INVERSE PROBLEMS, TRACE FORMULAE FOR DISCRETE SCHRÖDINGER OPERATORS

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Abstract. We study discrete Schrödinger operators with compactly supported potentials on $\mathbf{Z}^d$. Constructing spectral representations and representing S-matrices by the generalized eigenfunctions, we show that the potential is uniquely reconstructed from the S-matrix of all energies. We also study the spectral shift function $\xi(\lambda)$ for the trace class potentials, and estimate the discrete spectrum in terms of the moments of $\xi(\lambda)$ and the potential.

1. Introduction

In this paper, we consider trace formulas and inverse scattering problems for Schrödinger operators on the square lattice $\mathbf{Z}^d$ with $d \geq 2$. We restrict ourselves to the case of compactly supported, or trace class, potentials. Our aim is two-fold : the reconstruction of the potential from the scattering matrix, and the computation of trace formula using the spectral shift function. We begin with the forward problem. We shall construct the generalized Fourier transform and represent the S-matrix by generalized eigenfunctions. We then show that given the S-matrix $\mathcal{S}(\lambda)$ for all energies, one can uniquely reconstruct the potential (Theorem 4.4). We next compute the asymptotic expansion of the perturbation determinant associated with the discrete Hamiltonian. By virtue of Krein's spectral shift function, one can compute the moments of $\log\det\mathcal{S}(\lambda)$. As a by-product, one can estimate the discrete spectrum using these moments (Theorem 6.4).

In the continuous model, the first mathematical result on the inverse scattering for multi-dimensional Schrödinger operators was that of Faddeev [14] : the reconstruction of the potential from the high-energy behavior of the scattering matrix using the Born approximation. This result was extended by Saito [38] for more slowly decreasing potentials. A time-dependent approach was given by Enss-Weder [13]. In this paper, we give a discrete analogue of stationary method. Instead of high-energy, however, we consider the analytic continuation of the S-matrix with respect to the energy parameter and use the complex Born approximation. The analytic property of the resolvent of the discrete Laplacian is more complicated than the continuous case, which requires harder analysis in studying the inverse scattering problem. In the continuous case, Faddeev proposed a multi-dimensional analogue of the Gel'fand-Levitan theory using new Green's function of the Helmholtz equation ([16], [17]). Faddeev's Green function was rediscovered and developed in 1980's by Sylvester-Uhlmann [40], Nachman [32], Khenkin-Novikov [28] (see the survey article [23]). Reconstruction of the potential from the S-matrix of a fixed energy is one of the novelties of this idea. In the forthcoming paper, we shall study the inverse scattering from one fixed energy in the discrete model.

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Our next purpose is the trace formula. It is well-known that the scattering matrix, Krein's spectral shift function and the perturbation determinant for a pair of self-adjoint operators $\widehat{H}_0$ and $\widehat{H} = \widehat{H}_0 + \widehat{V}$ are mutually related. We shall write down the first 5 moments of the spectral shift function for our discrete model in terms of the traces of the potential $\widehat{V}$. If the potential admits a definite sign, we can obtain estimates of the discrete spectrum by the traces of $\widehat{V}$.

The computation of trace constitutes the central part of the study of spectral theory, since it provides quantitative information of the operator in question, hence serves as a clue to the inverse problem. In the continuous case, the trace formula was first obtained by Buslaev-Faddeev [11] in the one-dimensional problem and by Buslaev [9], [10] in the three-dimensional problem. Since then, an abundance of articles have been devoted to this subject, see e.g. [12] and [22], [33], [36], [18], [20]. The case of electric and magnetic fields was considered in [29], [30]. Gesztesy-Holden-Simon-Zhao [19] computed the trace $\mathrm{Tr}\,(L - L_A)$, where $L = -\Delta + V$ is a Schrödinger operator for the continuous case, and L_A is L with Dirichlet condition on a subset $A \subset \mathbf{R}^\nu$. Shirai [39] studied this problem on a graph. Karachalios [26] and Rosenblum-Solomjak [37] computed the Cwikel-Lieb-Rosenblum type bound for the discrete Schrödinger operator. The well-known Effimov effect has a different property in the case of the discrete model. See e.g. Albeverio, Dell Antonio and Lakaev [2]. See also [3].

In §2, we shall prove the limiting absorption principle with the aid of Mourre's commutator theory [31]. This is already done by A. Boutet de Monvel and J. Sahbani ([8]). However, we shall reproduce the proof in order to introduce the necessary notation and basic facts. We then derive the spectral representation in §3, and represent the S-matrix by generalized eigenfunctions. The inverse scattering problem is solved in §4, and §6 is devoted to the trace formula.

The essential spectrum of our discrete Schrödinger operator $\widehat{H} = \widehat{H}_0 + \widehat{V}$ on $\mathbf{Z}^d$ fills the interval $[0, d]$, and the set $[0, d] \cap \mathbf{Z}$ is that of critical points, since $\widehat{H}_0$ is unitarily equivalent to the operator of multiplication by $(d - \sum_{j=1}^d \cos x_j)/2$ on the torus $\mathbf{R}^d/(2\pi\mathbf{Z})^d$. In fact, the resolvent estimates in §2 are proved outside $[0, d] \cap \mathbf{Z}$. The behavior of the free resolvent $(\widehat{H}_0 - z)^{-1}$ near the critical points depends on the dimension d. This is itself interesting and is studied in §5 (Lemmas 5.3, 5.4 and 5.5), although we do not use it in this paper.

The notation used in this paper is standard. For two Banach spaces X and Y, $\mathbf{B}(X; Y)$ denotes the set of all bounded operators from X to Y. For a self-adjoint operator A, $\sigma(A)$, $\sigma_p(A)$, $\sigma_d(A)$, $\sigma_e(A)$, $\sigma_{ac}(A)$ and $\rho(A)$ denote its spectrum, point spectrum (= the set of all eigenvalues), discrete spectrum, essential spectrum, absolutely continuous spectrum and resolvent set, respectively. For a trace class operator K, $\mathrm{Tr}\,(K)$ denotes the trace of K.

2. Schrödinger operators on the lattice

2.1. **Discrete Schrödinger operator.** Let $\mathbf{Z}^d = \{n = (n_1, \cdots, n_d)\,;\, n_i \in \mathbf{Z}\}$, and $e_1 = (1, 0, \cdots, 0), \cdots, e_d = (0, \cdots, 0, 1)$ be the standard bases of $\mathbf{Z}^d$. The Schrödinger operator $\widehat{H}$ on $\mathbf{Z}^d$ is defined by

$$\widehat{H} = \widehat{H}_0 + \widehat{V},$$

where for $\widehat{f} = \{\hat{f}(n)\}_{n\in\mathbf{Z}^d} \in l^2(\mathbf{Z}^d)$ and $n \in \mathbf{Z}^d$

$$\big(\widehat{H}_0\widehat{f}\big)(n) = \frac{d}{2}\,\widehat{f}(n) - \frac{1}{4}\sum_{j=1}^{d}\big\{\widehat{f}(n+e_j) + \widehat{f}(n-e_j)\big\},$$

$$(\widehat{V}\widehat{f})(n) = \widehat{V}(n)\widehat{f}(n).$$

Until the end of §4, we impose the following assumption on $\widehat{V}$:

(A-1) *$\widehat{V}$ is real-valued, and $\widehat{V}(n) = 0$ except for a finite number of n.*

Define the 1-dimensional projection $\widehat{P}(n)$ by

$$\left(\widehat{P}(n)\widehat{f}\right)(m) = \delta_{nm}\widehat{f}(m).$$

Then $\widehat{V}$ is rewritten as

$$\widehat{V} = \sum_n \widehat{V}(n)\widehat{P}(n).$$

Let us introduce the shift operator

$$\big(\widehat{S}_j\widehat{f}\big)(n) = \widehat{f}(n+e_j), \quad \big((\widehat{S}_j)^*\widehat{f}\big)(n) = \widehat{f}(n-e_j),$$

and the position operator

$$\big(\widehat{N}_j\widehat{f}\big)(n) = n_j\widehat{f}(n).$$

A direct computation yields the following lemma.

Lemma 2.1. *$\widehat{S}_j$ is unitary, $\widehat{N}_j$ is self-adjoint with its natural domain and*

$$\big[\widehat{S}_j, \widehat{N}_j\big] = \widehat{S}_j.$$

Letting $\widehat{N} = (\widehat{N}_1, \cdots, \widehat{N}_d)$, $\widehat{H}$ is rewritten as

$$\widehat{H} = \frac{d}{2} - \frac{1}{4}\sum_{j=1}^{d}\left(\widehat{S}_j + (\widehat{S}_j)^*\right) + \widehat{V}(\widehat{N}).$$

The spectral properties of $\widehat{H}$ is easier to describe by passing to its unitary transformation by the Fourier series. Let

$$\mathbf{T}^d = \mathbf{R}^d/(2\pi\mathbf{Z})^d = [-\pi, \pi]^d$$

be the flat torus and $\mathcal{U}$ the unitary operator from $l^2(\mathbf{Z}^d)$ to $L^2(\mathbf{T}^d)$ defined by

$$(\mathcal{U}\,\widehat{f})(x) = (2\pi)^{-d/2}\sum_{n\in\mathbf{Z}^d}\widehat{f}(n)e^{-in\cdot x}.$$

The shift operator and the position operator are rewritten as

$$S_j := \mathcal{U}\,\widehat{S}_j\,\mathcal{U}^* = e^{ix_j}, \quad N_j := \mathcal{U}\,\widehat{N}_j\,\mathcal{U}^* = i\partial/\partial x_j.$$

Letting

$$H_0 = \mathcal{U}\,\widehat{H}_0\,\mathcal{U}^*, \quad V = \mathcal{U}\,\widehat{V}\,\mathcal{U}^*,$$

we have

$$H := \mathcal{U}\widehat{H}\mathcal{U}^* = H_0 + V, \tag{2.1}$$

$$H_0 = \frac{1}{2}\Big(d - \sum_{j=1}^{d}\cos x_j\Big) =: h(x), \tag{2.2}$$

$$(Vf)(x) = (2\pi)^{-d/2} \int_{\mathbf{T}^d} V(x-y) f(y) dy,$$
$$V(x) = (2\pi)^{-d/2} \sum_{n \in \mathbf{Z}^d} \widehat{V}(n) e^{-in\cdot x}.$$

In fact, this is a special case of the Friedrichs model (see e.g. [15]). The following theorem is easily proven by (2.1) and Weyl's theorem.

Theorem 2.2. *(1)* $\sigma(H_0) = \sigma_{ac}(H_0) = [0, d]$.
(2) $\sigma_e(H) = [0, d], \quad \sigma_d(H) \subset \mathbf{R} \setminus [0, d]$.

2.2. **Sobolev and Besov spaces.** We put $N = (N_1, \cdots, N_d)$, and let N^2 be the self-adjont operator defined by

$$N^2 = \sum_{j=1}^d N_j^2 = -\Delta, \quad \text{on} \quad \mathbf{T}^d,$$

where Δ denotes the Laplacian on $\mathbf{T}^d = [-\pi, \pi]^d$ with periodic boundary condition. We put

$$|N| = \sqrt{N^2} = \sqrt{-\Delta}.$$

We introduce the norm

$$\|u\|_s = \|(1 + N^2)^{s/2} u\|, \quad s \in \mathbf{R},$$

$\|\cdot\|$ being the norm on $L^2(\mathbf{T}^d)$, and let $\mathcal{H}^s$ be the completion of $D(|N|^s)$, the domain of $|N|^s$, with respect to the norm $\|u\|_s$:

$$\mathcal{H}^s = \{u \in \mathcal{D}'(\mathbf{T}^d)\, ;\, \|u\|_s < \infty\},$$

where $\mathcal{D}'(\mathbf{T}^d)$ denotes the space of distribution on $\mathbf{T}^d$. Put $\mathcal{H} = \mathcal{H}^0 = L^2(\mathbf{T}^d)$.

For a self-adjoint operator T, let $\chi(a \le T < b)$ denote the operator $\chi_I(T)$, where $\chi_I(\lambda)$ is the characteristic function of the interval $I = [a, b)$. The operators $\chi(T < a)$ and $\chi(T \ge b)$ are defined similarly. Using the sequence $\{r_j\}_{j=0}^\infty$ with $r_{-1} = 0$, $r_j = 2^j$ $(j \ge 0)$, we define the Besov space $\mathcal{B}$ by

$$\mathcal{B} = \Big\{ f \in \mathcal{H}\, ;\, \|f\|_{\mathcal{B}} = \sum_{j=0}^\infty r_j^{1/2} \|\chi(r_{j-1} \le |N| < r_j) f\| < \infty \Big\}.$$

Its dual space $\mathcal{B}^*$ is the completion of $\mathcal{H}$ by the following norm

$$\|u\|_{\mathcal{B}^*} = \sup_{j \ge 0} r_j^{-1/2} \|\chi(r_{j-1} \le |N| < r_j) u\|.$$

The following Lemmas 2.3 and 2.4 are proved in the same way as in the continuous case ([1]). We omit the proof.

Lemma 2.3. *There exists a constant* $C > 0$ *such that*

$$C^{-1} \|u\|_{\mathcal{B}^*} \le \left(\sup_{R>1} \frac{1}{R} \|\chi(|N| < R) u\|^2 \right)^{1/2} \le C \|u\|_{\mathcal{B}^*}.$$

Therefore, in the following, we use

$$\|u\|_{\mathcal{B}^*} = \left(\sup_{R>1} \frac{1}{R} \|\chi(|N| < R) u\|^2 \right)^{1/2}$$

as the norm on $\mathcal{B}^*$.

Lemma 2.4. *For $s > 1/2$, the following inclusion relations hold :*

$$\mathcal{H}^s \subset \mathcal{B} \subset \mathcal{H}^{1/2} \subset \mathcal{H} \subset \mathcal{H}^{-1/2} \subset \mathcal{B}^* \subset \mathcal{H}^{-s}.$$

We also put $\widehat{\mathcal{H}} = l^2(\mathbf{Z}^d)$, and define $\widehat{\mathcal{H}}^s$, $\widehat{\mathcal{B}}$, $\widehat{\mathcal{B}}^*$ by replacing N by $\widehat{N}$. Note that $\widehat{\mathcal{H}}^s = \mathcal{U}^*\mathcal{H}^s$ and so on. In particular, Parseval's formula implies that

$$\|u\|^2_{\mathcal{H}^s} = \|\widehat{u}\|^2_{\widehat{\mathcal{H}}^s} = \sum_{n\in Z^d}(1+|n|^2)^s|\widehat{u}(n)|^2,$$

$$\|u\|^2_{\mathcal{B}^*} = \|\widehat{u}\|^2_{\widehat{\mathcal{B}}^*} = \sup_{R>1}\frac{1}{R}\sum_{|n|<R}|\widehat{u}(n)|^2,$$

$\widehat{u}(n)$ being the Fourier coefficient of $u(x)$.

2.3. **Mourre estimate.** Let $\widehat{\mathcal{H}}^\infty = \cap_{s>0}\widehat{\mathcal{H}}^s$, and define a symmetric operator $\widehat{A}$ with domain $\widehat{\mathcal{H}}^\infty$ by

$$\widehat{A} = i\sum_{j=1}^d\left(\big((\widehat{S}_j)^* - \widehat{S}_j\big)\widehat{N}_j + \frac{\widehat{S}_j + (\widehat{S}_j)^*}{2}\right). \tag{2.3}$$

Then $\widehat{A}$ is essentially self-adjoint. In fact, letting $\widehat{M} = 1 + \widehat{N}^2$, we can find a constant $C > 0$ such that

$$\|\widehat{A}\widehat{u}\| \le C\|\widehat{M}\widehat{u}\|, \quad |(\widehat{A}\widehat{u}, \widehat{M}\widehat{u}) - (\widehat{M}\widehat{u}, \widehat{A}\widehat{u})| \le C\|\widehat{M}^{1/2}\widehat{u}\|^2, \quad \forall \widehat{u} \in \widehat{\mathcal{H}}^\infty. \tag{2.4}$$

Nelson's commutator theorem ([34], p. 193) then implies the result.

By Lemma 2.1, (2.3) is rewritten as

$$\widehat{A} = -i\sum_{j=1}^d\left(\widehat{N}_j\widehat{S}_j - (\widehat{S}_j)^*\widehat{N}_j + \frac{\widehat{S}_j - (\widehat{S}_j)^*}{2}\right).$$

Let us note that in [8], $-i\sum_{j=1}^d\left(\widehat{N}_j\widehat{S}_j - (\widehat{S}_j)^*\widehat{N}_j\right)$ is used as $\widehat{A}$. Our choice of $\widehat{A}$ comes from the following reasoning. Let $h(x)$ be defined by (2.2). Passing to the Fourier series, we have

$$A = \mathcal{U}\,\widehat{A}\,\mathcal{U}^* = i\sum_{j=1}^d\left(2\sin x_j\frac{\partial}{\partial x_j} + \cos x_j\right) = 2i\big(\nabla_x h\cdot\nabla_x + \nabla_x\cdot(\nabla_x h)\big).$$

This is an analogue of the generator of dilation group on $\mathbf{R}^d$. We then have

$$i[H_0, A] = 4|\nabla_x h|^2 = \sum_{j=1}^d(\sin x_j)^2.$$

Let $E_{H_0}(\lambda)$ and $E_H(\lambda)$ be the spectral decompositions of H_0 and H, respectively.

Lemma 2.5. *Let $\lambda \in (0, d)\setminus\mathbf{Z}$. Then there exist constants $\delta, C > 0$ and a compact operator K such that*

$$E_H(I)[H, iA]E_H(I) \ge CE_H(I) + K, \quad I = (\lambda-\delta, \lambda+\delta).$$

Proof. For $\lambda \in (0,d)\setminus \mathbf{Z}$, let

$$M_\lambda = \{x \in \mathbf{T}^d\,;\, h(x) = \lambda\}.$$

If $\nabla h(x) = 0$, then $\cos x_j = \pm 1$, and $h(x) \in \mathbf{Z}$. Therefore, the assumption $\lambda \not\in \mathbf{Z}$ implies that $\nabla h(x) \neq 0$ on M_λ, hence M_λ is a real analytic manifold. We put

$$C_0(\lambda) = \inf_{x\in M_\lambda} |\nabla h(x)|^2.$$

Then for any small $\epsilon > 0$, there exists $\delta > 0$ such that

$$|\nabla h(x)|^2 \geq C_0(\lambda) - \epsilon \quad \text{on} \quad h^{-1}([\lambda-\delta, \lambda+\delta]).$$

We have, therefore,

$$E_{H_0}(I)[H_0, iA]E_{H_0}(I) \geq (C_0(\lambda)-\epsilon)E_{H_0}(I), \quad I = (\lambda-\delta,\lambda+\delta).$$

Since $\widehat{V}$ is a compact operator, so are V and $E_H(I) - E_{H_0}(I)$. This proves the lemma. □

Let $R(z) = (H-z)^{-1}$ be the resolvent of H.

Theorem 2.6. *(1) $\sigma_p(H) \cap \big((0,d)\setminus \mathbf{Z}\big)$ is discrete and finite multiplicities with possible accumulation points in $\mathbf{Z}$.*
(2) Let $s > 1/2$ and $\lambda \in (0,d)\setminus\big(\mathbf{Z}\cup\sigma_p(H)\big)$. Then, thers exists a norm limit $R(\lambda \pm i0) := \lim_{\epsilon\to 0} R(\lambda \pm i\epsilon) \in \mathbf{B}(\mathcal{H}^s;\mathcal{H}^{-s})$. Moreover, we have

$$\sup_{\lambda\in J} \|R(\lambda\pm i0)\|_{\mathbf{B}(\mathcal{B};\mathcal{B}^*)} < \infty, \tag{2.5}$$

for any compact interval J in $(0,d)\setminus\big(\mathbf{Z}\cup\sigma_p(H)\big)$. The mapping $(0,d)\setminus\big(\mathbf{Z}\cup\sigma_p(H)\big) \ni \lambda \to R(\lambda\pm i0)$ is norm continuous in $\mathbf{B}(\mathcal{H}^s;\mathcal{H}^{-s})$ and weakly continuous in $\mathbf{B}(\mathcal{B};\mathcal{B}^*)$.
(3) H has no singular continuous spectrum.

This theorem follows from the well-known Mourre theory. We shall give here a brief explanation. First we introduce an abstract Besov space. We define

$$\mathcal{B}_A = \Big\{ f \in \mathcal{H}\,;\, \|f\|_{\mathcal{B}_A} = \sum_{j=0}^{\infty} r_j^{1/2}\|\chi(r_{j-1} \leq |A| < r_j)f\| < \infty \Big\},$$

where $\mathcal{H} = L^2(\mathbf{T}^d)$. Its dual space ${\mathcal{B}_A}^*$ is the completion of $\mathcal{H}$ by the norm

$$\|u\|_{{\mathcal{B}_A}^*} = \sup_j r_j^{-1/2}\|\chi(r_{j-1}\leq |A| < r_j)u\|.$$

The abstract theory of Mourre based on Lemma 2.5 then yields

Lemma 2.7. *Let J be as in Theorem 2.6 (2). Then there exists a constant $C > 0$ such that*

$$\sup_{\mathrm{Re}\, z\in J, \mathrm{Im}\, z\neq 0} \|(H-z)^{-1}f\|_{{\mathcal{B}_A}^*} \leq C\|f\|_{\mathcal{B}_A}, \quad \forall f \in \mathcal{B}_A.$$

For the proof of the lemma, see [4], [8], [25]. Therefore, to prove Theorem 2.6, we have only to replace $\mathcal{B}_A$ by $\mathcal{B}$ using the following lemma.

Lemma 2.8. *There is a constant $C > 0$ such that*

$$\|f\|_{\mathcal{B}_A} \leq C\|f\|_{\mathcal{B}}, \quad \forall f \in \mathcal{B}.$$

Proof. For $t \in \mathbf{R}$, let $\langle t\rangle = (1+t^2)^{1/2}$. By definitions of A and N we have

$$\langle A\rangle\langle N\rangle^{-1} \in \mathbf{B}(\mathcal{H}\,;\mathcal{H}).$$

For $f \in \mathcal{B}$, we put $f_j = \chi(r_{j-1} \le |N| < r_j)f$. Then

$$\|\langle A\rangle f_j\| \le C\|\langle N\rangle f_j\| \le Cr_j\|f_j\|,$$

which implies

$$\begin{aligned}\|\chi(r_{k-1} \le |A| < r_k)f_j\| &= \|\chi(r_{k-1} \le |A| < r_k)\langle A\rangle^{-1}\langle A\rangle f_j\| \\ &\le Cr_k^{-1}\|\langle A\rangle f_j\| \le Cr_k^{-1}r_j\|f_j\|.\end{aligned}$$

Then we have

$$\sum_{k>j} r_k^{1/2}\|\chi(r_{k-1} \le |A| < r_k)f_j\| \le C\sum_{k>j} r_k^{-1/2}r_j\|f_j\| \le Cr_j^{1/2}\|f_j\|,$$

$$\sum_{k\le j} r_k^{1/2}\|\chi(r_{k-1} \le |A| < r_k)f_j\| \le \sum_{k\le j} r_k^{1/2}\|f_j\| \le Cr_j^{1/2}\|f_j\|.$$

We have, therefore,

$$\|f_j\|_{\mathcal{B}_A} \le Cr_j^{1/2}\|f_j\|, \quad j = 0, 1, 2, \cdots .$$

Summing up these inequalities with respect to j, we obtain the lemma. □

3. Spectral representations and S-matrices

3.1. **Spectral representation on the torus.** For $t \in (0, d) \setminus \mathbf{Z}$, let dM_t be the measure on M_t induced from dx. By taking $t = h(x)$ as a new variable, one can show that for $f \in C(\mathbf{T}^d)$ supported in $\{x \in \mathbf{T}^d\,;\,h(x) \notin \mathbf{Z}\}$

$$\int_{\mathbf{T}^d} f(x)dx = \int_0^d \left(\int_{M_t} f\frac{dM_t}{|\nabla_x h|}\right)dt. \tag{3.1}$$

For $f, g \in L^2(\mathbf{T}^d)$, we have

$$(R_0(z)f, g) = \int_{\mathbf{T}^d} \frac{f(x)\overline{g(x)}}{h(x)-z}dx.$$

Therefore, if $f, g \in C^1(\mathbf{T}^d)$ and $\lambda \in (0, d) \setminus \mathbf{Z}$,

$$(R_0(\lambda \pm i0)f, g) = \pm i\pi\int_{M_\lambda} f\overline{g}\,\frac{dM_\lambda}{|\nabla_x h|} + \text{p.v.}\int_{\mathbf{T}^d}\frac{f\overline{g}}{h(x)-\lambda}dx. \tag{3.2}$$

Let $L^2(M_\lambda)$ be the Hilbert space equipped with the inner product

$$(\varphi, \psi)_{L^2(M_\lambda)} = \int_{M_\lambda} \varphi\,\overline{\psi}\,\frac{dM_\lambda}{|\nabla_x h|}. \tag{3.3}$$

We define

$$\mathcal{F}_0(\lambda)f = f\Big|_{M_\lambda}, \tag{3.4}$$

where the right-hand means the trace on , i.e. the restriction to, M_λ. Then we have by (3.2)

Lemma 3.1. *For $\lambda \in (0, d) \setminus \mathbf{Z}$, and $f, g \in C^1(\mathbf{T}^d)$,*

$$\frac{1}{2\pi i}\big((R_0(\lambda + i0) - R_0(\lambda - i0))f, g\big) = \big(\mathcal{F}_0(\lambda)f, \mathcal{F}_0(\lambda)g\big)_{L^2(M_\lambda)}.$$

By (2.5), this lemma implies

$$\mathcal{F}_0(\lambda) \in \mathbf{B}(\mathcal{B}; L^2(M_\lambda)). \tag{3.5}$$

Moreover,

$$(f, g)_{L^2(T^d)} = \int_0^d (\mathcal{F}_0(\lambda)f, \mathcal{F}_0(\lambda)g)_{L^2(M_\lambda)} d\lambda, \quad f, g \in \mathcal{B}. \tag{3.6}$$

The adjoint operator $\mathcal{F}_0(\lambda)^*$ is defined by

$$(\mathcal{F}_0(\lambda)f, \phi)_{L^2(M_\lambda)} = (f, \mathcal{F}_0(\lambda)^*\phi)_{L^2(\mathbf{T}^d)}.$$

By (3.5), $\mathcal{F}_0(\lambda)^* \in \mathbf{B}(L^2(M_\lambda); \mathcal{B}^*)$, and by (3.4), $\mathcal{F}_0(\lambda)(H_0 - \lambda) = 0$. Hence we have

$$(H_0 - \lambda)\mathcal{F}_0(\lambda)^* = 0.$$

In view of (3.1), we can identify $L^2(\mathbf{T}^d)$ with the space of L^2-functions $f(\lambda)$ over $(0, d)$ with respect to the measure $d\lambda$ such that for a.e. $\lambda \in (0, d)$, $f(\lambda)$ takes values in $L^2(M_\lambda)$. We denote this space by $L^2((0, d); L^2(M_\lambda); d\lambda)$.

We put $(\mathcal{F}_0 f)(\lambda) = \mathcal{F}_0(\lambda)f$ for $f \in \mathcal{B}$. The following Theorem 3.2 is essentially a reinterpretation of the identification $L^2(\mathbf{T}^d) \simeq L^2((0, d); L^2(M_\lambda); d\lambda)$. However, we give a functional analytic proof for the later convenience.

Theorem 3.2. *(1) $\mathcal{F}_0$ is uniquely extended to a unitary operator*

$$\mathcal{F}_0 : L^2(T^d) \to L^2((0, d); L^2(M_\lambda); d\lambda).$$

(2) $\mathcal{F}_0$ diagonalizes H_0 :

$$(\mathcal{F}_0 H_0 f)(\lambda) = \lambda(\mathcal{F}_0 f)(\lambda), \quad \forall f \in L^2(\mathbf{T}^d).$$

(3) For any compact interval $I \subset (0, d) \setminus \mathbf{Z}$,

$$\int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda \in L^2(T^d), \quad \forall g \in L^2((0, d); L^2(M_\lambda); d\lambda).$$

Moreover, for $I_N = \cup_{j=1}^d (j - 1 + 1/N, j - 1/N)$, the inversion formula holds:

$$f = \lim_{N \to \infty} \int_{I_N} \mathcal{F}_0(\lambda)^*(\mathcal{F}_0 f)(\lambda) d\lambda, \quad \forall f \in L^2(\mathbf{T}^d),$$

where the limit is taken in the norm of $L^2(\mathbf{T}^d)$.

Proof. By (3.6), $\mathcal{F}_0$ is uniquely extended to an isometric operator from $L^2(T^d)$ to $L^2((0, d); L^2(M_\lambda); d\lambda)$. To show that it is onto, we have only to note that the range of $\mathcal{F}_0$ is dense. For $f \in \mathcal{B}$, we have $\mathcal{F}_0(\lambda)(H_0 - \lambda)f = 0$ by definition, which proves (2). To show (3), we first note that for a compact interval $I \subset (0, d) \setminus \mathbf{Z}$, $\int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda \in \mathcal{B}^*$. We use $(\, , \,)$ to denote the inner product of $L^2(\mathbf{T}^d)$ as well as the coupling of $\mathcal{B}$ and $\mathcal{B}^*$. Then we have

$$\begin{aligned}\left(\int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda, f\right) &= \int_I (\mathcal{F}_0(\lambda)^* g(\lambda), f)\, d\lambda \\ &= \int_I (g(\lambda), \mathcal{F}_0(\lambda) f)_{L^2(M_\lambda)}\, d\lambda, \quad f \in \mathcal{B}.\end{aligned}$$

Therefore

$$\left|\left(\int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda, f\right)\right| \leq \|g\| \cdot \|\mathcal{F}_0 f\| = \|g\| \cdot \|f\|.$$

By Riesz' theorem, we then have

$$\int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda \in L^2(\mathbf{T}^d), \quad \| \int_I \mathcal{F}_0(\lambda)^* g(\lambda) d\lambda \| \le \|g\|.$$

Therefore for any compact interval $J \subset (0,d) \setminus \mathbf{Z}$,

$$\| \int_J \mathcal{F}_0(\lambda)^* (\mathcal{F}_0 f)(\lambda) d\lambda \| \le \|\mathcal{F}_0 \chi_J(H_0) f\| = \|\chi_J(H_0) f\|,$$

where χ_J is the characteristic function of J. One can then show the existence of the strong limit

$$\lim_{N\to\infty} \int_{I_N} \mathcal{F}_0(\lambda)^* (\mathcal{F}_0 f)(\lambda) d\lambda =: \tilde{f}.$$

By Parseval's formula, we have for any $h \in L^2(\mathbf{T}^d)$

$$\begin{aligned} (\tilde{f}, h) &= \lim_{N\to\infty} \int_{I_N} (\mathcal{F}_0 f(\lambda), \mathcal{F}_0(\lambda) h) d\lambda \\ &= (\mathcal{F}_0 f, \mathcal{F}_0 h) = (f, h), \end{aligned}$$

which implies $\tilde{f} = f$. □

Next let us construct the spectral representation for H. We put

$$\mathcal{F}^{(\pm)}(\lambda) = \mathcal{F}_0(\lambda)\left(1 - VR(\lambda \pm i0)\right), \quad \lambda \in (0,d) \setminus \left(\mathbf{Z} \cup \sigma_p(H)\right).$$

Then by (2.5)

$$\mathcal{F}^{(\pm)}(\lambda) \in \mathbf{B}(\mathcal{B}\,; L^2(M_\lambda)).$$

Lemma 3.3. *For $\lambda \in (0,d) \setminus (\mathbf{Z} \cup \sigma_p(H))$, and $f, g \in \mathcal{B}$*

$$\left(\big(R(\lambda + i0) - R(\lambda - i0)\big) f, g\right) = \Big(\mathcal{F}^{(\pm)}(\lambda) f, \mathcal{F}^{(\pm)}(\lambda) g\Big)_{L^2(M_\lambda)}.$$

Proof. We put

$$H_1 = H_0, \quad H_2 = H, \quad R_j(z) = (H_j - z)^{-1},$$

$$G_{jk}(z) = (H_j - z) R_k(z),$$

$$E_j'(\lambda) = \frac{1}{2\pi i}\left(R_j(\lambda + i0) - R_j(\lambda - i0)\right).$$

Then we have, by the resolvent equation,

$$\begin{aligned} &\frac{1}{2\pi i}\left(R_k(\lambda + i\epsilon) - R_k(\lambda - i\epsilon)\right) \\ &= G_{jk}(\lambda \pm i\epsilon)^* \frac{1}{2\pi i}\left(R_j(\lambda + i\epsilon) - R_j(\lambda - i\epsilon)\right) G_{jk}(\lambda \pm i\epsilon). \end{aligned}$$

Letting $\epsilon \to 0$, we have for $f, g \in \mathcal{B}$

$$(E_k'(\lambda) f, g) = \left(E_j'(\lambda) G_{jk}(\lambda \pm i0) f, G_{jk}(\lambda \pm i0) g\right). \tag{3.7}$$

Let $j = 1$, $k = 2$. Since $\mathcal{F}^{(\pm)}(\lambda) = \mathcal{F}_0(\lambda) G_{12}(\lambda \pm i0)$, the lemma follows if we replace f, g in Lemma 3.1 by $G_{jk}(\lambda \pm i0) f$, $G_{jk}(\lambda \pm i0) g$. □

We define the operator $\mathcal{F}^{(\pm)}$ by $\big(\mathcal{F}^{(\pm)} f\big)(\lambda) = \mathcal{F}^{(\pm)}(\lambda) f$ for $f \in \mathcal{B}$. Let $\mathcal{H}_{ac}(H)$ be the absolutely continuous subspace for H.

Theorem 3.4. *(1) $\mathcal{F}^{(\pm)}$ is uniquely extended to a partial isometry with initial set $\mathcal{H}_{ac}(H)$ and final set $L^2((0,d);L^2(M_\lambda);d\lambda)$. Moreover it diagonalizes H :*

$$\big(\mathcal{F}^{(\pm)}Hf\big)(\lambda) = \lambda\big(\mathcal{F}^{(\pm)}f\big)(\lambda), \quad \forall f \in L^2(\mathbf{T}^d). \tag{3.8}$$

(2) The following inversion formula holds:

$$f = \mathrm{s}-\lim_{N\to\infty}\int_{I_N}\mathcal{F}^{(\pm)}(\lambda)^*\big(\mathcal{F}^{(\pm)}f\big)(\lambda)d\lambda, \quad \forall f \in \mathcal{H}_{ac}(H), \tag{3.9}$$

where I_N is a union of compact intervals $\subset (0,d)\setminus(\mathbf{Z}\cup\sigma_p(H))$ such that $I_N \to (0,d)\setminus(\mathbf{Z}\cup\sigma_p(H))$ as $N\to\infty$.
(3) $\mathcal{F}^{(\pm)}(\lambda)^* \in \mathbf{B}(L^2(M_\lambda);\mathcal{B}^*)$ is an eigenoperator for H in the sense that

$$(H-\lambda)\mathcal{F}^{(\pm)}(\lambda)^*\phi = 0, \quad \forall \phi \in L^2(M_\lambda).$$

(4) The wave operators

$$W^{(\pm)} = \mathrm{s}-\lim_{t\to\pm\infty} e^{itH}e^{-itH_0} \tag{3.10}$$

exist and are complete, i.e. the range of $W^{(\pm)}$ is equal to $\mathcal{H}_{ac}(H)$. Moreover,

$$W^{(\pm)} = \big(\mathcal{F}^{(\pm)}\big)^*\mathcal{F}_0. \tag{3.11}$$

Proof. The proof of (1), (2), (3) is the same as that for Theorem 3.2 except for the surjectivity of $\mathcal{F}^{(\pm)}$. Since V is trace class, the existence and completeness of wave operators (3.10) can be proven by Rosenblum-Kato theory (see [27], p. 542). The relation (3.11) is also well-known, and we omit the proof (see e.g. [24]). We then have $\mathcal{F}^{(\pm)} = \mathcal{F}_0\left(W^{(\pm)}\right)^*$. The completeness of $W^{(\pm)}$ implies the surjectivity of $\mathcal{F}^{(\pm)}$. □

3.2. **Spectral representation on the lattice.** Theorem 3.4 is transferred on the lattice space by $\mathcal{U}$. We put $\widehat{\mathcal{F}}_0(\lambda)$, $\widehat{\mathcal{F}}^{(\pm)}(\lambda)$, $\widehat{\mathcal{F}}_0$ and $\widehat{\mathcal{F}}^{(\pm)}$ by

$$\widehat{\mathcal{F}}_0(\lambda) = \mathcal{F}_0(\lambda)\mathcal{U}, \quad \widehat{\mathcal{F}}^{(\pm)}(\lambda) = \mathcal{F}^{(\pm)}(\lambda)\mathcal{U},$$
$$\widehat{\mathcal{F}}_0 = \mathcal{F}_0\mathcal{U}, \quad \widehat{\mathcal{F}}^{(\pm)} = \mathcal{F}^{(\pm)}\mathcal{U}.$$

We also define

$$\widehat{\mathcal{B}} = \mathcal{U}^{-1}\mathcal{B}, \quad \widehat{\mathcal{B}}^* = \mathcal{U}^{-1}\mathcal{B}^*.$$

Theorem 3.5. *(1) $\widehat{\mathcal{F}}^{(\pm)}$ is uniquely extended to a partial isometry with initial set $\mathcal{H}_{ac}(\widehat{H})$ and final set $L^2(\mathbf{T}^d)$. Moreover it diagonalizes $\widehat{H}$:*

$$\big(\widehat{\mathcal{F}}^{(\pm)}\widehat{H}\widehat{f}\big)(\lambda) = \lambda\big(\widehat{\mathcal{F}}^{(\pm)}\widehat{f}\big)(\lambda). \tag{3.12}$$

(2) The following inversion formula holds:

$$\widehat{f} = \mathrm{s}-\lim_{N\to\infty}\int_{I_N}\widehat{\mathcal{F}}^{(\pm)}(\lambda)^*\left(\widehat{\mathcal{F}}^{(\pm)}\widehat{f}\right)(\lambda)d\lambda, \quad \forall \widehat{f} \in \mathcal{H}_{ac}(\widehat{H}), \tag{3.13}$$

where I_N is a union of compact intervals $\subset (0,d)\setminus\Big(\mathbf{Z}\cup\sigma_p(\widehat{H})\Big)$ such that $I_N \to (0,d)\setminus\Big(\mathbf{Z}\cup\sigma_p(\widehat{H})\Big)$ as $N\to\infty$.
(3) $\widehat{\mathcal{F}}^{(\pm)}(\lambda) \in \mathbf{B}(L^2(M_\lambda)\,;\widehat{\mathcal{B}}^*)$ is an eigenoperator for $\widehat{H}$ in the sense that

$$(\widehat{H}-\lambda)\widehat{\mathcal{F}}^{(\pm)}(\lambda)^*\phi = 0, \quad \forall \phi \in L^2(M_\lambda).$$

(4) The wave operators

$$\widehat{W}^{(\pm)} = \mathrm{s} - \lim_{t\to\pm\infty} e^{it\widehat{H}} e^{-it\widehat{H}_0}$$

exist and are complete. Moreover,

$$\widehat{W}^{(\pm)} = \big(\widehat{\mathcal{F}}^{(\pm)}\big)^* \widehat{\mathcal{F}}_0.$$

3.3. **Generalized eigenvector.** It is customary to define the distribution $\delta(h(x)-\lambda) \in \mathcal{D}'(\mathbf{T}^d)$ by

$$\int_{\mathbf{T}^d} f(x)\delta(h(x)-\lambda)dx = \int_{M_\lambda} f(x)\frac{dM_\lambda}{|\nabla_x h(x)|}, \quad f \in C(\mathbf{T}^d).$$

We then see that $\mathcal{F}_0(\lambda)^*$ defines a distribution on $\mathbf{T}^d$ by the following formula

$$\mathcal{F}_0(\lambda)^*\phi = \phi(x)\delta(h(x)-\lambda).$$

The right-hand side makes sense when, for example, $\phi \in C^\infty(M_\lambda)$ and is extended to a C^∞-function near M_λ, which is denoted by $\phi(x)$ again. The Fourier coefficients of $\mathcal{F}_0(\lambda)^*\phi$ are then computed as

$$(2\pi)^{-d/2}\int_{\mathbf{T}^d} e^{in\cdot x}\delta(h(x)-\lambda)\phi(x)dx = (2\pi)^{-d/2}\int_{M_\lambda} e^{in\cdot x}\phi(x)\frac{dM_\lambda}{|\nabla_x h(x)|}. \tag{3.14}$$

We look for a parametrization of M_λ suitable for the computation in the next section. Let us note

$$\frac{1}{2}\Big(d - \sum_{j=1}^d \cos x_j\Big) = \sum_{j=1}^d \sin^2\left(\frac{x_j}{2}\right),$$

which suggests that the variables $y = (y_1, \cdots, y_d) \in [-1,1]^d$:

$$y_j = \sin\frac{x_j}{2}, \quad x_j = 2\arcsin y_j$$

are convenient to describe H_0. In fact, the map $x \to y$ is a diffeomorphism between two tori:

$$\mathbf{R}^d/(2\pi\mathbf{Z})^d = [-\pi,\pi]^d \ni x \to y \in [-1,1]^d = \mathbf{R}^d/(2\mathbf{Z})^d.$$

Consequently,

$$x(\sqrt{\lambda}\theta) = \Big(2\arcsin(\sqrt{\lambda}\theta_1), \cdots, 2\arcsin(\sqrt{\lambda}\theta_d)\Big), \quad \theta \in S^{d-1}, \tag{3.15}$$

gives a parameter representation of M_λ. Passing to the polar coordinates $y = \sqrt{\lambda}\theta$, we also have

$$dx = J(y)dy = \frac{(\sqrt{\lambda})^{d-2}J(\sqrt{\lambda}\theta)}{2}d\lambda d\theta, \tag{3.16}$$

which implies

$$\frac{dM_\lambda}{|\nabla_x h(x)|} = \frac{(\sqrt{\lambda})^{d-2}J(\sqrt{\lambda}\theta)}{2}d\theta. \tag{3.17}$$

We define $\widehat{\psi}^{(0)}(n,\lambda,\theta)$ by

$$\begin{aligned}\widehat{\psi}^{(0)}(n,\lambda,\theta) &= (2\pi)^{-d/2}\frac{(\sqrt{\lambda})^{d-2}}{2}\, e^{in\cdot x(\sqrt{\lambda}\theta)}\, J(\sqrt{\lambda}\theta) \\ &= (2\pi)^{-d/2}2^{d-1}(\sqrt{\lambda})^{d-2}\, e^{in\cdot x(\sqrt{\lambda}\theta)}\, \frac{\chi(\sqrt{\lambda}\theta)}{\Pi_{j=1}^d \cos\big(x_j(\sqrt{\lambda}\theta)/2\big)}.\end{aligned} \tag{3.18}$$

where $\chi(y)$ is the characteristic function of $[-1,1]^d$. By (3.14) and (3.17), we have for $\phi \in L^2(M_\lambda)$

$$\big(\widehat{\mathcal{F}}_0(\lambda)^*\phi\big)(n) = \int_{S^{d-1}} \widehat{\psi}^{(0)}(n,\lambda,\theta)\phi(x(\sqrt{\lambda}\theta))d\theta. \tag{3.19}$$

One can also see that if $\widehat{f}$ is compactly supported

$$\big(\widehat{\mathcal{F}}_0(\lambda)\widehat{f}\big)(x(\sqrt{\lambda}\theta)) = (2\pi)^{-d/2}\sum_{n\in\mathbf{Z}^d} e^{-in\cdot x(\sqrt{\lambda}\theta)}\widehat{f}(n). \tag{3.20}$$

3.4. **Scattering matrix.** The scattering operator $\widehat{S}$ is defined by

$$\widehat{S} = \big(\widehat{W}_+\big)^*\widehat{W}_-.$$

We conjugate it by the spectral representation. Let

$$\mathcal{S} = \widehat{\mathcal{F}}_0\,\widehat{S}\,\big(\widehat{\mathcal{F}}_0\big)^*,$$

which is unitary on $L^2((0,d);L^2(M_\lambda);d\lambda)$. Since $\mathcal{S}$ commutes with $\widehat{H}_0$, $\mathcal{S}$ is written as a direct integral

$$\mathcal{S} = \int_{(0,d)} \oplus\mathcal{S}(\lambda)d\lambda.$$

The S-matrix, $\mathcal{S}(\lambda)$, is unitary on $L^2(M_\lambda)$ and has the following representation.

Theorem 3.6. *Let $\lambda \in (0,d)\setminus\big(\mathbf{Z}\cup\sigma_p(H)\big)$. Then $\mathcal{S}(\lambda)$ is written as*

$$\mathcal{S}(\lambda) = 1 - 2\pi i A(\lambda),$$

$$A(\lambda) = \widehat{\mathcal{F}}_0(\lambda)\widehat{V}\widehat{\mathcal{F}}_0(\lambda)^* - \widehat{\mathcal{F}}_0(\lambda)\widehat{V}\widehat{R}(\lambda+i0)\widehat{V}\widehat{\mathcal{F}}_0(\lambda)^*. \tag{3.21}$$

Since the proof is well-known, we omit it (see e.g. [24]).

By (3.18) and (3.20), the first term of the right-hand side of (3.21) has an integral kernel

$$(2\pi)^{-d}\frac{\lambda^{d-2}}{4}J(\sqrt{\lambda}\theta)J(\sqrt{\lambda}\theta')\sum_{n\in\mathbf{Z}^d} e^{-in\cdot(x(\sqrt{\lambda}\theta)-x(\sqrt{\lambda}\theta'))}\widehat{V}(n). \tag{3.22}$$

The 2nd term of the right-hand side of (3.21) has the following kernel

(3.23)
$$-(2\pi)^{-d/2}\frac{(\sqrt{\lambda})^{d-2}}{2}J(\sqrt{\lambda}\theta)\sum_{n\in\mathbf{Z}^d} e^{-in\cdot x(\sqrt{\lambda}\theta)}\widehat{V}(n)\Big(\widehat{R}(\lambda+i0)\widehat{V}\widehat{\psi}^{(0)}(\lambda,\theta')\Big)(n).$$

4. Inverse scattering

In this section we prove that the potential $\widehat{V}$ is uniquely reconstructed from the scattering matrix for all energies. We first consider the analytic continuation of $x(\sqrt{\lambda}\theta)$ defined by (3.15).

Lemma 4.1. *Let τ be a constant such that $-1<\tau<1$, $\tau\neq 0$. Then $f(z,\tau) = 2\arcsin(z\tau)$ is analytic with respect to $z\in\mathbf{C}\setminus\Big((-\infty,-1/|\tau|]\cup[1/|\tau|,\infty)\Big)$. Moreover, letting $\epsilon(\tau)=\tau/|\tau|$, we have as $N\to\infty$,*

$$\mathrm{Re}\, f(N+i,\tau) \equiv \epsilon(\tau)\Big(\pi - \frac{2}{N} + O(\frac{1}{N^3})\Big), \quad \bmod \quad 2\pi\mathbf{Z}$$

$$\mathrm{Im}\, f(N+i,\tau) = \epsilon(\tau)\Big(2\log N + \log(4\tau^2) + O(\frac{1}{N^2})\Big).$$

Proof. We take the branch of $\arcsin(z) = u(z) + iv(z)$ so that it is single-valued analytic on $\mathbf{C} \setminus \big((-\infty, -1] \cup [1, \infty)\big)$, and $0 < u(s) < \pi/2$ when $0 < s < 1$. Then we have

$$\sin(u)\cosh(v) = \operatorname{Re} z, \quad \cos(u)\sinh(v) = \operatorname{Im} z. \tag{4.1}$$

Let us note that

$$\cos(u) > 0 \quad \text{and} \quad \pm\sinh(v) > 0, \quad \text{if} \quad \pm\operatorname{Im} z > 0. \tag{4.2}$$

In fact, by the 2nd equation of (4.1), $\cos(u(z))$ and $\sinh(v(z))$ do not vanish if $\operatorname{Im} z \neq 0$, and $\cos(u(s)) > 0$, $v(s) = 0$ when $s \in (0, 1)$. So, $\cos(u(z)) > 0$ when $\operatorname{Im} z \neq 0$, and again by the 2nd equation of (4.1), $\sinh(v(z))$ and $\operatorname{Im} z > 0$ have the same sign.

Let $u_N = u((N + i)\tau), v_N = v((N + i)\tau)$. Then by (4.1) we have $\sinh(v_N) = \tau/\cos(u_N)$. Plugging this with

$$\big(1 - \cos^2(u_N)\big)\big(1 + \sinh^2(v_N)\big) = N^2\tau^2,$$

and letting $t_N = \cos^2(u_N)$, we get the equation

$$t_N^2 + (N^2\tau^2 + \tau^2 - 1)t_N - \tau^2 = 0.$$

Since $t_N > 0$, by solving this equation, we have

$$t_N = N^{-2} + O(N^{-4}).$$

Since $\cos(u_N) > 0$, we have

$$\cos(u_N) = N^{-1} + O(N^{-3}). \tag{4.3}$$

This, combined with (4.1) for $z = (N + i)\tau$, then yields

$$\sinh(v_N) = \tau N + O(N^{-1}). \tag{4.4}$$

If $\tau > 0$, then $v_N > 0$, and by (4.1) with $z = (N + i)\tau$, $\sin(u_N) > 0$. From (4.3), we then get

$$u_N \equiv \frac{\pi}{2} - N^{-1} + O(N^{-3}) \mod 2\pi\mathbf{Z}. \tag{4.5}$$

From (4.4), we have

$$e^{2v_N} - 2\left(\tau N + O(N^{-1})\right)e^{v_N} - 1 = 0,$$

which implies

$$v_N = \log(2\tau N) + O(N^{-2}). \tag{4.6}$$

Since $f(z, \tau) = 2\arcsin(z\tau)$ and $\arcsin(-z) = -\arcsin(z)$, (4.5) and (4.6) prove the lemma. □

We define the l^1-norm of $n = (n_1, \cdots, n_d) \in \mathbf{Z}^d$ by

$$|n|_{l^1} = \sum_{j=1}^{d} |n_j|. \tag{4.7}$$

We also introduce the following notation. For $n \in \mathbf{Z}^d$, we define $\widehat{B}(n) \in \mathbf{B}(l^2(\mathbf{Z}^d); \mathbf{C})$ and $\widehat{K}(n) \in \mathbf{B}(\mathbf{C}; l^2(\mathbf{Z}^d))$ by

$$\widehat{B}(n)\widehat{f} = \widehat{f}(n), \tag{4.8}$$

$$\big(\widehat{K}(n)c\big)(m) = c\,\delta_{mn}. \tag{4.9}$$

Note that

$$\widehat{P}(n) = \widehat{K}(n)\widehat{B}(n). \tag{4.10}$$

For $k \in \mathbf{Z}^d$ and $z \in \mathbf{C} \setminus \mathbf{R}$, let $r_0(k, z)$ be defined by

$$r_0(k, z) = (2\pi)^{-d} \int_{T^d} \frac{e^{ik\cdot x}}{h(x) - z} dx. \tag{4.11}$$

Then the resolvent $\widehat{R}_0(z) = (\widehat{H}_0 - z)^{-1}$ is written as

$$\big(\widehat{R}_0(z)\widehat{f}\big)(m) = \sum_{n\in\mathbf{Z}^d} r_0(m - n, z)\widehat{f}(n). \tag{4.12}$$

Lemma 4.2. *For any m, n and $|z| > d$*

$$\widehat{B}(m)\widehat{R}_0(z)\widehat{K}(n) = \sum_{s=|m-n|}^{\infty} c_s(m - n)\, z^{-s-1}, \tag{4.13}$$

where $c_s(k)$ is a constant satisfying

$$|c_s(k)| \le d^s, \quad s = 0, 1, 2, \cdots . \tag{4.14}$$

In particular, for $|z| > 2d$

$$\|\widehat{B}(m)\widehat{R}_0(z)\widehat{K}(n)\| \le |z|^{-1-|m-n|_{l^1}}. \tag{4.15}$$

Proof. Using $(h(x) - z)^{-1} = -\sum_{s=0}^{\infty} z^{-s-1}h(x)^s$, we have for large $|z|$

$$r_0(k, z) = \sum_{s=0}^{\infty} z^{-s-1}c_s(k), \tag{4.16}$$

$$c_s(k) = -(2\pi)^{-d} \int_{T^d} h(x)^s e^{ik\cdot x} dx.$$

Since $|h(x)| \le d$, we have

$$|c_s(k)| \le d^s. \tag{4.17}$$

Hence the series (4.16) is absolutely convergent for $|z| > d$. Note that $h(x)^s$ is a sum of terms of the form

$$(\cos x_1)^{\alpha_1} \cdots (\cos x_d)^{\alpha_d}, \quad 0 \le \alpha_1 + \cdots + \alpha_d \le s, \quad 0 \le \alpha_j \le s.$$

If $s < |k|_{l^1}$, we have $\alpha_j < |k_j|$ for some j, which implies

$$\int_{T^d} h(x)^s e^{ik\cdot x} dx = 0, \quad \text{if} \quad s < |k|_{l^1}.$$

Then we have

$$c_s(k) = 0, \quad \text{if} \quad s < |k|_{l^1}. \tag{4.18}$$

By (4.12) and (4.16), we have

$$\widehat{B}(m)\widehat{R}_0(z)\widehat{K}(n) = \sum_{s=0}^{\infty} z^{-s-1}c_s(m - n).$$

Then lemma then follows from (4.17) and (4.18). □

Lemma 4.3. *For any m, n, there exists a constant C_{mn} such that if $|z| > \|\widehat{H}\| + 1$,*

$$\|\widehat{B}(m)\widehat{R}(z)\widehat{K}(n)\| \le C_{mn}(1 + |z|)^{-1-|m-n|_{l^1}}.$$

Proof. Let $p = |m-n|_{l^1}$. By the perturbation expansion, we have

$$\widehat{R}(z) = \widehat{R}_0(z) - \widehat{R}_0(z)\widehat{V}\widehat{R}_0(z) + \cdots + (-1)^p\widehat{R}_0(z)\widehat{V}\cdots\widehat{V}\widehat{R}_0(z) + O(z^{-p-2}).$$

Multiply this equality by $\widehat{B}(m)$ and $\widehat{K}(n)$. Then by Lemma 4.2, the first term decays like $O(|z|^{-p-1})$. Next we look at the term

$$\widehat{B}(m)\widehat{R}_0(z)\widehat{V}\cdots\widehat{V}\widehat{R}_0(z)\widehat{K}(n),$$

consisting of k numbers of $\widehat{V}$ and $k+1$ numbers of $\widehat{R}_0(z)$, where $1 \le k \le p$. It is rewritten as a finite linear combination of terms

$$\widehat{B}(m)\widehat{R}_0(z)\widehat{P}(r^{(1)})\widehat{R}_0(z)\widehat{P}(r^{(2)})\cdots\widehat{P}(r^{(k)})\widehat{R}_0(z)\widehat{K}(n), \tag{4.19}$$

since $\widehat{V} = \sum_{|r|<c}\widehat{V}(r)\widehat{P}(r)$ for some $c > 0$. We put

$$\epsilon_1 = |m - r^{(1)}|_{l^1}, \quad \epsilon_2 = |r^{(1)} - r^{(2)}|_{l^1}, \quad \cdots, \epsilon_{k+1} = |r^{(k)} - n|_{l^1}.$$

By (4.10), (4.19) is written as the product

$$\widehat{B}(m)\widehat{R}_0(z)\widehat{K}(r^{(1)})\cdot\widehat{B}(r^{(1)})\widehat{R}_0(z)\widehat{K}(r^{(2)})\cdot\cdots\cdot\widehat{B}(r^{(k)})\widehat{R}_0(z)\widehat{K}(r^{(n)}).$$

By (4.15), this decays like $|z|^{-(k+1+\epsilon_1+\cdots+\epsilon_{k+1})}$. Since $|m-n|_{l^1} = p$, we have

$$\epsilon_1 + \cdots + \epsilon_{k+1} \ge p.$$

Taking notice of $k+1+\epsilon_1+\cdots+\epsilon_{k+1} \ge 2+p$, we have proven the lemma. □

We can now solve the inverse problem for $\widehat{H}$.

Theorem 4.4. *Suppose $\widehat{V}$ is compactly supported. Then from the scattering amplitude $A(\lambda)$ for all $\lambda \in (0,d)\setminus(\mathbf{Z}\cup\sigma_p(H))$, one can reconstruct $\widehat{V}$.*

Proof. Let $A(\lambda;\theta,\theta)$ be the integral kernel of $A(\lambda)$. Let $\sqrt{\lambda} = k$, and put

$$B(k;\theta,\theta') = \frac{4(2\pi)^d}{k^{2d-4}}\left(J(k\theta)J(k\theta')\right)^{-1}A(k^2;\theta,\theta').$$

In view of (3.18), (3.22) and (3.23), we can rewrite it as

$$B(k;\theta,\theta') = B_0(k;\theta,\theta') - B_1(k;\theta,\theta'), \tag{4.20}$$

$$B_0(k;\theta,\theta') = \sum_{n\in\mathbf{Z}^d} e^{-in\cdot(x(k\theta)-x(k\theta'))}\widehat{V}(n), \tag{4.21}$$

$$B_1(k;\theta,\theta') = -\sum_{n\in\mathbf{Z}^d} e^{-in\cdot x(k\theta)}\widehat{V}(n)\left(\widehat{R}(k^2+i0)\widehat{V}\widehat{\varphi}^{(0)}(k,\theta')\right)(n), \tag{4.22}$$

$$\widehat{\varphi}^{(0)}(k,\theta') = \left(e^{in\cdot x(k\theta')}\right)_{n\in\mathbf{Z}^d}. \tag{4.23}$$

Let $\theta_j \ne 0$, $\theta'_j \ne 0$ $(j = 1,\cdots,d)$, and put $\zeta(z,\theta) = (f(z,\theta_1),\cdots,f(z,\theta_d))$, where $f(z,\tau)$ is defined in Lemma 4.1. Then $B_0(k;\theta,\theta')$ and $B_1(k;\theta,\theta')$ have analytic continuations $B_0(z;\theta,\theta')$ and $B_1(z;\theta,\theta')$, which are defined with k replaced by z in the upper-half plane and $x(k\theta)$ by $\zeta(z,\theta)$. We put

$$S(n) = n_1 + \cdots + n_d, \quad n \in \mathbf{Z^d}.$$

We now take $\theta_j > 0$ and $\theta'_j < 0$, $(j = 1, \cdots, d)$. Then by Lemma 4.1, as $z = N + i \to \infty$,

$$e^{-in\cdot\zeta(z,\theta)} = e^{-iS(n)\pi}(4N^2)^{S(n)} \prod_{j=1}^{d} (\theta_j)^{2n_j} (1 + O(N^{-1})), \tag{4.24}$$

$$e^{in\cdot\zeta(z,\theta')} = e^{iS(n)\pi}(4N^2)^{S(n)} \prod_{j=1}^{d} \left(\theta'_j\right)^{2n_j} (1 + O(N^{-1})). \tag{4.25}$$

The reconstruction procedure for $\widehat{V}(n)$ goes inductively with respect to $S(n)$. Let us assume that

$$\mathrm{supp}\, \widehat{V} \subset \{(n_1, \cdots, n_d)\, ;\, |n_j| \leq M\}. \tag{4.26}$$

We use (4.21), (4.24) and (4.25) to compute the asymptotic expansion of $B_0(z_N; \theta, \theta')$, $z_N = N + i$, as $N \to \infty$. Then the largest contribution arises from the term for which $S(n)$ is the largest, i.e. $n = (M, \cdots, M)$. Therefore, we have

$$B_0(z_N\, ;\, \theta, \theta') \sim (2N)^{4dM} \prod_{j=1}^{d} \left(\theta_j\theta'_j\right)^{2M} \widehat{V}(n^{(M)}), \tag{4.27}$$

where $n^{(M)} = (M, \cdots, M)$. Since

$$\|\hat{R}((N + i)^2)\| = O(N^{-2}), \tag{4.28}$$

using (4.22), (4.24) and (4.25), we see that

$$B_1(z_N\, ;\, \theta, \theta') = O(N^{4dM-2}). \tag{4.29}$$

By (4.27) and (4.29), we can compute $\widehat{V}(n^{(M)})$ from the asymptotic expansion of $B(z_N\, ;\, \theta, \theta')$.

Assume that we have computed $\widehat{V}(n)$ for $S(n) > p$. Then

$$\begin{aligned} B_0(z_N\, ;\, \theta, \theta') - \sum_{S(n)>p} e^{-in\cdot(\zeta(z,\theta)-\zeta(z,\theta'))}\widehat{V}(n) \\ \sim (2N)^{4p} \sum_{S(n)=p} \prod_{j=1}^{d} (\theta_j\theta'_j)^{2n_j} \widehat{V}(n). \end{aligned} \tag{4.30}$$

The image of the map

$$S^{d-1}_{-} \times S^{d-1}_{+} \ni (\theta, \theta') \to (\theta_1\theta'_1, \cdots, \theta_d\theta'_d)$$

contains an open set in $\mathbf{R}^d$, where

$$S^{d-1}_{+} = \{\theta \in S^{d-1}\, ;\, \theta_j > 0,\ \forall j\}, \quad S^{d-1}_{-} = \{\theta \in S^{d-1}\, ;\, \theta_j < 0,\ \forall j\}.$$

Therefore, one can compute $\widehat{V}(n)$ for $S(n) = p$ from (4.30).

We show that $B_1(z_N; \theta, \theta') = O(N^{4p-2})$ up to terms which are already known. We rewrite $B_1(z_N; \theta, \theta')$ as

$$B_1(z_N; \theta, \theta') = \sum_{m,n} e^{-im\cdot\zeta(z_N,\theta)} e^{in\cdot\zeta(z_N,\theta')} \cdot \widehat{V}(m)\widehat{V}(n) \cdot \widehat{B}(m)\widehat{R}(z_N^2)\widehat{K}(n).$$

We split this sum into 4 parts:

$$\sum_{S(m),S(n)>p} + \sum_{S(m)>p,S(n)\leq p} + \sum_{S(m)\leq p,S(n)>p} + \sum_{S(m),S(n)\leq p} =: I_1 + I_2 + I_3 + I_4.$$

Note that by (4.24) and (4.25), we have

$$e^{-im\cdot\zeta(z_N,\theta)}e^{in\cdot\zeta(z_N,\theta')} = O(N^{2(S(m)+S(n))}). \tag{4.31}$$

Then by (4.28) and (4.31), we have

$$I_4 = O(N^{4p-2}). \tag{4.32}$$

By Lemma 4.3 and (4.31), $I_3 = O(N^{2(S(m)+S(n)-1-|m-n|_{l^1})})$. Since

$$S(n) - S(m) = \sum_{j=1}^{d}(n_j - m_j) \leq |m-n|_{l^1},$$

we have

$$\begin{aligned} &2S(m) + 2S(n) - 2|m-n|_{l^1} - 2 \\ &= 4S(m) + 2(S(n) - S(m) - |m-n|_{l^1}) - 2 \leq 4p - 2, \end{aligned}$$

which proves

$$I_3 = O(N^{4p-2}). \tag{4.33}$$

Similarly, we can prove

$$I_2 = O(N^{4p-2}). \tag{4.34}$$

We finally observe I_1. We put

$$\widehat{V}_{\leq p} = \sum_{S(n)\leq p}\widehat{V}(n)\widehat{P}(n), \quad \widehat{V}_{>p} = \sum_{S(n)>p}\widehat{V}(n)\widehat{P}(n),$$

$$\widehat{H}_{>p} = \widehat{H}_0 + \widehat{V}_{>p}, \quad \widehat{R}_{>p}(z) = (\widehat{H}_{>p} - z)^{-1}.$$

By the resolvent equation, I_1 is split into 2 parts

$$\begin{aligned} I_1 = &\sum_{S(m),S(n)>p} e^{-im\cdot\zeta(z_N,\theta)}e^{in\cdot\zeta(z_N,\theta')}\cdot\widehat{V}(m)\widehat{V}(n)\cdot\widehat{B}(m)\widehat{R}_{>p}(z_N^2)\widehat{K}(n) \\ &- \sum_{S(m),S(n)>p} e^{-im\cdot\zeta(z_N,\theta)}e^{in\cdot\zeta(z_N,\theta')}\cdot\widehat{V}(m)\widehat{V}(n)\cdot\widehat{B}(m)\widehat{R}_{>p}(z_N^2)\widehat{V}_{\leq p}\widehat{R}(z_N^2)\widehat{K}(n). \end{aligned}$$

The 1st term of the right-hand side is a known term, since we have already reconstructed $\widehat{V}(n)$ for $S(n) > p$. The 2nd term is a linear combination of terms

$$e^{-im\cdot\zeta(z_N,\theta)}e^{in\cdot\zeta(z_N,\theta')}\cdot\widehat{B}(m)\widehat{R}_{>p}(z_N^2)\widehat{P}(k)\widehat{R}(z_N^2)\widehat{K}(n), \tag{4.35}$$

where $S(k) \leq p$. By Lemma 4.3, it decays like $O(N^{2(S(m)+S(n)-|m-k|_{l^1}-|n-k|_{l^1}-2)})$. Using

$$\begin{aligned} S(m) - |m-k|_{l^1} &= \sum_j (m_j - k_j) - \sum_j |m_j - k_j| + \sum_j k_j \\ &\leq S(k) \leq p, \end{aligned}$$

we see that (4.35) decays like $O(N^{4p-4})$. Therefore, we have

$$I_1 = O(N^{4p-2}), \tag{4.36}$$

up to known terms. By virtute of (4.32) $\sim$ (4.36), we have completed the proof of the theorem. □

5. Estimates of the free resolvent near the critical values

The purpose of this section is to derive estimates of the resolvent $\widehat{R}_0(z) = (\widehat{H}_0 - z)^{-1}$ in weighted Hilbert spaces. Equivalently, we consider the operator norm on $L^2(\mathbf{Z}^d)$ of $\widehat{q}\,\widehat{R}_0(z)\,\widehat{q}$, where $\widehat{q}$ is the operator of multiplication by $\widehat{q} \in \ell^\infty(\mathbf{Z}^d)$: $(\widehat{q}\,\widehat{f})(n) = \widehat{q}(n)\widehat{f}(n)$. In particular, $\widehat{\rho}_s$ is the operator defined by

$$\widehat{\rho}_s(n) = (1 + |n|^2)^{-s/2}, \quad s \in \mathbf{R}.$$

We put

$$\mathbf{D}_1 = \{z \in \mathbf{C}\,;\, 0 < |z| < 1\},$$

$$\Lambda_d = \rho(\widehat{H}_0) = \mathbf{C} \setminus [0, d],$$

$$\lambda(z) = \frac{1}{4}\left(2 - z - \frac{1}{z}\right). \tag{5.1}$$

For $w = re^{i\theta}$ with $0 < \theta < 2\pi$, we take the branch $\sqrt{w} = \sqrt{r}e^{i\theta/2}$. For $a, b \in \mathbf{C}$, we put

$$I(a, b) = \{ta + (1 - t)b\,;\, 0 \le t \le 1\}.$$

Lemma 5.1. *$\lambda(z)$ is a conformal map from $\mathbf{D}_1$ onto Λ_1, and its inverse is given by*

$$z(\lambda) = 2\lambda - 1 - 2\sqrt{\lambda(\lambda - 1)}. \tag{5.2}$$

Proof. Since the map

$$\{0 < |z| < 1\} \ni z \to \frac{1}{2}\left(z + \frac{1}{z}\right) \in \mathbf{C} \setminus [-1, 1]$$

is conformal, so is $\lambda(z)$ from $\mathbf{D}_1$ onto Λ_1. By solving the equation $z^2 + (4\lambda - 2)z + 1 = 0$, we have the inverse map $z = 2\lambda - 1 \pm 2\sqrt{\lambda(\lambda - 1)}$. For $\lambda > 1$, $|2\lambda - 1 - 2\sqrt{\lambda(\lambda - 1)}| < 1$. Therefore, we obtain (5.2). □

The following lemma is proved by Lemma 2.4 and Theorem 2.6 (2). Note that $\widehat{H}_0$ has no eigenvalues.

Lemma 5.2. *For $s > 1/2$, the operator-valued function $\widehat{\rho}_s\,\widehat{R}_0(\lambda)\,\widehat{\rho}_s$ is analytic with respect to $\lambda \in \Lambda_d$, and has continuous boundary values when λ approaches $E \pm i0$, $E \in (0, d) \setminus \mathbf{Z}$.*

We study estimates for $\widehat{R}_0(E \pm i0)$ when $E \in \sigma(\widehat{H}_0) = [0, d]$ is close to $\{0, 1, \cdots, d\}$, the set of critical values of $h(x)$. Let us begin with the case $d = 1$.

Lemma 5.3. *Assume $d = 1$.*
(1) $r_0(n, z)$ defined by (4.11) has the following representation

$$r_0(n, \lambda(z)) = \frac{4z^{|n|}}{z - 1/z} = -\frac{z^{|n|}}{\sqrt{\lambda(z)(\lambda(z) - 1)}}, \quad \text{for} \quad (n, z) \in \mathbf{Z} \times \mathbf{D}_1.$$

Moreover, $r_0(n, \lambda(z))$ has a meromorphic continuation from $\mathbf{D}_1$ into $\mathbf{C}$.
(2) Let $\|\cdot\|_{HS}$ be the Hilbert-Schmidt norm on $\ell^2(\mathbf{Z})$, and take $\widehat{q}_j = (\widehat{q}_j(n))_{n\in\mathbf{Z}} \in \ell^2(\mathbf{Z})$, $j = 1, 2$. Then we have for $\lambda \in \Lambda_1$

$$\|\widehat{q}_1\,\widehat{R}_0(\lambda)\,\widehat{q}_2\|_{HS} \le \frac{\|\widehat{q}_1\|_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|_{\ell^2(\mathbf{Z})}}{|\sqrt{\lambda(\lambda - 1)}|}.$$

(3) Let $u(\nu)=\sqrt{\nu(\nu-1)}$*, and take* $\lambda,\lambda\in\Lambda_1$ *such that* $I(\lambda,\lambda_1)\subset\Lambda_1$*. We put*

$$M(\lambda,\lambda_1)=\left(1+2\max_{\nu\in I(\lambda,\lambda_1)}|u'(\nu)|\right)\left(1+\frac{1}{|u(\lambda)|}+\frac{1}{|u(\lambda_1)|}\right),$$

$$N(\lambda,\lambda_1)=\left|\frac{1}{u(\lambda)}-\frac{1}{u(\lambda_1)}\right|.$$

Then for any $0\le\alpha\le1$*, we have the following pointwise Hölder estimate*

$$|r_0(n,\lambda)-r_0(n,\lambda_1)|\le|\lambda-\lambda_1|^\alpha(1+|n|)^\alpha M(\lambda,\lambda_1)^\alpha N(\lambda,\lambda_1)^{1-\alpha}, \tag{5.3}$$

and the following Hölder estimate of the Hilbert-Schmidt norm

$$\|\widehat{\rho}_\alpha\widehat{q}_1\,(\widehat{R}_0(\lambda)-\widehat{R}_0(\lambda_1))\,\widehat{\rho}_\alpha\widehat{q}_2\|_{HS}\le|\lambda-\lambda_1|^\alpha C_\alpha(\lambda,\lambda_1)\|\widehat{q}_1\|_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|_{\ell^2(\mathbf{Z})}, \tag{5.4}$$

$$C_\alpha(\lambda,\lambda_1)=M(\lambda,\lambda_1)^\alpha N(\lambda,\lambda_1)^{1-\alpha}. \tag{5.5}$$

In particular, there exists a constant $C'_\alpha>0$ *such that*

$$\begin{aligned}&\|\widehat{\rho}_\alpha\widehat{q}_1\,(\widehat{R}_0(\lambda)-\widehat{R}_0(\lambda_1))\,\widehat{\rho}_\alpha\widehat{q}_2\|_{HS}\\ &\le\frac{C'_\alpha|\lambda-\lambda_1|^\alpha}{|\lambda(\lambda-1)\lambda_1(\lambda_1-1)|^{(1+3\alpha)/2}}\,\|\widehat{q}_1\|_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|_{\ell^2(\mathbf{Z})},\end{aligned} \tag{5.6}$$

if $|\lambda|,|\lambda_1|\le2$*, and* $I(\lambda,\lambda_1)\subset\Lambda_1$*.*

Proof. To prove (1), we first note by residue calculus

$$r_0(n,\lambda(z))=\frac{1}{\pi}\int_0^{2\pi}\frac{e^{-inx}dx}{1-\cos x-2\lambda(z)}=\frac{2}{\pi i}\int_{|w|=1}\frac{w^{-n}dw}{(w-z)(w-1/z)}=\frac{4z^{|n|}}{z-1/z}.$$

By (5.2), we have $1/z=2\lambda-1+2\sqrt{\lambda(\lambda-1)}$. Hence $z-1/z=-4\sqrt{\lambda(\lambda-1)}$, which proves (1).

Using (4.12) and (1), we obtain for $z\in\mathbf{D}_1$

$$\begin{aligned}\|\widehat{q}_1\,\widehat{R}_0(\lambda(z))\,\widehat{q}_2\|_{HS}^2&=\sum_{n,m\in\mathbf{Z}}\frac{|z|^{2|n-m|}}{|\lambda(z)(\lambda(z)-1)|}|\widehat{q}_1(n)|^2|\widehat{q}_2(m)|^2\\ &\le\frac{\|\widehat{q}_1\|^2\|\widehat{q}_2\|^2}{|\lambda(z)(\lambda(z)-1)|},\end{aligned}$$

where $\|\widehat{q}_j\|^2=\sum_{n\in\mathbf{Z}}|\widehat{q}_j(n)|^2$. This proves (2).

We prove (3). Let $\lambda_1,\lambda\in\mathbf{C}_+$ and $z=z(\lambda),z_1=z(\lambda_1)$. Then (1) and (5.2) give

$$r_0(n,\lambda)-r_0(n,\lambda_1)=-\frac{z^{|n|}}{u(\lambda)}+\frac{z_1^{|n|}}{u(\lambda_1)}=\frac{z_1^{|n|}-z^{|n|}}{u(\lambda)}+z_1^{|n|}\frac{u(\lambda)-u(\lambda_1)}{u(\lambda)u(\lambda_1)}.$$

Since $z,z_1\in\mathbf{D}_1$, we have

$$|z^{|n|}-z_1^{|n|}|=|(z-z_1)\sum_{j=0}^{|n|-1}z^{|n|-1-j}z_1^j|\le|(z-z_1)\sum_{j=0}^{|n|-1}1|\le|n||z-z_1|.$$

Moreover, we have by using (5.2)

$$|u(\lambda)-u(\lambda_1)|\le\left(\max_{\nu\in I(\lambda,\lambda_1)}|u'(\nu)|\right)|\lambda-\lambda_1|,$$

$$|z(\lambda)-z(\lambda_1)|\le2\left(1+\max_{\nu\in I(\lambda,\lambda_1)}|u'(\nu)|\right)|\lambda-\lambda_1|.$$

The above inequalities yield

$$|r_0(n,\lambda) - r_0(n,\lambda_1)| \leq |\lambda - \lambda_1| \left(\frac{2|n|}{|u(\lambda)|} + \max_{\nu \in I(\lambda,\lambda_1)} |u'(\nu)| \Big(2|n| + \frac{1}{|u(\lambda_1)|} \Big) \right).$$

Interchanging λ and λ_1, and adding the resulting inequalities, we have

$$|r_0(n,\lambda) - r_0(n,\lambda_1)| \leq |\lambda - \lambda_1|(1+|n|)M(\lambda,\lambda_1). \tag{5.7}$$

We also have by (1)

$$|r_0(n,\lambda) - r_0(n,\lambda_1)| \leq N(\lambda,\lambda_1). \tag{5.8}$$

By (5.7) and (5.8), we obtain (5.3).

Using (4.12) and (5.3), we have for $z \in \mathbf{D}_1$

$$\begin{aligned}
&\|\widehat{\rho}_\alpha \widehat{q}_1 \,(\widehat{R}_0(\lambda) - \widehat{R}_0(\lambda_1))\, \widehat{\rho}_\alpha \widehat{q}_2\|_{HS}^2 \\
&= \sum_{n,m \in \mathbf{Z}} |r_0(n-m,\lambda) - r_0(n-m,\lambda_1)|^2 |\widehat{\rho}_\alpha(n)\widehat{q}_1(n)|^2 |\widehat{\rho}_\alpha(m)\widehat{q}_2(m)|^2 \\
&\leq \sum_{n,m \in \mathbf{Z}} |\lambda - \lambda_1|^{2\alpha}(1+|n-m|)^{2\alpha} C_\alpha(\lambda,\lambda_1)^2 |\widehat{\rho}_\alpha(n)\widehat{q}_1(n)|^2 |\widehat{\rho}_\alpha(m)\widehat{q}_2(m)|^2 \\
&\leq |\lambda - \lambda_1|^{2\alpha} C_\alpha(\lambda,\lambda_1)^2 \sum_{n,m \in \mathbf{Z}} |\widehat{q}_1(n)|^2 |\widehat{q}_2(m)|^2,
\end{aligned}$$

which proves (5.4). The inequality (5.6) follows easily from (5.5). □

We study the case $d = 2$.

Lemma 5.4. *Let $d = 2$ and $\widehat{q}(n) = \widehat{q}_1(n_1)\,\widehat{q}_2(n_2)$, where $\widehat{q}_j \in \ell^2(\mathbf{Z})$ and $n = (n_1,n_2) \in \mathbf{Z}^2$. Then there exists a constant $C > 0$ such that*

$$\|\widehat{q}\,\widehat{R}_0(\lambda)\,\widehat{q}\| \leq C \|\widehat{q}_1\|_{\ell^2(\mathbf{Z})}^2 \|\widehat{q}_2\|_{\ell^2(\mathbf{Z})}^2 \big| \log\big(\lambda(\lambda-1)(\lambda-2)\big)\big|, \tag{5.9}$$

for all $\lambda \in \Lambda_2 \cap \{|\lambda| < 3\}$.

Proof. We prove the lemma by passing it on the torus. The idea consists in reducing it to the 1-dimensional case, regarding the remaining variable as a parameter. We put

$$q_j(x_j) = (2\pi)^{-1/2} \sum_{n_j \in \mathbf{Z}} \widehat{q}_j(n_j)\, e^{in_jx_j},$$

and define the convolution operator q_j* by

$$(q_j * f)(x) = \int_0^{2\pi} q_j(x_j - y_j) f(y) dy_j, \quad f \in L^2(\mathbf{T}^2),$$

where $y = (y_1, x_2)$ if $j = 1$, $y = (x_1, y_2)$ if $j = 2$. We put

$$\mu = \mu(\lambda, x_2) = \lambda - h(x_2), \quad h(x_2) = \frac{1}{2}\,(1 - \cos x_2)\,,$$

and define the 1-dimensional operator $A_1(\mu)$ with parameter μ by

$$A_1(\mu) = q_1 * (h(x_1) - \mu)^{-1}\, q_1 * = q_1 * (H_0 - \lambda)^{-1}\, q_1 * .$$

Take $f, f' \in L^2(\mathbf{T}^2)$, and let $\widehat{f}, \widehat{f'} \in \ell^2(\mathbf{Z}^2)$ be their Fourier coefficients. We are going to estimate

$$\begin{aligned}
C_2(\lambda) &:= (\widehat{q}_1\, \widehat{q}_2\, (\widehat{H}_0 - \lambda)^{-1} \widehat{q}_1\, \widehat{q}_2\, \widehat{f}, \widehat{f'})_{\ell^2(\mathbf{Z}^2)} \\
&= \big(q_1 * q_2 * (H_0 - \lambda)^{-1} q_1 * q_2 * f, f'\big)_{L^2(\mathbf{T}^2)}\,.
\end{aligned}$$

Letting

$$g = q_2 * f, \quad g' = q_2 * f',$$

we have

$$C_2(\lambda) = \int_0^{2\pi} \big(\big(A_1(\mu)g\big)(\cdot, x_2), g'(\cdot, x_2)\big)_{L^2(\mathbf{T}^1)}\, dx_2.$$

By Lemma 5.3 (2), we obtain

$$|C_2(\lambda)| \leq \|q_1\|^2_{L^2(\mathbf{T}^1)} \int_0^{2\pi} \frac{\|g(\cdot, x_2)\|_{L^2(\mathbf{T}^1)}\|g'(\cdot, x_2)\|_{L^2(\mathbf{T}^1)}}{|\mu(\lambda, x_2)(\mu(\lambda, x_2) - 1)|^{1/2}} dx_2.$$

Since

$$\|\left(q_2 * f\right)(\cdot, x_2)\|_{L^2(\mathbf{T}^1)} \leq \|q_2\|_{L^2(\mathbf{T}^1)}\|f\|_{L^2(\mathbf{T}^2)},$$

which follows from a simple application of Cauchy-Schwarz inequality, we have

$$|C_2(\lambda)| \leq \|q_1\|^2_{L^2(\mathbf{T}^1)}\|q_2\|^2_{L^2(\mathbf{T}^1)}\|f\|_{L^2(\mathbf{T}^2)}\|f'\|_{L^2(\mathbf{T}^2)} D_2(\lambda),$$

$$D_2(\lambda) = \int_0^{2\pi} \frac{dx_2}{|\mu(\lambda, x_2)(\mu(\lambda, x_2) - 1)|^{1/2}}.$$

Then the lemma is proved if we show for $|\lambda| < 4$

$$D_2(\lambda) \leq 8\left(K(\lambda) + K(\lambda - 1) + K(\lambda - 2)\right), \tag{5.10}$$

$$K(\lambda) = \sqrt{2}\left(2 + \log\frac{3\sqrt{2}}{|\lambda|}\right).$$

To prove (5.10), we let

$$J(\lambda) = \int_0^1 |(s - \lambda)s(1 - s)|^{-1/2} ds,$$

and first derive

$$D_2(\lambda) \leq 2J(\lambda) + 2J(\lambda - 1). \tag{5.11}$$

In fact, by the change of variable $s = (1 - \cos x_2)/2$, we have

$$D_2(\lambda) = 2\int_0^1 |(s - \lambda)(s + 1 - \lambda)s(1 - s)|^{-1/2} ds.$$

Using the inequality

$$\frac{1}{|a(a - 1)|^{1/2}} = \left|\frac{1}{a} - \frac{1}{a - 1}\right|^{1/2} \leq \frac{1}{|a|^{1/2}} + \frac{1}{|a - 1|^{1/2}} \tag{5.12}$$

with $a = s + 1 - \lambda$, we obtain (5.11).

In order to compute $J(\lambda)$, we put

$$J_0(\lambda) = \int_0^{1/2} |s(s - \lambda)|^{-1/2} ds.$$

Then we have

$$J(\lambda) \leq 2\int_0^{1/2} \frac{ds}{|s(s - \lambda)|^{\frac{1}{2}}} + 2\int_{1/2}^1 \frac{ds}{|(1 - s)(s - \lambda)|^{1/2}} = 2J_0(\lambda) + 2J_0(\lambda - 1).$$

This, combined with (5.11), implies

$$D_2(\lambda) \leq 4\left(J_0(\lambda) + 2J_0(\lambda - 1) + J_0(\lambda - 2)\right). \tag{5.13}$$

Let us first consider the case $|\lambda| \geq 1$. Estimating as in (5.12), we have for $0 \leq s \leq 1/2$

$$\frac{1}{|s(s-\lambda)|^{1/2}} \leq \frac{1}{|\lambda|^{1/2}}\left(\frac{1}{|s|^{1/2}} + \frac{1}{|s-\lambda|^{1/2}}\right) \leq \frac{1}{s^{1/2}} + \frac{1}{(1-s)^{1/2}}.$$

Hence for $|\lambda| \geq 1$

$$J_0(\lambda) \leq \int_0^{1/2}\left(\frac{1}{s^{1/2}} + \frac{1}{(1-s)^{1/2}}\right)ds = 2. \tag{5.14}$$

Next we consider the case $|\lambda| \leq 1$ and let $\lambda = \mu + i\nu$. If $|\nu| \geq 4|\mu|$, we put $s = |\nu|t$, $E = 1/(2|\nu|)$, $\mu_0 = \mu/|\nu|$. Note that $\sqrt{2}|\nu| \geq |\lambda| \geq |\nu|$ and if $t \geq 1/2$ then $t - \mu_0 \geq t/2$, hence $|(t-\mu_0)^2 + 1|^{1/4} \geq (t/2)^{1/2}$. We now compute

$$\begin{aligned} J_0(\lambda) &= \int_0^E \frac{dt}{\sqrt{t}|(t-\mu_0)^2+1|^{1/4}} \\ &= \int_0^{1/2} \frac{dt}{\sqrt{t}|(t-\mu_0)^2+1|^{1/4}} + \int_{1/2}^E \frac{dt}{\sqrt{t}|(t-\mu_0)^2+1|^{1/4}} \\ &\leq \int_0^{1/2}\frac{dt}{\sqrt{t}} + \sqrt{2}\int_{1/2}^E \frac{dt}{t} = \sqrt{2} + \sqrt{2}\log(2E) \leq 2\sqrt{2} + \sqrt{2}\log\frac{\sqrt{2}}{|\lambda|}. \end{aligned} \tag{5.15}$$

If $|\nu| \leq 4|\mu|$, we let $s = |\mu|t$, $R = 1/(2|\mu|)$, $\sigma(\mu) = \mu/|\mu|$, $\nu_0 = \nu/|\mu|$. We then obtain

$$\begin{aligned} J_0(\lambda) &= \int_0^R \frac{dt}{\sqrt{t}|(t-\sigma(\mu))^2+\nu_0|^{1/4}} \\ &= \int_0^{1/2} \frac{dt}{\sqrt{t}|(t-\sigma(\mu))^2+\nu_0^2|^{1/4}} + \int_{1/2}^R \frac{dt}{\sqrt{t}|(t-\sigma(\mu))^2+\nu_0^2|^{1/4}} \\ &\leq \int_0^{1/2} \frac{dt}{\sqrt{t}|t-1|^{1/2}} + \int_{1/2}^R \frac{dt}{t-1} \\ &\leq 2 + \log 2R \leq 2 + \log\frac{3\sqrt{2}}{|\lambda|}. \end{aligned} \tag{5.16}$$

In view of (5.14), (5.15) and (5.16), we have

$$J_0(\lambda) \leq \sqrt{2}\left(2 + \log\frac{3\sqrt{2}}{|\lambda|}\right),$$

which, together with (5.13), proves (5.10). □

Finally we consider the case $d \geq 3$.

Lemma 5.5. *(1) Let $d \geq 3$ and*

$$\widehat{Q}_s(n_1, \cdots, n_d) = \widehat{q}_1(n_1)\,\widehat{q}_2(n_2)\,\widehat{\rho}_s(n'),$$

where $n' = (n_3, \cdots, n_d) \in \mathbf{Z}^{d-2}$, $\widehat{q}_1, \widehat{q}_2 \in \ell^2(\mathbf{Z})$ and $\widehat{\rho}_s(n') = (1+|n'|^2)^{-s/2}$ with $0 < s \leq 1$. Then there exists a constant $C_s > 0$ such that the following estimate holds:

$$\|\widehat{Q}_s\,\widehat{R}_0(\lambda)\,\widehat{Q}_s\| \leq C_s\|\widehat{q}_1\|^2_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|^2_{\ell^2(\mathbf{Z})} \tag{5.17}$$

for all $\lambda \in \Lambda_d \cap \{\lambda \in \mathbf{C}\,;\, |\lambda| < 2d\}$.

(2) Moreover, let $\lambda, \lambda_1 \in \mathbf{C}_\pm \cap \{\lambda \in \mathbf{C}\,;\, |\lambda| < 2d\}$ and let $g > 0$ be small enough and

$$\widehat{Q}_{s,g}(n_1, \cdots, n_d) = \widehat{\rho}_g(n_1)\widehat{Q}_{s+2g}(n_1, \cdots, n_d), \qquad n \in \mathbf{Z}^d.$$

Then there exists a constant $C_{s,g} > 0$ such that the following estimate holds true:

$$\|\widehat{Q}_{s,g}\,(\widehat{R}_0(\lambda) - \widehat{R}_0(\lambda_1))\,\widehat{Q}_{s,g}\| \leq |\lambda - \lambda_1|^g C_{s,g}\|\widehat{q}_1\|^2_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|^2_{\ell^2(\mathbf{Z})}, \tag{5.18}$$

Proof. (1) The proof is similar to the one for the previous lemma. Let

$$A_2(\mu) = q_1 * q_2 * (H_0 - \lambda)^{-1} q_1 * q_2 * = q_1 * q_2 * (h_1 + h_2 - \mu)^{-1} q_1 * q_2 *,$$

$$h_j = h(x_j) = \frac{1}{2}(1 - \cos x_j), \quad \mu = \mu(\lambda, x') = \lambda - \sum_{j=3}^{d} h_j,$$

where $x' = (x_3, \cdots, x_d)$. For $f, f' \in L^2(\mathbf{T}^d)$, we put $g_s = \rho_s * f$, $g'_s = \rho_s * f'$. Then we have

$$\begin{aligned} C(\lambda) &:= (\widehat{q}_1\,\widehat{q}_2\,(\widehat{H}_0 - \lambda)^{-1}\widehat{q}_1\,\widehat{q}_2\,\widehat{\rho}\widehat{f}, \widehat{\rho}\,\widehat{f'}) \\ &= (q_1 * q_2 * (H_0 - \lambda)^{-1} q_1 * q_2 * \rho_s * f, \rho_s * f') \\ &= \int_{\mathbf{T}^{d-2}} (A_2(\mu) g_s(\cdot, x'), g'_s(\cdot, x'))_{L^2(\mathbf{T}^2)} dx'. \end{aligned}$$

Lemma 5.4 then implies

$$\begin{aligned} |C(\lambda)| &\leq C\|\widehat{q}_1\|^2_{\ell^2(\mathbf{Z})}\|\widehat{q}_2\|^2_{\ell^2(\mathbf{Z})} \\ &\quad \times \int_{\mathbf{T}^{d-2}} |\log(\mu(\mu - 1)(\mu - 2)|\|g_s(\cdot, x')\|_{L^2(\mathbf{T}^2)}\|g'_s(\cdot, x')\|_{L^2(\mathbf{T}^2)} dx', \end{aligned}$$

where C is a constant independent of $\lambda \in \Lambda_d$. We now put

$$D_s(\lambda) = \int_{\mathbf{T}^{d-2}} |\log(\mu(\lambda, x')(\mu(\lambda, x') - 1)(\mu(\lambda, x') - 2)|\|(\rho_s * f)(\cdot, x')\|^2_{L^2(\mathbf{T}^2)} dx'.$$

Lemma 5.5 will then be proved if we show the existence of a constant C_s independent of $\lambda \in \Lambda_d \cap \{|\lambda| < 2d\}$ such that

$$D_s(\lambda) \leq C_s\|f\|^2_{L^2(\mathbf{T}^d)}. \tag{5.19}$$

We define the set **SP** by

$$\mathbf{SP} = \{(x_3, \cdots, x_d)\,;\, x_j = 0 \text{ or } \pi,\ j = 3, \cdots, d\}.$$

This is the set of singular points for $\mu(\lambda, x')$, since $\nabla_{x'}\mu(\lambda, x') = 0$ if and only if $x' \in \mathbf{SP}$. We label the points in **SP** by $p^{(1)}, \cdots, p^{(N)}$, $N = 2^{d-2}$:

$$\mathbf{SP} = \{p^{(1)}, \cdots, p^{(N)}\}.$$

For a sufficiently small $\epsilon > 0$, we put

$$\mathbf{T}^{(j)} = \{x' \in \mathbf{T}^{d-2}\,;\, |x' - p^{(j)}| < \epsilon\}, \quad 1 \leq j \leq N,$$

$$\mathbf{T}^{(0)}(\lambda) = \mathbf{T}^{d-2} \setminus \left(\cup_{j=1}^N \mathbf{T}^{(j)}\right),$$

and let

$$E_s^{(j)}(\lambda) = \int_{\mathbf{T}^{(j)}} |\log(\mu(\lambda, x')(\mu(\lambda, x') - 1)(\mu(\lambda, x') - 2)|\|(\rho_s * f)(\cdot, x')\|^2_{L^2(\mathbf{T}^2)} dx',$$

$$E_s^{(j,k)}(\lambda) = \int_{\mathbf{T}^{(j)}} |\log(\mu(\lambda, x') - k)|\|(\rho_s * f)(\cdot, x')\|^2_{L^2(\mathbf{T}^2)} dx'.$$

Then we have

$$D_s(\lambda) = \sum_{j=0}^{N} E_s^{(j)}(\lambda) \leq \sum_{j=0}^{N}\sum_{k=0}^{2} E_s^{(j,k)}(\lambda). \tag{5.20}$$

We shall make use of the following version of Heinz' inequality. For the proof, see p. 232 of [6].

Proposition 5.6. *Let A, B be self-adjoint operators satisfying*

$$A \geq 1, \quad B \geq 0, \quad D(A) \subset D(B), \quad \|BA^{-1}\| \leq 1.$$

Then for any $0 < \theta < 1$, we have

$$D(A^\theta) \subset D(B^\theta), \quad \|B^\theta A^{-\theta}\| \leq 1.$$

Let us estimate $E_s^{(j,k)}(\lambda)$. We take $\theta = \dfrac{s}{n-2}$, and define self-adjoint operators A and B in $L^2(\mathbf{T}^{d-2})$ by

$$\widehat{Af}(n') = C_0(1 + |n'|^2)^{(n-2)/2}\widehat{f}(n'),$$

$$(Bf)(x') = \chi^{(j)}(x')\big|\log(\mu(\lambda, x') - k)\big|^{1/\theta} f(x'),$$

where $\chi^{(j)}(x')$ is the characteristic function of the set $\mathbf{T}^{(j)}$, and C_0 is a constant to be determined later. We compute the Hilbert-Schmidt norm of BA^{-1}. Let $k(x')$ be the inverse Fourier image of $(1+|n'|^2)^{-(n-2)}$. Then, up to a multiplicative constant, BA^{-1} has the integral kernel

$$K(x', y') = C_0\chi^{(j)}(x')\big|\log(\mu(\lambda, x') - k)\big|^{1/\theta} k(x' - y'). \tag{5.21}$$

One can show that for any $\alpha > 1$,

$$\sup_{\lambda \in \Lambda_d \cap \{|\lambda| < 2d\}} \int_{\mathbf{T}_j} |\log(\mu(\lambda, x') - k)|^\alpha dx' < \infty. \tag{5.22}$$

In fact, if $j = 0$, $\nabla_{x'}\mu(\lambda, x') \neq 0$ on $\mathbf{T}_0$. Then we can take $\sum_{j=3}^d \cos x_j$ as a new variable to compute (5.22). The case $j \neq 0$ is dealt with as follows. Suppose, for example, $p^{(j)} = (0, \cdots, 0)$. By the Morse Lemma, we can introduce new variables y_j, $3 \leq j \leq d$, around $p^{(j)}$ so that $\sum_{j=3}^d \cos x_j = (d-2) - \sum_{j=3}^d y_j^2$. One can then prove (5.22) by an elementary computation. The other cases are treated similarly.

On the other hand, by Parseval's formula

$$\int_{\mathbf{T}^{d-2}} |k(x')|^2 dx' = \sum (1 + |n'|^2)^{-(n-2)} < \infty.$$

Therefore BA^{-1} is of Hilbert-Schmidt type, in particular, bounded. By choosing C_0 small enough, we have $\|BA^{-1}\| \leq 1$. Then by Proposition 5.6, $B^\theta A^{-\theta}$ is bounded on $L^2(\mathbf{T}^{d-2})$, which implies that

$$\|E_s^{(j,k)}(\lambda)f\| \leq C_s\|f\|^2_{L^2(\mathbf{T}^d)},$$

This proves (5.19).

The proof of (2) repeats the arguments from the proof of (1). □

As a consequence of the above lemma, we show the following theorem.

Theorem 5.7. *Let $d \geq 3$, and $\widehat{H}_\gamma = \widehat{H}_0 + \gamma \widehat{V}$, where $\widehat{V}$ is a complex-valued potential such that $\widehat{V}(n) = O(|n|^{-s})$, $s > 2$, as $|n| \to \infty$, γ being a complex parameter. Then there exists a constant $\delta > 0$ such that $\widehat{H}_\gamma$ has no eigenvalues when $|\gamma| < \delta$.*

Proof. We put $\widehat{Q}(n_1, \cdots, n_d) = \widehat{q}_1(n_1)\, \widehat{q}_2(n_2)\, \widehat{\rho}(n')$, where

$$\widehat{q}_1(n_1) = (1+|n_1|^2)^{-(1+\epsilon)/4}, \quad \widehat{q}_2(n_2) = (1+|n_2|^2)^{-(1+\epsilon)/4}, \quad \widehat{\rho}(n') = (1+|n'|^2)^{-\epsilon/2}.$$

If there exists $E \in \mathbf{R}$ and $\widehat{f} \in \ell^2(\mathbf{Z}^d)$ such that $(\widehat{H}_0 + \gamma \widehat{V} - E)\widehat{f} = 0$, we have

$$\widehat{Q}\, \widehat{f} = -\gamma\, \widehat{Q}\, (\widehat{H}_0 - E)^{-1}\, \widehat{Q} \cdot \widehat{Q}^{-1}\, \widehat{V}\, \widehat{Q}^{-1}\, \widehat{f}.$$

Choosing $\epsilon > 0$ small enough, we have $\widehat{Q}^{-1}\, \widehat{V}\, \widehat{Q}^{-1} \in \mathbf{B}(\ell^2(\mathbf{Z}^d))$. Using Lemma 5.5 and taking

$$\frac{1}{\delta} = \|\widehat{Q}\, (\widehat{H}_0 - E)^{-1} \widehat{Q} \cdot \widehat{Q}^{-1}\, \widehat{V}\, \widehat{Q}^{-1}\|,$$

we obtain Theorem 5.7. □

6. Traces formulas

6.1. **Fredholm determinant.** In contrast to sections 2-5, the material in this section is discussed from an abstract point of view. Let $\mathcal{H}$ be a Hilbert space endowed with inner product $(\ ,\ )$ and norm $\|\cdot\|$. Let $\mathcal{C}_1$ be the set of all trace class operators on $\mathcal{H}$ equipped with the trace norm $\|\cdot\|_{\mathcal{C}_1}$. Recall that for $K \in \mathcal{C}_1$ and $z \in \mathbf{C}$, the following formula holds:

$$\det(I - zK) = \exp\left(- \int_0^z \mathrm{Tr}\, \big(K(1 - sK)^{-1}\big) ds \right) \tag{6.1}$$

(see e.g. [5], [21], p.167, or [35], p.331). As is well-known if $A \in \mathbf{B}(\mathcal{H};\mathcal{H})$ and $B \in \mathcal{C}_1$, we have

$$\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA), \tag{6.2}$$

$$\det(I + AB) = \det(I + BA). \tag{6.3}$$

Suppose we are given an operator $H = H_0 + V$ on $\mathcal{H}$ satisfying the following conditions:

(B-1) H_0 is bounded self-adjoint.

(B-2) V is self-adjoint and trace class.

We put

$$R_0(\lambda) = (H_0 - \lambda)^{-1}, \quad \lambda \in \Lambda := \rho(H_0),$$

and define $D(\lambda)$ by

$$D(\lambda) = \det(I + V R_0(\lambda)), \quad \lambda \in \Lambda. \tag{6.4}$$

Lemma 6.1. *(1) $D(\lambda)$ is analytic in Λ. Moreover*

$$D(\lambda) = 1 + O(1/\lambda) \quad as \quad |\lambda| \to \infty, \tag{6.5}$$

$$\log D(\lambda) = - \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \mathrm{Tr}\, \left(V R_0(\lambda)\right)^n, \tag{6.6}$$

where the right-hand side is absolutely convergent for $|\lambda| > r_0$, $r_0 > 0$ *being a sufficiently large constant.*
(2) The set $\{\lambda \in \Lambda\,;\, D(\lambda) = 0\}$ *is finite and coincides with* $\sigma_d(H)$.

Proof. Letting $E_V(t)$ be the spectral decomposition of V, we define

$$V^{1/2} = \int_{-\infty}^{\infty} \mathrm{sgn}\, t\, |t|^{1/2} dE_V(t), \quad |V|^{1/2} = \int_{-\infty}^{\infty} |t|^{1/2} dE_V(t).$$

There exists $r_0 > 0$ such that $\|R_0(\lambda)\| \leq C/|\lambda|$ for $|\lambda| > r_0$, which implies

$$|\mathrm{Tr}\,(VR_0(\lambda))\,| \leq C/|\lambda| \quad \text{for} \quad |\lambda| > r_0. \tag{6.7}$$

By (6.2), taking r_0 large enough, we have for $|\lambda| > r_0$

$$\begin{aligned}
&\mathrm{Tr}\,\big(VR_0(\lambda)(1 + sVR_0(\lambda))^{-1}\big) \\
&= \mathrm{Tr}\,\Big(V^{1/2}R_0(\lambda)(1 + sVR_0(\lambda))^{-1}|V|^{1/2}\Big) \\
&= \sum_{n=0}^{\infty}(-s)^n \mathrm{Tr}\,\Big(V^{1/2}R_0(\lambda)\,\overbrace{VR_0(\lambda)\cdots VR_0(\lambda)}^{n}\,|V|^{1/2}\Big) \\
&= \sum_{n=0}^{\infty}(-s)^n \mathrm{Tr}\,(VR_0(\lambda))^{n+1}.
\end{aligned}$$

We then have (6.5) and (6.6) by (6.1). For $\lambda \notin \sigma(H_0)$, the eigenvalue problem $(H - \lambda)u = 0$ is equivalent to $(I + (H_0 - \lambda)^{-1}V)u = 0$, which has a non-trivial solution if and only if $\det(I + (H_0 - \lambda)^{-1}V) = 0$. This proves (2) by (6.3). □

Lemma 6.2. *The following identity holds:*

$$\log D(\lambda) = -\sum_{n\geq 1} \frac{F_n}{n}\left(\frac{1}{\lambda}\right)^n, \quad F_n = \mathrm{Tr}\,(H^n - H_0^n), \quad n \geq 1, \tag{6.8}$$

where the right-hand side is unifomly convergent on $\{|\lambda| \geq r_0\}$ *for* $r_0 > 0$ *large enough. In particular,*

$$F_1 = \mathrm{Tr}\,(V), \quad F_2 = \mathrm{Tr}\,(2VH_0 + V^2). \tag{6.9}$$

Proof. Let $R(\lambda) = (H - \lambda)^{-1}$. Take $r_0 > 0$ large enough. Then for $|\lambda| > r_0$, we have by the resolvent equation

$$R(\lambda) - R_0(\lambda) = \sum_{n=1}^{\infty}(-1)^n R_0(\lambda)\,\overbrace{VR_0(\lambda)\cdots VR_0(\lambda)}^{n}. \tag{6.10}$$

Let $F(\lambda) = \log D(\lambda)$. Since $\frac{d}{d\lambda}R_0(\lambda) = R_0(\lambda)^2$, we have by (6.6) and (6.10)

$$\begin{aligned}
-\frac{d}{d\lambda}F(\lambda) &= \sum_{n=1}^{\infty}(-1)^n \mathrm{Tr}\,\Big(R_0(\lambda)\,\overbrace{VR_0(\lambda)\cdots VR_0(\lambda)}^{n}\Big) \\
&= \mathrm{Tr}\,\Big(R(\lambda) - R_0(\lambda)\Big).
\end{aligned}$$

Using the equation

$$R(\lambda) = -\sum_{n=0}^{\infty} \lambda^{-n-1}H^n,$$

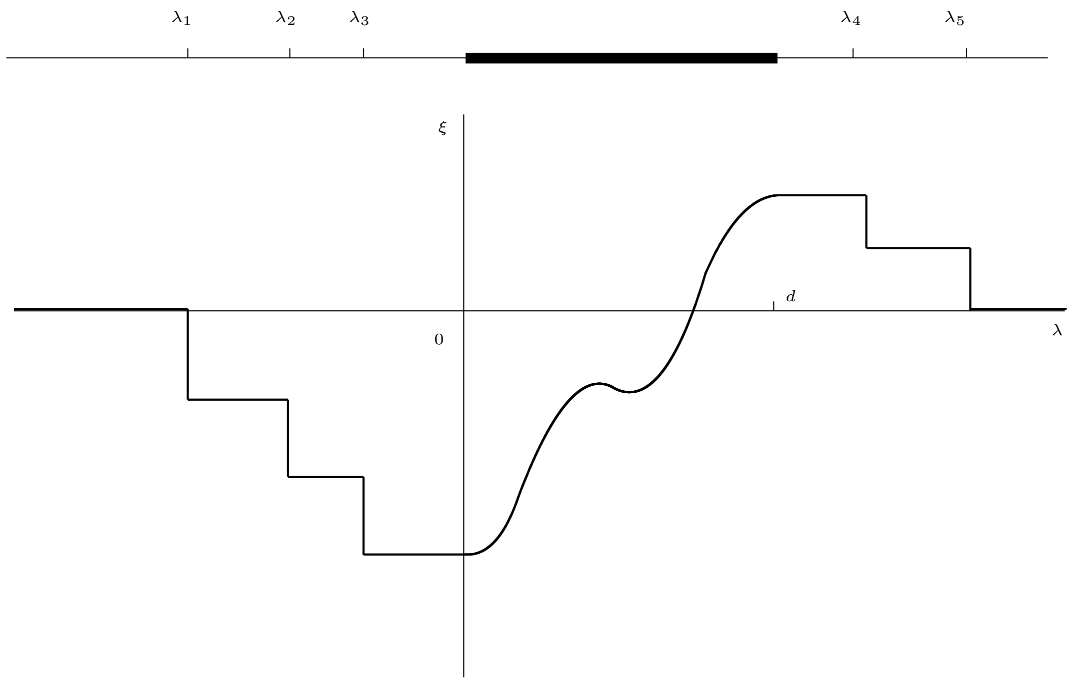

FIGURE 1. The spectral shift function $\xi(\lambda)$ and five eigenvalues $l_1, \cdots, l_5$ for H

we obtain

$$F'(\lambda) = \sum_{n=0}^{\infty} \lambda^{-n-1} \mathrm{Tr}\big(H^n - H_0^n\big).$$

In view of (6.5), we get (6.8). □

6.2. **Spectral shift function and trace formula.** Let $H = H_0 + V$ satisfy (B-1), (B-2). Then there exists a function $\xi(\lambda)$ such that the following equality

$$\mathrm{Tr}\,(f(H) - f(H_0)) = \int_{\mathbf{R}} \xi(\lambda) df(\lambda) \tag{6.11}$$

holds, where f is an arbitrary function from some suitable class. If f is absolutely continuous, then df can be replaced by $f'(\lambda)d\lambda$. We call (6.11) a *trace formula*, and $\xi(\lambda)$ the *spectral shift function* for the pair H, H_0. A typical form of $\xi(\lambda)$ for our case of discrete Schrödinger operator $\widehat{H}$ in §2 is drawn in Figure 1.

Let us recall the basic properties of $\xi(\lambda)$ (see [7], [41]).

(1) *The following identity holds:*

$$\log D(\lambda) = \int_{\mathbf{R}} \frac{\xi(t)}{t - \lambda} dt, \quad \lambda \in \mathbf{C}_+,$$

where $D(\lambda)$ is the perturbation determinant defined by (6.4), and the branch of $\log D(\lambda)$ *is chosen so that* $\log D(\lambda) = o(1)$ *as* $|\lambda| \to \infty$*, and* $\xi(t) \in L^1(\mathbf{R})$*. We have*

$$\xi(\lambda) = \lim_{\varepsilon \to +0} \frac{1}{\pi} \arg D(\lambda + i\varepsilon), \qquad a.e.\ \lambda \in \mathbf{R},$$

where the limit in the right-hand side exists for a.e. $\lambda \in \mathbf{R}$ *The support of* $\xi(\lambda)$ *is equal to* $\sigma(H)$ *and*

$$\int_{\mathbf{R}} |\xi(\lambda)| d\lambda \le \|V\|_{\mathcal{C}_1},$$

$$\int_{\mathbf{R}} \xi(\lambda) d\lambda = \mathrm{Tr}\,(V).$$

(2) Its relation to the S-matrix is

$$\det \mathcal{S}(\lambda) = e^{-2\pi i \xi(\lambda)}, \quad \textit{for a.e. } \lambda \in \sigma_{ac}(H_0). \tag{6.12}$$

(3) If H *have* $N_- \ge 0$ *negative eigenvalues and* $N_+ \ge 0$ *positive eigenvalues, then*

$$-N_- \le \xi(\lambda) \le N_+, \quad \textit{for a.e. } \lambda \in \mathbf{R}.$$

(4) Suppose H_0 *has no eigenvalues in the interval* $(a,b) \subset \mathbf{R}$*. Assume that* $\lambda_0 \in (a,b)$ *is an isolated eigenvalue of finite multiplicity* d_0 *of* H*. Then* $\xi(\lambda)$ *takes an integer value* n_- (n_+) *on the interval* (a,λ_0) *(on the interval* (λ_0,b)*). Moreover, we have*

$$\xi(\lambda_0+0) - \xi(\lambda_0-0) = -d_0. \tag{6.13}$$

(5) If $V \ge 0$*, then* $\xi(\lambda) \ge 0$ *for all* $\lambda \in \mathbf{R}$*.*

(6) If $V \le 0$*, then* $\xi(\lambda) \le 0$ *for all* $\lambda \in \mathbf{R}$*.*

(7) If the perturbation V *has rank* $N < \infty$*, then* $-N \le \xi(\lambda) \le N$ *for all* $\lambda \in \mathbf{R}$*.*

As will be shown in the following lemma, F_n/n, the Taylor coefficients of $-\log D(\lambda)$ around $\lambda = \infty$ are equal to the moments of the spectral shift function $\xi(\lambda)$. The first two terms were computed in Lemma 6.2. To compute the terms for $n \ge 3$, we impose the following assumption.

(B-3) *There exist unitary operators* S_j $(1 \le j \le d)$ *such that*

$$H_0 = -\frac{1}{4}(S+S^*), \quad S = \sum_{j=1}^d S_j, \quad S_jS_i = S_iS_j, \quad \forall\, i,j, \tag{6.14}$$

$$\mathrm{Tr}\,\big(S_j^k V^p\big) = 0, \quad \forall\, j = 1,..,d, \quad k \neq 0, \quad p \ge 1. \tag{6.15}$$

Note that by (6.14) and (6.15), we have

$$\mathrm{Tr}\,\big(S^k V^p\big) = 0, \quad \mathrm{Tr}\,\big(V^p (S^*)^k\big) = 0, \quad k \ge 1, \quad p \ge 1, \tag{6.16}$$

$$\mathrm{Tr}\,\big(S^a (S^*)^b V^p\big) = 0, \quad a \neq b, \quad p \ge 1. \tag{6.17}$$

Lemma 6.3. *Let* $H = H_0 + V$ *satisfy (B-1), (B-2) and (B-3). Then*

$$F_n = \mathrm{Tr}\,(H^n - H_0^n) = n \int_{\mathbf{R}} \xi(\lambda) \lambda^{n-1} d\lambda, \quad n \ge 1. \tag{6.18}$$

In particular, letting $\tau = -1/4$*, and*

$$\Delta V = \tau \sum_{i=1}^d (S_j V S_j^* + S_j^* V S_j), \tag{6.19}$$

we have

$$F_1 = \mathrm{Tr}\,(V), \quad F_2 = \mathrm{Tr}\,(V^2), \quad F_3 = \mathrm{Tr}\,\big(V^3 + 6d\tau^2 V\big), \tag{6.20}$$

$$F_4 = \mathrm{Tr}\,\big(V^4 + 8d\tau^2V^2 + 2\tau(\Delta V)V\big), \tag{6.21}$$

$$F_5 = \mathrm{Tr}\,\big(V^5 + 30d(2d-1)\tau^4V + 10d\tau^2V^3 + 5\tau(\Delta V)V^2\big). \tag{6.22}$$

Proof. By taking $f(\lambda) = \lambda^k$ in (6.11), we get (6.18). In Lemma 6.2, we have proven that $F_1 = \mathrm{Tr}\,(V)$. F_2 and F_3 are computed by the use of (6.15) as follows:

$$\begin{aligned}
F_2 &= \mathrm{Tr}\,((H_0+V)^2 - H_0^2) = \mathrm{Tr}\,(2H_0V + V^2) = \mathrm{Tr}\,(V^2),\\
F_3 &= \mathrm{Tr}\,((H_0+V)^3 - H_0^3) = \mathrm{Tr}\,(3H_0^2V + 3H_0V^2 + V^3) = \mathrm{Tr}\,(3H_0^2V + V^3),
\end{aligned}$$

$$\begin{aligned}
\mathrm{Tr}\,\big(H_0^2V\big) &= \tau^2\mathrm{Tr}\,\big((S^2 + 2SS^* + S^{*2})V\big) = 2\tau^2\mathrm{Tr}\,(SS^*V)\\
&= 2\tau^2\mathrm{Tr}\,\big((d + \sum_{i\neq j} S_iS_j^*)V\big) = 2d\tau^2\mathrm{Tr}\,(V).
\end{aligned}$$

To calculate F_4, we first compute

$$\begin{aligned}
F_4 &= \mathrm{Tr}\,\big((H_0+V)^4 - H_0^4)\big)\\
&= \mathrm{Tr}\,(V^4 + 4H_0^3V + 4H_0V^3 + 4H_0^2V^2 + 2H_0VH_0V).
\end{aligned}$$

Due to (6.16), we have

$$\mathrm{Tr}\,(H_0^3V) = 0, \quad \mathrm{Tr}\,(H_0V^3) = 0, \quad \mathrm{Tr}\,(H_0^2V^2) = 2d\tau^2\mathrm{Tr}\,(V^2).$$

Using $\mathrm{Tr}\,(SVSV) = 0$, we get

$$\begin{aligned}
\mathrm{Tr}\,(H_0VH_0V) &= \tau^2\mathrm{Tr}\,((S+S^*)V(S+S^*)V\big)\\
&= \tau^2\mathrm{Tr}\,\big((SVS^* + S^*VS)V\big) = \tau\mathrm{Tr}\,\big((\Delta V)V,\big),
\end{aligned}$$

since $\mathrm{Tr}\,\big(\sum_{i\neq j} S_iVS_j^*V\big) = 0$.

Finally we compute F_5. Firstly,

$$\begin{aligned}
F_5 &= \mathrm{Tr}\,\big((H_0+V)^5 - H_0^5\big)\\
&= \mathrm{Tr}\,\big(V^5 + 5H_0^4V + 5H_0V^4 + 5H_0^2V^3\\
&\qquad + 5H_0^3V^2 + 5H_0^2VH_0V + 5H_0VH_0V^2\big).
\end{aligned}$$

By (6.16), we have $\mathrm{Tr}\,(H_0V^4) = 0$, $\mathrm{Tr}\,(H_0^3V^2) = 0$, and $\mathrm{Tr}\,(H_0^2VH_0V) = 0$. We then have

$$\begin{aligned}
\mathrm{Tr}\,\big(H_0VH_0V^2\big) &= \tau^2\mathrm{Tr}\,\big((S+S^*)V(S+S^*)V^2\big)\\
&= \tau^2\mathrm{Tr}\,\big((SVS^* + S^*VS)V^2\big)\\
&= \tau\mathrm{Tr}\,\big((\Delta V)V^2\big) = \mathrm{Tr}\,\big(H_0^4V\big) = \tau^4\mathrm{Tr}\,\big((S+S^*)^4V\big)\\
&= 6\tau^4\mathrm{Tr}\,\big(S^2S^{*2}V\big) = 6\tau^4d(2d-1)\mathrm{Tr}\,(V). \qquad \square
\end{aligned}$$

The above lemma enables us to estimate the eigenvalues in terms of the spectral shift function.

Theorem 6.4. *Let $H = H_0 + V$ satisfy (B-1), (B-2) and (B-3). Assume that $\sigma(H_0) = [\alpha,\beta]$, and put*

$$E_n = n\int_{\mathbf{R}\setminus[\alpha,\beta]} \xi(\lambda)\lambda^{n-1}d\lambda. \tag{6.23}$$

Let m_j be the multiplicity of $\lambda_j \in \sigma_d(H)$. Then we have for any $n \geq 0$

$$E_n = \sum_{\lambda_j<\alpha} m_j\big(\lambda_j^n - \alpha^n\big) + \sum_{\lambda_j>\beta} m_j\big(\lambda_j^n - \beta^n\big). \tag{6.24}$$

(1) If $V \geq 0$, then $\sigma_d(H) \subset (\beta, \infty)$ and

$$\sum_{\lambda_j\in\sigma_d(H)} m_j\big(\lambda_j - \beta\big) \leq \mathrm{Tr}\,(V) \tag{6.25}$$

$$\sum_{\lambda_j\in\sigma_d(H)} m_j\big(\lambda_j^3 - \beta^3\big) \leq \mathrm{Tr}\,\big(V^3 + \frac{3d}{8}V\big). \tag{6.26}$$

(2) If $V \leq 0$, then $\sigma_d(H) \subset (-\infty, \alpha)$ and

$$\sum_{\lambda_j\in\sigma_d(H)} m_j\big(\lambda_j - \alpha\big) \geq \mathrm{Tr}\,(V), \tag{6.27}$$

$$\sum_{\lambda_j\in\sigma_d(H)} m_j\big(\lambda_j^3 - \alpha^3\big) \geq \mathrm{Tr}\,\big(V^3 + \frac{3d}{8}V\big). \tag{6.28}$$

Proof. For small $t > 0$, we define the set

$$\mathcal{O}_t = (-\infty, \alpha - t) \cup (\beta + t, \infty).$$

For $\lambda_j \in \sigma_d(H)$, we take $\epsilon > 0$ small enough so that the interval $I_j = (\lambda_j - \epsilon, \lambda_j + \epsilon)$ satisfies $I_j \cap \sigma_d(H) = \{\lambda_j\}$. Then we have, by the property (6.13),

$$\xi'(\lambda)d\lambda = -m_j\delta(\lambda - \lambda_j)d\lambda, \quad \text{on} \quad I_j$$

(see Fig. 1). More precisely, see (3.28), (3.29) of [7]. We then obtain

$$\begin{aligned}
E_n(t) &:= n\int_{\mathcal{O}_t} \xi(\lambda)\lambda^{n-1}d\lambda \\
&= -(\alpha - t)^n \sum_{\lambda_j<\alpha} m_j - (\beta + t)^n \sum_{\lambda_j>\beta} m_j - \int_{\mathcal{O}_t} \xi'(\lambda)\lambda^n d\lambda \\
&= \sum_{\lambda_j<\alpha} m_j\big(\lambda_j^n - (\alpha - t)^n\big) + \sum_{\lambda_j>\beta} m_j\big(\lambda_j^n - (\beta + t)^n\big) \\
&\to E_n(0) = \sum_{\lambda_j<\alpha} m_j\big(\lambda_j^n - \alpha^n\big) + \sum_{\lambda_j>\beta} m_j\big(\lambda_j^n - \beta^n\big) = E_n,
\end{aligned}$$

which proves (6.24).

If $V \geq 0$, then $\lambda_j > \beta$ and $\xi(\lambda) \geq 0$ on $[\beta, \infty)$, which implies $E_{2n-1} \leq F_{2n-1}$. Then (6.24) and (6.20) give (6.25) and (6.26). The proof for the case $V \leq 0$ is similar. □

Remark 6.5 For our discrete Schrödinger operator discussed in sections 1, 2, 3, $\widehat{V} = \sum_{n\in\mathbf{Z}^d} \widehat{V}(n)P(n)$ is trace class if

$$\sum_{n\in\mathbf{Z}^d} |\widehat{V}(n)| < \infty.$$

The assumptions **(B-1)**, **(B-2)**, **(B-3)** are then satisfied if we shift our Hamiltonian $\widehat{H}_0$ in §2 by $d/2$.

Remark 6.6 For the continuous model, it is well-known that H has no embedded eigenvalues for the short-range perturbation. The (non) existence of embedded eigenvalues for the discrete model is an interesting open question.

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