parabola (as a function of $\mu \in \mathbb{R}$)

$$P_z(\lambda, \mu) := \frac{1}{a(z)} - \frac{2b(z)}{a(z)} \mu - \frac{d(z)}{a(z)} \mu^2 - \lambda = 0.$$

2. Properties of $\Delta(\lambda, \mu; z)$ and $P_z(\lambda, \mu)$

For a fixed $x \in \mathbb{Z}^3$ consider the function

$$r(x, z) = \frac{1}{(2\pi)^3} \int_{\mathbb{T}^3} \frac{e^{i(x,t)}}{\mathcal{E}(t) - z} dt, \quad z \in (-\infty, \mathcal{E}_{\min}),$$

then the functions $a(z), b(z)$ and $c(z)$ can be expressed as $a(z) = r(0, z)$, $b(z) = r(x_0, z)$ and $c(z) = \frac{1}{2} \left(r(0, z) + r(x_0, z) \right)$, respectively.

For the readers convenience we state the lemma from [14] which reveals some useful properties of the function $r(x,z)$:

Lemma 2: *For any fixed* $x \in \mathrm{Z}^3$, $r(x,z)$ *is positive and monotonically increasing. Moreover, the following asymptotical relation holds*

$$r(x,z) = O\left(\frac{1}{|z|^{|x|_1+1}}\right) \quad as \quad z \to -\infty,$$

where

$$|x|_1 = |x_1| + |x_2| + |x_3|$$

and

$$\lim_{z \to e_{\min}} r(x,z) = r(x, e_{\min}).$$

Lemma 3: *The functions* $a(z), b(z), c(z)$ *and* $d(z)$ *are monotonically increasing and positive in* $(-\infty, 0)$, *and the followings are valid*

$$\lim_{z \to e_{\min}} a(z) = a(e_{\min}), \quad \lim_{z \to e_{\min}} b(z) = b(e_{\min}),$$

$$\lim_{z \to e_{\min}} c(z) = c(e_{\min}), \quad \lim_{z \to e_{\min}} d(z) = d(e_{\min}).$$

We also have the aymptotic relations

$$a(z) = O\left(\frac{1}{|z|}\right) \quad as \quad z \to -\infty, \ b(z) = O\left(\frac{1}{|z|^{|x_0|_1+1}}\right) \quad as \quad z \to -\infty,$$

$$c(z) = O\left(\frac{1}{|z|}\right) \quad as \quad z \to -\infty, \ d(z) = O\left(\frac{1}{|z|^2}\right) \quad as \quad z \to -\infty,$$

$$\frac{a(z)}{d(z)} = O(|z|) \quad as \quad z \to -\infty. \qquad (3)$$

Proof. Proofs of the statements involving the functions $a(z)$ and $b(z)$ follow from the equalities $a(z) = r(0,z)$, $b(z) = r(x_0, z)$ and Lemma 2. The relation

$$d(z) = a^2(z) - b^2(z) = (a(z) - b(z))(a(z) + b(z)),$$

the limits

$$a_0 = \lim_{z \to 0-} a(z) = \frac{1}{(2\pi)^3} \int_{\mathrm{T}^3} \frac{1}{e(t) - e_{\min}},$$

$$b_0 = \lim_{z \to 0-} b(z) = \frac{1}{(2\pi)^3} \int_{\mathrm{T}^3} \frac{cos(x_0, t)}{e(t) - e_{\min}},$$

$$c_0 = \lim_{z \to 0-} c(z) = \frac{1}{(2\pi)^3} \int_{\mathrm{T}^3} \frac{cos^2(x_0, t)}{e(t) - e_{\min}}$$

and the properties of $a(z)$ and $b(z)$ yield the proof of the statements related to $d(z)$

2.1 Properties of the parabola $P_z(\lambda,\mu)$

Let us start our subsection with the following obvious lemma.

Lemma 4: *(a) For any* $z\in(-\infty,e_{\min})$, *the numbers*

$$\mu_2(z)=\frac{1}{b(z)+\sqrt{a(z)c(z)}} \quad \text{and} \quad \mu_1(z)=\frac{1}{b(z)-\sqrt{a(z)c(z)}} \tag{4}$$

are μ*-intercepts and*

$$A\left(-\frac{b(z)}{d(z)},\frac{\sqrt{a(z)c(z)}}{d(z)}\right)$$

is the vertex of the parabola $P_z(\lambda,\mu)=0$.

(b) For any $\zeta, z\in(-\infty,e_{\min})$ *with* $\zeta<z$, *the inequalities*

$$\mu_1(\zeta)<\mu_1(z)<0<\mu_2(z)<\mu_2(\zeta) \quad (5)$$

and

$$|\mu_1(z)|>\mu_2(z) \quad (6)$$

hold.

Moreover, we have

$$\mu_1^0:=\lim_{z\to e_{\min}-}\mu_1(z)=\frac{1}{b_0-\sqrt{a_0c_0}}<0, \quad \lim_{z\to-\infty}\mu_1(z)=-\infty \tag{7}$$

and

$$\mu_2^0:=\lim_{z\to e_{\min}-}\mu_2(z)=\frac{1}{b_0+\sqrt{a_0c_0}}, \quad \lim_{z\to-\infty}\mu_2(z)=+\infty. \tag{8}$$

Proof. Simple calculations yield the statement (a).

(b) Due to Lemma 2, the functions $a(z)\pm b(z)$ are monotonically increasing in the interval $(-\infty,e_{\min})$, therefore the relations

$$\sqrt{a(z)c(z)}+b(z)>\sqrt{a(\zeta)c(\zeta)}+b(\zeta)>0>b(\zeta)-\sqrt{a(\zeta)c(\zeta)}>b(z)-\sqrt{a(z)c(z)}$$

and

$$0>b(z)-\sqrt{a(z)c(z)}>-(\sqrt{a(z)c(z)}+b(z))$$

provide the proof of inequalities (5) and (6).

Next, we prove that in the $\lambda-\mu$ plane, the parabolas $P_z(\lambda,\mu)=0$ corresponding to different values of the parameter $z\in(-\infty,e_{\min})$, have no common points.

3. Threshold eigenvalues and threshold resonances of $H_{\lambda\mu}$

So far, we have studied the equation $H_{\lambda\mu}f=zf$ for $z\in(-\infty,e_{\min})$. Now, we consider it at the left edge $z=e_{\min}$ of the essential spectrum with $(\lambda,\mu)\in\Gamma_l$.

Definition 1: In the equation $H_{\lambda\mu}f=e_{\min}f$, $e_{\min}$ is called

- a lower threshold eigenvalue if $f\in L^2(\mathrm{T}^3)$,
- a lower threshold resonance if $f\in L^1(\mathrm{T}^3)\setminus L^2(\mathrm{T}^3)$,
- a lower super-threshold resonance if $f\in L^m(\mathrm{T}^3)\setminus L^1(\mathrm{T}^3)$ for any $0<m<1$.

If $H_{\lambda\mu} f = e_{\min} f$ has no solutions in $L^1(\mathrm{T}^3)$, then $e_{\min}$ is a regular point of the essential spectrum.

For a continuous function $\varphi \in C(\mathrm{T}^3)$ define $h(p) = \varphi(p) / e(p)$. The function $1 / e(p)$ has a unique singular point at the origin $p = 0$, and approximated as $e(p) \approx |p|^2$ at this point. The lemma below is a straightforward consequence of the definition of h and the properties of $e(\cdot)$

Lemma 7: *The followings hold:*

(a) $h \in L^1(\mathrm{T}^3)$,

(b) if $h \in L^2(\mathrm{T}^3)$, *then* $\varphi(0) = 0$,

(c) if $|\varphi(p)| < C|p|^\alpha$ *for some* $C > 0$ *and* $\alpha > \dfrac{1}{2}$, *then* $h \in L^2(\mathrm{T}^3)$.

In the theorem below, we describe the conditions for $e_{\min}$ to be a regular point, an eigenvalue or a threshold resonance.

Theorem 2: *(a) For any* $(\lambda, \mu) \in G_1$ *or* $(\lambda, \mu) \in G_0$, *the threshold* $e_{\min}$ *is a regular point.*

(b) The equation $H_{\lambda\mu} f = e_{\min} f$ *has a solution* $f \in L^1(\mathrm{T}^3)$ *if and only if* $(\lambda, \mu) \in \Gamma_l$ *. Also,* $e_{\min}$ *is*

(b1) an eigenvalue if $\mu = \mu_1^0$;

(b2) a threshold resonance if $\mu \neq \mu_1^0$.

Proof. (a) Regularity of the threshold point $e_{\min}$ for $(\lambda, \mu) \in G_1$ or $(\lambda, \mu) \in G_0$ follows from the fact that the corresponding equation $H_{\lambda\mu} f = e_{\min} f$ has no solutions, by Theorem 1.

(b) To prove part (b) we use the the system of linear equations

$$\begin{cases} (1 - \mu b_0 - \lambda a_0) C_1 - \mu a_0 C_2 = 0, \\ (-\lambda b_0 - \mu c_0) C_1 + (1 - \mu b_0) C_2 = 0, \end{cases} \tag{9}$$

which we have shown is equivalent to the equation

$$(H_\mu - e_{\min}) f = 0, \quad f \in L^1(\mathrm{T}^3)$$

in the proof of Lemma 1.4. The solution f and the coefficients C_1 and C_2 are related as

$$C_1 = \frac{1}{(2\pi)^3} \int_{\mathrm{T}^3} f(t) dt, \quad C_2 = \frac{1}{(2\pi)^3} \int_{\mathrm{T}^3} \cos(x_0, t) f(t) dt \tag{10}$$

and

$$f(p) = \frac{\phi(p)}{e(p) - e_{\min}}, \quad \phi(p) = \big((\lambda + \mu \cos(x_0, p)) C_1 + \mu C_2\big). \tag{11}$$

Also, consider the different form of the Fredholm determinant of the system of (9)

$$\Delta(\lambda, \mu; z) = a_0 P_m(\lambda, \mu).$$

Next, we prove the statements (b1) and (b2).

(b1) For the function ϕ in (11), assume that $\phi(0) = 0$, then

$$\phi(0) = \left((\lambda + \mu)C_1 + \mu C_2\right) = 0.$$

Then, the functions ϕ and f can be written as

$$\phi(p) = (\cos(x_0, p) - 1)\mu C_1 \quad and \quad f(p) = \frac{(\cos(x_0, p) - 1)}{e(p) - e_{\min}}\mu C_1.$$

Taking this into account in (10), we obtain

$$(1 - \mu(b_0 - a_0))C_1 = 0, \quad i.e. \quad \mu = \mu_1^0$$

and hence, according to Lemma (3) we obtain that the solution f belongs to $L^2(\mathrm{T}^3)$.

(b2) Let $\mu \neq \mu_1^0$. Then the inequalities $\lambda \neq 0$ and $\phi(0) \neq 0$ and Lemma (3) provide the proof of (b2).

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