Bound states of the two-particle Hamiltonians on lattices

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Goal

The main goal of this report is to give *new threshold phenomena* that are not present in the continuous case for the two-particle discrete Schrödinger operators $h(k), k \in \mathbb{T}^d$, associated to the Hamiltonian h of a system of two identical particles on the d-dimensional lattice $\mathbb{Z}^d$ interacting via short-range pair potentials.

Dispersion relations

The free Hamiltonian $\hat{h}^0$ of a quantum particle on the d-dimensional lattice ^{d}, $d \geq 1$, is associated with the following self-adjoint (bounded) multidimensional Toeplitz-type operator on the Hilbert space $\ell^2(^d)$:

$$(\hat{h}^0\hat{\psi})(x) = \sum_{s\in\mathbb{Z}^d} \hat{\varepsilon}(s)\hat{\psi}(x+s), \quad \hat{\psi} \in \ell^2(\mathbb{Z}^d).$$

Here the series $\sum_{s\in\mathbb{Z}^d} \hat{\varepsilon}(s)$ is assumed to be absolutely convergent,i.e.,

$$\{\hat{\varepsilon}(s)\}_{s\in\mathbb{Z}^d} \in \ell^1(\mathbb{Z}^d).$$

We also assume that the “self-adjointness” property is fulfilled

$$\hat{\varepsilon}(s) = \overline{\hat{\varepsilon}(-s)}, \quad s \in \mathbb{Z}^d.$$

Dispersion relations

In the physical literature, the symbol of the Toeplitz operator $\hat{h}^0$ given by the Fourier series

$$\varepsilon(p) = \sum_{s\in\mathbb{Z}^d} \hat{\varepsilon}(s) e^{\mathrm{i}(p,s)}, \quad p \in \mathbb{T}^d, \tag{1}$$

being a real valued-function on $\mathbb{T}^d$, is called

the dispersion relations of normal modes

associated with the free particle in question.

Dispersion relations

The one-particle free Hamiltonian is required to be of the form

$$\hat{h}^0 = \varepsilon(-\mathrm{i}\nabla),$$

where ∇ is the generator of the infinitesimal translations. Under the mild assumption that

$$\hat{v} \in \ell^\infty(\mathbb{Z}^d),$$

where $\hat{v} = \{\hat{v}(s)\}_{s\in\mathbb{Z}^d}$ is a sequence of reals, the one-particle Hamiltonian $\hat{h}$,

$$\hat{h} = \hat{h}^0 + \hat{v},$$

describing the quantum particle moving in the potential field $\hat{v}$, is a bounded self-adjoint operator on the Hilbert space $\ell^2(\mathbb{Z}^d)$.

Dispersion relations

The one-particle Hamiltonian h in the momentum representation is introduced as

$$h = \mathcal{F}^{-1}\hat{h}\mathcal{F},$$

where $\mathcal{F}$ stands for the Fourier transform

$$\mathcal{F} : L^2(\mathbb{T}^d) \longrightarrow \ell^2(\mathbb{Z}^d),$$

and $\mathbb{T}^d$ denotes the three-dimensional torus, the cube $(-\pi, \pi]^d$ with appropriately identified sides.
Throughout the paper the torus $\mathbb{T}^d$ will be considered as an abelian group with respect to the addition and multiplication by real numbers regarded as operations on $\mathbb{R}^d$ modulo $(2\pi\mathbb{Z})^d$.

The following important subclass of the one-particle systems is of certain interest. It is introduced by the additional requirement that the dispersion relation $\varepsilon(p)$ is a real-valued continuous conditionally negative definite function and hence

(i) ε is an even function,

(ii) $\varepsilon(p)$ has a minimum at $p = 0$.

Recall that a complex-valued bounded function $\varepsilon : \mathbb{T}^d \longrightarrow \mathbb{C}$ is called conditionally negative definite if $\varepsilon(p) = \overline{\varepsilon(-p)}$ and

$$\sum_{i,j=1}^{n} \varepsilon(p_i - p_j) z_i \bar{z}_j \leq 0 \tag{2}$$

for $n \in \mathbb{N}$, $p_1, p_2, .., p_n \in \mathbb{T}^d$, $\mathbf{z} = (z_1, z_2, ..., z_n) \in \mathbb{C}^n$ satisfying $\sum_{i=1}^{n} z_i = 0$.

It is known that in this case the dispersion relation $\varepsilon(p)$ admits the (Lévy-Khinchin) representation

$$\varepsilon(p) = \varepsilon(0) + \sum_{s\in\mathbb{Z}^d\setminus\{0\}} (e^{\mathrm{i}(p,s)} - 1)\hat{\varepsilon}(s), \quad p \in \mathbb{T}^d,$$

which is equivalent to the requirement that the Fourier coefficients $\hat{\varepsilon}(s)$ with $s \neq 0$ are non-positive, that is,

$$\hat{\varepsilon}(s) \leq 0, \quad s \neq 0,$$

and the series $\sum_{s\in\mathbb{Z}^d\setminus\{0\}} \hat{\varepsilon}(s)$ converges absolutely. In turn, this is also equivalent to the requirement that the lattice Hamiltonian $\hat{h} = \hat{h}^0 + \hat{v}$ generates the positivity preserving semi-group $e^{-t\hat{h}}$, $t > 0$, on $\ell^2(\mathbb{Z}^d)$.

Example

For the one-particle free Hamiltonian $\ell^2(\mathbb{Z}^d)$

$$(\hat{h}^0\hat{\psi})(x) = (-\Delta\hat{\psi})(x) = \sum_{|s|=1}[\hat{\psi}(x) - \hat{\psi}(x+s)], \quad x \in \mathbb{Z}^d,$$

the (Fourier) coefficients $\hat{\varepsilon}(s)$, $s \in \mathbb{Z}^d$, from (1) are necessarily of the form

$$\hat{\varepsilon}(s) = \begin{cases} 2d, & s = 0 \\ -1, & |s| = 1 \\ 0, & \text{otherwise.} \end{cases}$$

Hence, the corresponding dispersion relation

$$\varepsilon(p) = 2\sum^{d}(1 - \cos p_i), \ \ p = (p_1, p_2, \dots, p_d) \in \mathbb{T}^d,$$

Recall that the two-particle operators $h(k)$, $k \in \mathbb{T}^d$, are unitary equivalent to the following operator

$$h(k) = h_0(k) - v,\ \ k \in \mathbb{T}^d.$$

Here the operators $h_0(k)$ and v are defined on the Hilbert space $L^2_e(\mathbb{T}^d)$ by

$$(h_0(k)f)(q) = \mathcal{E}_k(q)f(q), \quad f \in L^2_e(\mathbb{T}^d),$$

where

$$\mathcal{E}_k(q) = \varepsilon(\frac{k}{2}+q) + \varepsilon(\frac{k}{2}-q) = 2\sum_{j=1}^{d}[1 - \cos{(\frac{k_j}{2})}\cos q_j]$$

and

$$(vf)(p) = (2\pi)^{-\frac{d}{2}} \int\limits_{\mathbb{T}^d} v(p-q)f(q)dq, \quad f \in L^2_e(\mathbb{T}^d).$$

Two-particle Schrödinger operators

Example

$$(vf)(p) = (2\pi)^{-\frac{d}{2}} \int\limits_{\mathbb{T}^d} f(q)dq, \quad f \in L^2_e(\mathbb{T}^d).$$

Hypothesis

Assume, that $v(\cdot)$ is a continuous function on $\mathbb{T}^d$ with real even nonnegative Fourier coefficients $\hat{v}(s), s \in \mathbb{Z}^d$.

Two-particle Schrödinger operators

Since the perturbation operator v is compact according to Weyl's theorem the essential spectrum $\sigma_{\text{ess}}(h(k))$ of the operator $h(k), k \in \mathbb{T}^d$ coincides with the spectrum $\sigma(h_0(k))$ of the non-perturbed operator $h_0(k)$. More specifically,

$$\sigma_{\text{ess}}(h(k)) = [\mathcal{E}_{\min}(k), \mathcal{E}_{\max}(k)],$$

where

$$\mathcal{E}_{\min}(k) \equiv \min_{p \in \mathbb{T}^d} \mathcal{E}_k(p) = 2 \sum [1 - \cos(\frac{k_j}{2})],$$

$$\mathcal{E}_{\max}(k) \equiv \max_{p \in \mathbb{T}^d} \mathcal{E}_k(p) = 2 \sum [1 + \cos(\frac{k_j}{2})].$$

Let $d \geq 1$ and $z < \mathcal{E}_{\min}(k)$. Define by

$$G(k,z) = v^{\frac{1}{2}} r_0(k,z) v^{\frac{1}{2}},\ k \in \mathbb{T}^d$$

the Birman-Schwinger integral operator with the kernel

$$G(k,z;p,q) = (2\pi)^{-d} \int\limits_{\mathbb{T}^d} v^{\frac{1}{2}}(p-t)(\mathcal{E}_k(t)-z)^{-1} v^{\frac{1}{2}}(t-q)dt,$$

where $r_0(k,z)$ is the resolvent of the operator $h_0(k)$ and

$$v^{\frac{1}{2}}(p) = (2\pi)^{-\frac{d}{2}} \sum_{s \in \mathbb{Z}^d} \hat{v}^{\frac{1}{2}}(s) e^{\mathrm{i}(p,s)}.$$

The following lemma is the Birman-Schwinger principle for the two-particle Schrödinger operators on the lattice $\mathbb{Z}^d$.

Lemma

(i)A number $z < \mathcal{E}_{\min}(k), k \in \mathbb{T}^d$ is an eigenvalue for $h(k)$, if and only if the number "1" is eigenvalue for $G(k,z)$.
(ii)For any $z < \mathcal{E}_{\min}(k), k \in \mathbb{T}^d$ the following equality holds

$$N(z, h(k)) = n(1, G(k,z)), k \in \mathbb{T}^d.$$

Remark

Let $d \geq 3$*. Then for any* $z \leq \mathcal{E}_{\min}(k), k \in \mathbb{T}^d$ *the function*

$$G_\mu(k, z; p, q) = (2\pi)^{-d} \int_{\mathbb{T}^d} v^{\frac{1}{2}}(p - t)(\mathcal{E}_k(t) - z)^{-1} v^{\frac{1}{2}}(t - q)dt,$$

defines a Hilbert-Schmidt operator on $L^2_e(\mathbb{T}^d)$*.*

$$(h_0(k) - z)f = vf, \ \ f = (h_0(k) - z)^{-1} vf$$

or

$$v^{1/2} f = v^{1/2}(h_0(k) - z)^{-1} v^{1/2} v^{1/2} f.$$

Thus $\psi(p) = (v^{1/2} f)(p)$ *is associated eigenfunction of*

$$G(k, z), z \leq \mathcal{E}_{\min}(k), k \in \mathbb{T}^d.$$

If $d = 3$ or 4, then the function

$$f(p) = \frac{(v^{1/2}\psi)(p)}{\mathcal{E}_k(p) - \mathcal{E}_{\min}(k)}$$

belongs to $L^1_e(\mathbb{T}^d) \setminus L^2_e(\mathbb{T}^d)$, where $L^1_e(\mathbb{T}^d)$ is the Banach space of integrable functions. If $d \geq 5$, then the function

$$f(p) = \frac{(v^{1/2}\psi)(p)}{\mathcal{E}_k(p) - \mathcal{E}_{\min}(k)}$$

belongs to $L^2_e(\mathbb{T}^d)$.

Definition

Let $d \geq 3$. The $h(k)$ is said to have a singular point of multiplicity m (resp.regular point) at the bottom $z = \mathcal{E}_{\min}(k)$ if the number 1 is an eigenvalue of multiplicity m (resp.no eigenvalue) for the Birman-Schwinger operator $G(k, \mathcal{E}_{\min}(k))$.

Definition

Let $d = 3 or 4$. The singular point is called a virtual level of the operator $h(k)$ if the number 1 is a simple eigenvalue for the operator

$$G(k, \mathcal{E}_{\min}(k)) = v^{\frac{1}{2}} r_0(k, \mathcal{E}_{\min}(k)) v^{\frac{1}{2}}.$$

and the associated eigenfunction ψ satisfies the condition $(v^{1/2}\psi)(\mathcal{E}_{\min}(k)) \neq 0$. Without loss of generality we can always normalise $(v^{1/2}\psi)(\cdot)$ so that $(v^{1/2}\psi)(\mathcal{E}_{\min}(k)) = 1$.

For a bounded self-adjoint operator A, we define $n(\lambda, A)$ as

$$n(\lambda, A) = sup\{dimF : (Au, u) > \lambda,\ u \in F,\ ||u|| = 1\}. \qquad (3)$$

If $n(\lambda, A)$ is finite, the number $n(\lambda, A)$ is equal to the number of the eigenvalues of A bigger than λ.

Let $\hat{v}(s), s \in \mathbb{Z}^d$ *is real even non-negative function and* $\hat{v}(s) \to 0, s \to \infty$.

Theorem

Let either $d = 1$ *or* 2*. For any* $v > 0$ *for any* $k \in \mathbb{T}^d$ *the operator* $h(k)$ *has an eigenvalue* $z(k) < \mathcal{E}_{min}(k)$ *below the bottom of the essential spectrum* $\sigma_{ess}(h(k))$.

Remark

The eigenfunction of $h(k)$ associated to the eigenvalue $z(k) < \mathcal{E}_{min}(k)$ is of the form

$$f(p) = (\mathcal{E}_k(p) - z(k))^{-1}(v^{1/2}\psi)(p)$$

where ψ is a solution (up to a constant factor) of the equation $G(k, \mathcal{E}_{min}(k))\psi = \psi$.

To formulate our results in case that $d \geq 3$, we introduce a parameter $\eta(\mathcal{E}_0) \geq 0$ by

$$\eta(\mathcal{E}_0) = [\frac{1}{(2\pi)^d} \int\limits_{\mathbb{T}^d} \frac{dq}{\mathcal{E}_0(q)})]^{-1} < (\mathcal{E}_{max}(0) = 4d)^{-1}.$$

Note that $\eta(\mathcal{E}_0) < \infty$ is finite because all critical points of $\mathcal{E}_0$ are non-degenerate.

Theorem

Let $d \geq 3$. If $\max \hat{v}(s) > \eta(\mathcal{E}_0)$ holds, then for any $k \in \mathbb{T}^d$ the operator $h(k)$ has an eigenvalue $z(k)$ lying below the bottom $z = \mathcal{E}_{min}(k)$ of the essential spectrum $\sigma_{ess}(h(k))$.

The following Theorem states the existence of bound states of $h(k)$ for all $k \in \mathbb{T}_0^d = \mathbb{T}^d \setminus \{0\}$.

Theorem

(See. [1]) Assume Hypothesis 3. Let the operator $h(0)$ is positive and the bottom $z = 0$ is singular point of the essential spectrum of $h(0)$. Then, for all $k \in \mathbb{T}_0^d = \mathbb{T}^d \setminus \{0\}$ the discrete spectrum of the fiber Hamiltonian $h(k)$ below the bottom $\mathcal{E}_{\min}(k)$ of its essential spectrum is a non-empty set.

Theorem

Assume that the assumptions of Theorem 11 are fulfilled. Then there exists a unique even continuous positive function $z(\cdot)$ on $\mathbb{T}^d$ and for any $k \in \mathbb{T}_0^d$ the number $z(k) > 0$ is an eigenvalue of $h(k)$ lying below the bottom $\mathcal{E}_{\min}(k)$.

Remark

We remark that it may exists a region $G \subset \mathbb{T}_0^d, G \neq \mathbb{T}_0^d$ *and several continuous positive functions* $z_1(\cdot), ..., z_n(\cdot)$ *defined on it and for any* $k \in G$ *the numbers* $0 < z_1(k) \leq ... \leq z_n(k)$ *are eigenvalues of* $h(k)$ *lying below the bottom* $\mathcal{E}_{\min}(k)$.

Theorem

Let $d \geq 3$. *Assume Hypothesis 3.Let the bottom* $z = 0$ *is singular point of multiplicity m for the essential spectrum of the operator* $h(0)$. *Then for any* $k \in \mathbb{T}_0^d$ *the op-r* $h(k)$ *has at least m eigenvalues lying below the bottom* $\mathcal{E}_{\min}(k)$ *of the essential spectrum of* $h(k)$.

Theorem
Let $d \geq 3$. Assume Hypothesis 3.Let the operator $h(0)$ has n negative eigenvalues (counting multiplicities). Then for any $k \in \mathbb{T}_0^d$ the $h(k)$ has at least n eigenvalues lying below the bottom $\mathcal{E}_{\min}(k)$.

Theorem
Let $d \geq 3$. Assume Hypothesis 3.Let $z_2(0) < z_1(0) < 0$ are two negative eigenvalues(counting multiplicities) of the operator $h(0)$. Then for any $k \in \mathbb{T}_0^d$ the inequality $z_2(k) < z_1(k)$ holds.

Remark

We underline that these results are in contrast to the similar one for the continuous two-particle Schrödinger operators, where the number of eigenvalues does not depend on the two-particle total momentum $k \in \mathbb{R}^d$.

The proofs of above stated Theorems 12, 14, 15,16 are based on the following inequality.

Remark

Assume that the dispersion relation $\varepsilon(\cdot)$ is a real-valued even conditionally negative definite function on $\mathbb{T}^d$ with the unique minimum $\varepsilon(0)$. Then for all $q \in \mathbb{T}^d \setminus \{0\}$ the inequality

$$\varepsilon(p) + \varepsilon(q) > \frac{\varepsilon(p+q) + \varepsilon(p-q)}{2} + \varepsilon(0), \quad a.e. \quad p \in \mathbb{T}^3,$$

olds.

Lemma

For any $s \in \mathbb{Z}^d$ the number $\lambda = \hat{v}(s)$ is an eigenvalue of the operator $\hat{v}$ with the multiplicity N_λ, where $N_\lambda = |\{x \in \mathbb{Z}^d : \hat{v}(x) = \lambda\}|$ is number of points of the set $\{x \in \mathbb{Z}^d : \hat{v}(x) = \lambda\}$.

Note that the number $\lambda = \hat{v}(s)$ is eigenvalue and the function

$$\psi_s(p) = (2\pi)^{-1/2} e^{isp}, s \in \mathbb{Z}^d,$$

is an associated eigenfunction for the operator

$$v = \mathcal{F}^{-1} \hat{v} \mathcal{F},$$

in momentum space.

For any [$z < 0$,if $d = 1$ or 2 (resp.$z \leq 0$,if $d \geq 3$)] and

$$\psi_s(p) = (2\pi)^{-1/2} e^{isp}, s \in \mathbb{Z}^d,$$

we conclude that

$$(G(0,z)\psi_s, \psi_s) = \frac{1}{(2\pi)^d} \int\limits_{\mathbf{T}^d} \frac{|(v^{\frac{1}{2}}\psi)(p)|^2 dp}{\mathcal{E}_0(q) - z}$$

$$= \frac{1}{(2\pi)^d} \int\limits_{\mathbb{T}^d} \frac{|v^{\frac{1}{2}}(s)\psi_s(p)|^2 dq}{\mathcal{E}_0(q) - z} = \frac{\hat{v}(s)}{(2\pi)^d} \int\limits_{\mathbb{T}^d} \frac{dq}{\mathcal{E}_0(q) - z}$$

$\psi_s \in L^2(\mathbb{T}^d)$

Let $d = 1$ or 2. Then for any $v(x) \geq 0$ there exists $E(0) < 0$ such that the inequality

$$\frac{\hat{v}(x)}{(2\pi)^d} \int\limits_{\mathbb{T}^d} \frac{dq}{\mathcal{E}_0(q) - E(0)} > 1 \qquad (4)$$

holds. Let $d \geq 3$. Let for some $x \in \mathbb{Z}^d$ the inequality holds

$$\max \hat{v}(x)[\frac{1}{(2\pi)^d} \int\limits_{\mathbb{T}^d} \frac{dq}{\mathcal{E}_0(q)})] > 1$$

.

Thus there exist $\psi \in L^2(\mathbb{T}^d)$ and $E(0) < 0$(resp.$E(0) = 0$) such that $(G(0, E(0))\psi, \psi) > 1$, i.e.,the self-adjoint bounded operator $G(0, E(0))$ has an eigenvalue in $(1, +\infty)$. By the Birman-Schwinger principle the operator $h(0)$ has an eigenvalue in $(-\infty, 0)$.

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