Discrete Laplacian in a half-space with a periodic surface potential: an overview on analytical investigations

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Abstract

In this conference proceeding's paper we summarize some recent investigations on a scattering system given by the Neumann Laplacian on the discrete half-space perturbed by a periodic potential at the boundary. This material is borrowed from a joint paper [9] with H.S. Nguyen and R. Tiedra de Aldecoa. For more precise statements and details, we refer to this reference.

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Overview

For the last 20 years, Schrödinger operators with potentials supported on lower dimensional subspaces have been the subject of an intensive study motivated by both physical applications and mathematical interest, see for example [2, 3, 4, 5, 6, 7, 13] and references therein. These systems exhibit properties that are intermediate between the ones of standard scattering systems (with potentials decaying in all space directions) and the ones of bulk systems (with potentials having no specific space decay). A fundamental example of such property, appearing in discrete and in continuous settings, is the presence of surface states propagating along the lower dimensional subspace. Our goal is to present a detailed study of these surface states from a C^*-algebraic point of view and for a two-dimensional system on the discrete lattice. In particular, we plan to establish an index-type theorem relating the surface states to the scattering part of system. Note that relations of this type in various contexts have already appeared in [1, 8, 20, 23]. However, before any C^*-algebraic construction and prior to any index theorem, a lot of analysis is needed. This is the subject of this first part of a series of two papers.

The model that we consider is a simple and natural quantum system exhibiting surface states. It is given by a Laplace operator on a discrete half-space, subject to a periodic potential at the boundary, see Figure 1. Despite its simplicity, this model requires a non-trivial analysis, and reveals some unexpected properties. Note that this model has already been studied, for instance in [2, 3], but our paper contains more precise scattering results, presented within an up-to-date framework.

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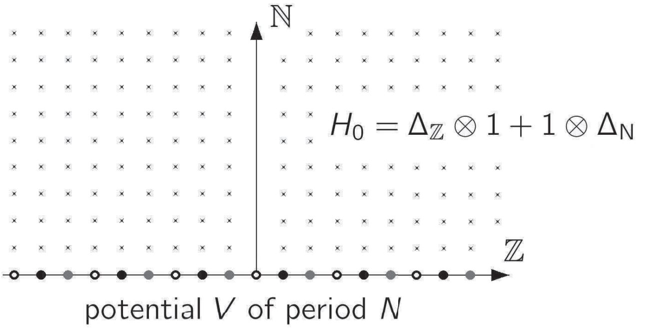

Figure 1: Representation of the discrete model

Let us now give rather complete description of our results, and refer to the following sections for more rigorous statements. In the Hilbert space $\mathcal{H} := \ell^2(\mathbb{Z}\times\mathbb{N}) \cong \ell^2(\mathbb{Z}) \otimes \ell^2(\mathbb{N})$ we consider the free Hamiltonian H_0 given by

$$H_0 := \Delta_{\mathbb{Z}} \otimes 1 + 1 \otimes \Delta_{\mathrm{N}},$$

where $\Delta_{\mathbb{Z}}$ denote the adjacency operator in $\ell^2(\mathbb{Z})$ given by

$$(\Delta_{\mathbb{Z}}\varphi)(x) := \varphi(x+1) + \varphi(x-1), \quad \varphi \in \ell^2(\mathbb{Z}),\ x \in \mathbb{Z},$$

and where Δ_{N} denote the discrete Neumann adjacency operator on $\mathbb{N}$ whose action on $\phi \in \ell^2(\mathbb{N})$ is described by

$$(\Delta_{\mathrm{N}}\phi)(n) = \begin{cases} 2^{1/2}\phi(1) & \text{if } n = 0 \\ 2^{1/2}\phi(0) + \phi(2) & \text{if } n = 1 \\ \phi(n+1) + \phi(n-1) & \text{if } n \geq 2. \end{cases}$$

The full Hamiltonian H describing our discrete quantum model is then given by

$$H := H_0 + V,$$

where V is the multiplication operator by a nonzero, periodic, real-valued function with support on $\mathbb{Z}\times\{0\}$. In other words, there exists a nonzero periodic function $v : \mathbb{Z} \to \mathbb{R}$ of period $N \in \mathbb{N}$ ($N \geq 2$) such that

$$(H\psi)(x,n) = (H_0\psi)(x,n) + \delta_{0,n}\, v(x)\psi(x,0), \quad \psi \in \mathcal{H},\ x \in \mathbb{Z},\ n \in \mathbb{N},$$

with $\delta_{0,n}$ the Kronecker delta function. Note that the multiplication operator V associated to the potential v is not a compact perturbation of H_0.

Since H_0 and H are N-periodic in the x-variable, it is a rather standard fact that they can be decomposed by using a Bloch-Floquet transformation. Namely, let us set

$$\mathfrak{h} := \mathrm{L}^2\left([0,\pi), \tfrac{\mathrm{d}\omega}{\pi}; \mathbb{C}^N\right)$$

and consider the direct integral Hilbert space $\mathfrak{H} := \int_{[0,2\pi]}^{\oplus} \mathfrak{h}\, \frac{\mathrm{d}\theta}{2\pi}$. Then, the operator H_0 and H are unitarily equivalent to the operators direct integral operators in $\mathfrak{H}$ given by

$$\int_{[0,2\pi]}^{\oplus} H_0^\theta \, \frac{\mathrm{d}\theta}{2\pi} \quad \text{with} \quad H_0^\theta := 2\cos(\Omega) + A^\theta \tag{1}$$

and

$$\int_{[0,2\pi]}^{\oplus} H^\theta \tfrac{\mathrm{d}\theta}{2\pi} \quad \text{with} \quad H^\theta := 2\cos(\Omega) + A^\theta + \mathrm{diag}(v)P_0 \tag{2}$$

where $\cos(\Omega)$ denotes the multiplication operator by the function $\omega \to \cos(\omega)$ in $\mathfrak{h}$, A^θ corresponds to the $N \times N$ hermitian matrix

$$A^\theta := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & \mathrm{e}^{-i\theta} \\ 1 & 0 & 1 & \ddots & & 0 \\ 0 & 1 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 1 & 0 \\ 0 & & \ddots & 1 & 0 & 1 \\ \mathrm{e}^{i\theta} & 0 & \cdots & 0 & 1 & 0 \end{pmatrix}. \tag{3}$$

and

$$\big(\mathrm{diag}(v)\mathfrak{f}(\theta,\cdot)\big)_j := v(j)\,\mathfrak{f}_j(\theta,\cdot) \quad \text{and} \quad \big(P_0\,\mathfrak{f}(\theta,\cdot)\big)_j := \int_0^\pi \mathfrak{f}_j(\theta,\omega)\tfrac{\mathrm{d}\omega}{\pi} \tag{4}$$

for $\mathfrak{f} \in \mathfrak{H}$, $j \in \{1,\dots,N\}$ and a.e. $\theta \in [0,2\pi]$. The main advantage of the above representation is that for each fixed θ the operator $\mathrm{diag}(v)P_0$ is a finite rank perturbation of the operator H_0^θ.

Remark 1. *A direct inspection shows that the matrix A^θ has eigenvalues*

$$\lambda_j^\theta := 2\cos\left(\frac{\theta + 2\pi j}{N}\right), \quad j \in \{1,\dots,N\},$$

with corresponding eigenvectors $\xi_j^\theta \in \mathbb{C}^N$ having components $\big(\xi_j^\theta\big)_k := \mathrm{e}^{i(\theta+2\pi j)k/N}$, $j,k \in \{1,\dots,N\}$. Using the notation $\mathcal{P}_j^\theta$ for the orthogonal projection associated to ξ_j^θ, we thus can write A^θ as $A^\theta = \sum_{j=1}^N \lambda_j^\theta \mathcal{P}_j^\theta$.

As a consequence these unitary equivalences, the analysis of the pair of operators (H, H_0) is reduced to the analysis of the family of pairs of operators (H^θ, H_0^θ) indexed by a quasi-momentum $\theta \in [0,2\pi]$. We emphasize that all operators H^θ and H_0^θ act in the fixed Hilbert space $\mathfrak{h} = \mathrm{L}^2\big([0,\pi), \frac{\mathrm{d}\omega}{\pi}; \mathbb{C}^N\big)$. From now on, we shall study the operators H^θ and H_0^θ for fixed θ, and come back to the pair (H, H_0) later on.

A spectral representation of H_0^θ is now easy to find, and since it plays an important role in the sequel, we provide its construction. Roughly speaking, it consists in diagonalizing the matrix A^θ and in linearizing the function cos. More precisely, we first define for $\theta \in [0,2\pi]$ and $j \in \{1,\dots,N\}$ the sets

$$I_j^\theta := \big(\lambda_j^\theta - 2, \lambda_j^\theta + 2\big) \quad \text{and} \quad I^\theta := \cup_{j=1}^N I_j^\theta,$$

with λ_j^θ the eigenvalues of A^θ exhibited in Remark 1. Also, we define the fiber Hilbert spaces

$$\mathscr{H}^\theta(\lambda) := \mathrm{span}\big\{\mathcal{P}_j^\theta \mathbb{C}^N \mid j \in \{1,\dots,N\} \text{ such that } \lambda \in I_j^\theta\big\} \subset \mathbb{C}^N, \quad \lambda \in I^\theta,$$

and the corresponding direct integral Hilbert space

$$\mathscr{H}^\theta := \int_{I^\theta}^{\oplus} \mathscr{H}^\theta(\lambda)\,\mathrm{d}\lambda.$$

Then, we define the operator $\mathscr{F}^\theta : \mathfrak{h} \to \mathscr{H}^\theta$ by

$$\big(\mathscr{F}^\theta g\big)(\lambda) := \pi^{-1/2} \sum_{\{j \mid \lambda \in I_j^\theta\}} \big(4 - (\lambda - \lambda_j^\theta)^2\big)^{-1/4} \mathcal{P}_j^\theta g\left(\arccos\left(\tfrac{\lambda - \lambda_j^\theta}{2}\right)\right), \quad g \in \mathfrak{h}, \text{ a.e. } \lambda \in I^\theta.$$

It is easily verified that $\mathscr{F}^\theta$ is unitary, with adjoint $(\mathscr{F}^\theta)^* : \mathscr{H}^\theta \to \mathfrak{h}$ given by

$$\big((\mathscr{F}^\theta)^*\zeta\big)(\omega) := \big(2\pi\sin(\omega)\big)^{1/2}\sum_{j=1}^N \mathcal{P}_j^\theta\zeta\big(2\cos(\omega)+\lambda_j^\theta\big), \quad \zeta\in\mathscr{H}^\theta, \text{ a.e. } \omega\in[0,\pi). \tag{5}$$

In addition, $\mathscr{F}^\theta$ diagonalises the Hamiltonian H_0^θ, namely for all $\zeta\in\mathscr{H}^\theta$ and a.e. $\lambda\in I^\theta$ one has

$$\big(\mathscr{F}^\theta H_0^\theta(\mathscr{F}^\theta)^*\zeta\big)(\lambda) = \lambda\,\zeta(\lambda) = \big(X^\theta\zeta\big)(\lambda),$$

with X^θ the (bounded) operator of multiplication by the variable in $\mathscr{H}^\theta$. One directly infers from it that H_0^θ has purely absolutely continuous spectrum equal to

$$\sigma(H_0^\theta) = \overline{\operatorname{Ran}(X^\theta)} = \overline{I^\theta} = \big[\big(\min_j\lambda_j^\theta\big)-2, \big(\max_j\lambda_j^\theta\big)+2\big] \subset [-4,4]. \tag{6}$$

and also that $\sigma(H_0) = \overline{\bigcup_{\theta\in[0,2\pi]}\sigma(H_0^\theta)} = [-4,4]$. Note that the spectral representation of H_0^θ leads also naturally to the notion of thresholds: these real values correspond to a change of multiplicity of the spectrum. Clearly, the set $\mathcal{T}^\theta$ of thresholds for the operator H_0^θ is given by

$$\mathcal{T}^\theta := \big\{\lambda_j^\theta \pm 2 \mid j\in\{1,\dots,N\}\big\}. \tag{7}$$

The next step is to analyse the operator H^θ. In brief, we establish the spectral properties of this operator, and provide resolvent expansions near the thresholds of its spectrum. Based on the resolvent expansion we also provide information on the scattering operator for the pair (H^θ, H_0^θ).

For the spectral analysis, the main result is a necessary and sufficient condition for the existence of an eigenvalue for the operator H^θ. For its statement, we follow some standard constructions borrowed from [14] and [24]. First of all, let us decompose the matrix $\operatorname{diag}(v) := (v(1),\dots,v(N))$ as a product $\operatorname{diag}(v) = \mathfrak{u}\mathfrak{v}^2$, where $\mathfrak{v} := |\operatorname{diag}(v)|^{1/2}$ and $\mathfrak{u} := \operatorname{sgn}\big(\operatorname{diag}(v)\big)$ is the diagonal matrix with components

$$\mathfrak{u}_{jj} = \operatorname{sgn}\big(\operatorname{diag}(v)\big)_{jj} = \begin{cases} +1 & \text{if } v(j)\geq 0 \\ -1 & \text{if } v(j)<0, \end{cases} \qquad j\in\{1,\dots,N\}.$$

We also introduce the expression

$$\beta_j^\theta(z) := \big|\big(z-\lambda_j^\theta\big)^2 - 4\big|^{1/4}, \quad j\in\{1,\dots,N\},\ z\in\mathbb{C}. \tag{8}$$

The main spectral result for H^θ then reads (see Remark 1 for the notation $\mathcal{P}_j^\theta$) :

Proposition 2. *A value $\lambda\in\mathbb{R}\setminus\mathcal{T}^\theta$ is an eigenvalue of H^θ if and only if*

$$\mathcal{K} := \ker\left(\mathfrak{u} + \sum_{\{j\mid\lambda<\lambda_j^\theta-2\}}\frac{\mathfrak{v}\mathcal{P}_j^\theta\mathfrak{v}}{\beta_j^\theta(\lambda)^2} - \sum_{\{j\mid\lambda>\lambda_j^\theta+2\}}\frac{\mathfrak{v}\mathcal{P}_j^\theta\mathfrak{v}}{\beta_j^\theta(\lambda)^2}\right)\bigcap\Big(\cap_{\{j\mid\lambda\in I_j^\theta\}}\ker\big(\mathcal{P}_j^\theta\mathfrak{v}\big)\Big) \neq \{0\},$$

in which case the multiplicity of λ equals the dimension of $\mathcal{K}$.

After this spectral result, we use a general approach for resolvent expansions [14, 21] to derive precise asymptotic expansions for the operators H^θ. For that purpose, let us introduce the bounded operator $G : \mathfrak{h}\to\mathbb{C}^N$ defined by

$$(Gg)_j := \mathfrak{v}_{jj}\int_0^\pi g_j(\omega)\,\tfrac{\mathrm{d}\omega}{\pi} = |v(j)|^{1/2}\int_0^\pi g_j(\omega)\,\tfrac{\mathrm{d}\omega}{\pi}, \quad g\in\mathfrak{h}. \tag{9}$$

Then, investigations on the resolvent of H^θ are equivalent to the study of the expression

$$M^\theta(\lambda+i\varepsilon) := \big(\mathfrak{u} + G(H_0^\theta - \lambda - i\varepsilon)^{-1}G^*\big)^{-1}, \quad \lambda, \varepsilon \in \mathbb{R},\ \varepsilon \neq 0 \tag{10}$$

as ε approaches 0. The expansions that we obtain are expressed in terms of projections S_0, S_1, S_2 in $\mathbb{C}^N$ with decreasing range, with the most singular divergences of the expansions taking place in the ranges of the projections of higher indices (the greater the divergence, the smaller the subspace where it takes place). Our expansions are valid for any point λ in the spectrum of H^θ. That is, when λ is a threshold of H^θ, when λ is an eigenvalue of H^θ, and when λ is neither a threshold, nor an eigenvalue of H^θ. Note that the asymptotic expansion is too complicated and long to be stated in an introduction, but that the technics for deriving such results are nowadays rather standard. Let us also mention that a direct consequence of the asymptotic expansion is the finiteness of point spectrum of H^θ.

Once the asymptotic expansion of the operator (10) is obtained, the next key result of our investigations can be proved, namely the continuity of the scattering matrix. Indeed, early investigations on scattering theory usually deal with the existence and completeness of the wave operators. Such results lead to the existence and the unitarity of the scattering operator, but does not say anything about its continuity of the scattering matrix. On the other hand, the future C^*-algebraic framework requires the continuity of this operator.

For getting such a result, let us recall that the wave operators

$$W_\pm^\theta := \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{itH^\theta}\,\mathrm{e}^{-itH_0^\theta}$$

exist and are complete since the difference $H^\theta - H_0^\theta$ is a finite rank operator, see [15, Thm. X.4.4]. As a consequence, the scattering operator $S^\theta := (W_+^\theta)^* W_-^\theta$ is a unitary operator in $\mathfrak{h}$ commuting with H_0^θ, and thus S^θ is decomposable in the spectral representation of H_0^θ, that is,

$$\big(\mathscr{F}^\theta S^\theta (\mathscr{F}^\theta)^* h\big)(\lambda) = S^\theta(\lambda)h(\lambda), \quad h \in \mathscr{H}^\theta, \text{ a.e. } \lambda \in \sigma(H_0^\theta),$$

with the scattering matrix $S^\theta(\lambda)$ a unitary operator in $\mathscr{H}^\theta(\lambda)$.

To give an explicit formula for $S^\theta(\lambda)$, Proposition 2 and the asymptotic expansion play a key role. Indeed, it follows from them that that the operator

$$M^\theta(\lambda+i0) := \lim_{\varepsilon\searrow 0}\big(\mathfrak{u} + G(H_0^\theta - \lambda - i\varepsilon)^{-1}G^*\big)^{-1}$$

belongs to $\mathscr{B}(\mathbb{C}^N)$ for each $\lambda \in \sigma(H_0^\theta)\setminus\big(\mathcal{T}^\theta \cup \sigma_{\mathrm{p}}(H^\theta)\big)$. Here, we have used the notation $\sigma_{\mathrm{p}}(H^\theta)$ for the point spectrum of the operator H^θ. We also define for $j, j' \in \{1, \dots, N\}$ the operator $\delta_{jj'} \in \mathscr{B}\big(\mathcal{P}_{j'}^\theta\mathbb{C}^N; \mathcal{P}_j^\theta\mathbb{C}^N\big)$ by $\delta_{jj'} := 1$ if $j = j'$ and $\delta_{jj'} := 0$ otherwise. Then, a computation using stationary formulas as presented in [24, Sec. 2.8] shows that for $\lambda \in \big(I_j^\theta \cap I_{j'}^\theta\big) \setminus \big(\mathcal{T}^\theta \cup \sigma_{\mathrm{p}}(H^\theta)\big)$ the channel scattering matrix $S^\theta(\lambda)_{jj'} := \mathcal{P}_j^\theta S^\theta(\lambda)\mathcal{P}_{j'}^\theta$ satisfies the formula

$$S^\theta(\lambda)_{jj'} = \delta_{jj'} - 2i\,\beta_j^\theta(\lambda)^{-1}\mathcal{P}_j^\theta \mathfrak{v}\, M^\theta(\lambda+i0)\mathfrak{v}\,\mathcal{P}_{j'}^\theta \beta_{j'}^\theta(\lambda)^{-1}. \tag{11}$$

For the continuity of the scattering matrix, the explicit formula for $G(H_0^\theta - \lambda - i0)^{-1}G^*$ provided in [9] implies the continuity of the map

$$\big(I_j^\theta \cap I_{j'}^\theta\big) \setminus \big(\mathcal{T}^\theta \cup \sigma_{\mathrm{p}}(H^\theta)\big) \ni \lambda \mapsto S^\theta(\lambda)_{jj'} \in \mathscr{B}\big(\mathcal{P}_{j'}^\theta\mathbb{C}^N; \mathcal{P}_j^\theta\mathbb{C}^N\big).$$

Therefore, in order to completely establish the continuity of the channel scattering matrices $S^\theta(\lambda)_{jj'}$, what remains is to describe the behaviour of $S^\theta(\lambda)_{jj'}$ as $\lambda \to \lambda_\star \in \mathcal{T}^\theta \cup \sigma_{\mathrm{p}}(H^\theta)$. We will consider separately the behaviour of $S^\theta(\lambda)_{jj'}$ at thresholds and at embedded eigenvalues, starting with the thresholds. For that purpose, we first note that for each $\lambda \in \mathcal{T}^\theta$, a channel can already be opened at the energy λ (in which case one has to show the existence and the equality of the limits from the right and from the left), it can open at the energy λ (in which case one only has to show the existence of the limit from the right), or it can close at the energy λ (in which case one only has to show the existence of the limit from the left). Therefore, we will fix $\lambda \in \mathcal{T}^\theta$, and consider the matrix $S^\theta(\lambda+\varepsilon)_{jj'}$ for suitable ε. In this setting our main result is (see [9] for a statement with the operators at the limits):

Theorem 3. *Let $\lambda \in \mathcal{T}^\theta$, take $\varepsilon \in \mathbb{R}$ with $|\varepsilon|$ small enough, and let $j, j' \in \{1, \ldots, N\}$.*

(a) If $\lambda \in I_j^\theta \cap I_{j'}^\theta$, then the limit $\lim_{\varepsilon\to 0} S^\theta(\lambda+\varepsilon)_{jj'}$ exists.

(b) If $\lambda \in \overline{I_j^\theta} \cap \overline{I_{j'}^\theta}$ and $\lambda+\varepsilon \in I_j^\theta \cap I_{j'}^\theta$ for $\varepsilon > 0$ small enough, then the limit $\lim_{\varepsilon\searrow 0} S^\theta(\lambda+\varepsilon)_{jj'}$ exists.

(c) If $\lambda \in \overline{I_j^\theta} \cap \overline{I_{j'}^\theta}$ and $\lambda-\varepsilon \in I_j^\theta \cap I_{j'}^\theta$ for $\varepsilon > 0$ small enough, then the limit $\lim_{\varepsilon\searrow 0} S^\theta(\lambda-\varepsilon)_{jj'}$ exists.

For the statement about the continuity of the scattering matrix at embedded eigenvalues not located at thresholds.

Theorem 4. *Let $\lambda \in \sigma_{\rm p}(H^\theta) \setminus \mathcal{T}^\theta$, take $\varepsilon \in \mathbb{R}$ with $|\varepsilon| > 0$ small enough, and let $j, j' \in \{1, \ldots, N\}$. Then, if $\lambda \in I_j^\theta \cap I_{j'}^\theta$, the limit $\lim_{\varepsilon\to 0} S^\theta(\lambda+\varepsilon)_{jj'}$ exists.*

Let us now return to the wave operator W_-^θ, which is of primary interest for future investigations. By using the stationary approach of scattering theory and by looking at the representation of the wave operator inside the spectral representation of H_0^θ, we can express W_-^θ as the sum of two distinct contributions, namely for suitable $\xi, \zeta \in \mathscr{H}^\theta$

$$
\begin{aligned}
&\big\langle \mathscr{F}^\theta (W_-^\theta - 1)(\mathscr{F}^\theta)^*\xi, \zeta\big\rangle_{\mathscr{H}^\theta} \\
&= -\pi^{-1/2} \sum_{j=1}^N \int_{I_j^\theta} \lim_{\varepsilon\searrow 0} \left\langle \mathfrak{v} M^\theta(\lambda+i\varepsilon)\mathfrak{v}\gamma_0(\mathscr{F}^\theta)^*\delta_\varepsilon(X^\theta-\lambda)\xi, \int_{I_j^\theta} \frac{\beta_j^\theta(\mu)^{-1}}{\mu-\lambda+i\varepsilon}\zeta_j(\mu)\,\mathrm{d}\mu\right\rangle_{\mathbb{C}^N} \mathrm{d}\lambda \qquad (12)\\
&\quad - \pi^{-1/2} \sum_{j=1}^N \int_{\sigma(H_0^\theta)\setminus I_j^\theta} \lim_{\varepsilon\searrow 0} \left\langle \mathfrak{v} M^\theta(\lambda+i\varepsilon)\mathfrak{v}\gamma_0(\mathscr{F}^\theta)^*\delta_\varepsilon(X^\theta-\lambda)\xi, \int_{I_j^\theta} \frac{\beta_j^\theta(\mu)^{-1}}{\mu-\lambda+i\varepsilon}\zeta_j(\mu)\,\mathrm{d}\mu\right\rangle_{\mathbb{C}^N} \mathrm{d}\lambda. \qquad (13)
\end{aligned}
$$

where $\delta_\varepsilon(X^\theta-\lambda) := \frac{\pi^{-1}\varepsilon}{(X^\theta-\lambda)^2+\varepsilon^2}$ and $\gamma_0 : \mathfrak{h} \to \mathbb{C}^N$ is defined by

$$
(\gamma_0 g)_j := \int_0^\pi g_j(\omega)\,\tfrac{\mathrm{d}\omega}{\pi}, \quad g \in \mathfrak{h},\ j \in \{1, \ldots, N\}. \qquad (14)
$$

Note that the main term (12) could be called the *on shell* contribution while the remainder term (13) could be called the *off shell* contribution.

Our interest in such a decomposition is that main term is equal to the product of an explicit operator independent of the potential, and the operator $S^\theta - 1$. Namely, we show that the operator described by (12) is unitarily equivalent to the operator

$$
\tfrac{1}{2}\big(1 - \tanh(\pi\mathfrak{D}) - i\cosh(\pi\mathfrak{D})^{-1}\tanh(\mathfrak{X})\big)\big(S^\theta - 1\big) \qquad (15)
$$

where $\mathfrak{X}$ and $\mathfrak{D}$ are representations of the canonical position and momentum operators in the Hilbert space $\mathfrak{h}$. Let us emphasize that such a formula has been derived by looking at the on shell contribution into a *rescaled energy representation* whose importance has been revealed in [1, 23] and which was also used explicitly in [12] and implicitly in [18, 19].

The analysis of the remainder term (13) is more involved, and depends on the value of $\theta \in [0, 2\pi]$. For $\theta \neq 0$, then the operator defined by (13) extends continuously to a compact operator. Since (15) is never a compact operator it means that the remainder term can indeed be considered as small compared to the leading term. Note that the same result holds when $\theta = 0$ and N (the periodicity) is odd. On the other hand, when $\theta = 0$ and N is even, more analysis is required. In fact, it is interesting to observe that a compacity argument does not work exactly when two energy bands in the spectrum of H^0 touch but do not overlap (the energy bands are $[-4, 0]$ and $[0, 4]$). In the special case $\theta = 0$ and N even, one can still show that the remainder term is compact if the vectors $\mathfrak{v}\xi_N^0$ and $\mathfrak{v}\xi_{N/2}^0$ are linearly independent (see Remark 1 for the definition of the vectors ξ_N^0 and $\xi_{N/2}^0$). The very exceptional situation $\theta = 0$, N even and $\mathfrak{v}\xi_N^0$ and $\mathfrak{v}\xi_{N/2}^0$ are linearly dependent is called the *the exceptional case* and take place if and only if the matrix $\mathfrak{v}$ is of the special form

$$\mathfrak{v} = \begin{pmatrix} v(1) & & & 0 \\ & 0 & & \\ & & v(3) & \\ & & & 0 \\ 0 & & & & \ddots \end{pmatrix} \quad \text{or} \quad \mathfrak{v} = \begin{pmatrix} 0 & & & 0 \\ & v(2) & & \\ & & 0 & \\ & & & v(4) \\ 0 & & & & \ddots \end{pmatrix}. \tag{16}$$

In the exceptional case, the remainder term is bounded but not compact. Let us however already mention that this operator will still be smaller than the main term in a sense which will be fully explained in the second part of this work, once suitable C^*-algebras will be introduced.

By summing up the previous two paragraphs in a single statement:

Theorem 5. *For any $\theta \in [0, 2\pi]$, one has the equality*

$$W_-^\theta - 1 = \tfrac{1}{2}\big(1 - \tanh(\pi\mathfrak{D}) - i\cosh(\pi\mathfrak{D})^{-1}\tanh(\mathfrak{X})\big)(S^\theta - 1) + \mathfrak{K}^\theta,$$

with $\mathfrak{K}^\theta \in \mathscr{K}(\mathfrak{h})$ in the nondegenerate cases, and $\mathfrak{K}^0 \in \mathscr{B}(\mathfrak{h})$ in the degenerate case.

Let us mention that this kind of results for various models having a finite point spectrum are not new: The first appearance took place in [16, 17], it has then appeared in several papers and summarized in the review paper [20], and independently developed in [1] and in [12]. An extension for an infinite number of eigenvalues has also been provided in [10, 11]. However, our main interest is now to combine such formulas for all quasi-momenta, and derive a new representation formula for the full wave operators $W_\pm := \text{s-lim}_{t\to\pm\infty} e^{itH} e^{-itH_0}$ for the initial pair of Hamiltonians (H, H_0). Note that such an approach for the full wave operators has already been used for example in [6, 7, 22].

For this last step, it follows from the direct integral decompositions of H and H_0, from the existence and completeness of $W_\pm^\theta$ for each $\theta \in [0, 2\pi]$, and from [6, Sec. 2.4], that $W_\pm$ exist and have same range. In addition, both $W_\pm$ and S are unitarily equivalent to the direct integral operators

$$\int_{[0,2\pi]}^{\oplus} W_\pm^\theta \tfrac{d\theta}{2\pi} \quad \text{and} \quad \int_{[0,2\pi]}^{\oplus} S^\theta \tfrac{d\theta}{2\pi}$$

which act on the Hilbert space $\mathfrak{H}$. Therefore, by collecting the formulas obtained in Theorem 5 for $W_-^\theta - 1$ in each fiber Hilbert space $\mathfrak{h}$, we obtain a formula for $W_- - 1$ (and thus also for W_+ if we use the relation $W_+ = W_- S^*$):

Theorem 6. *The operator $W_- - 1$ is unitarily equivalent to the direct integral operator*

$$\int_{[0,2\pi]}^{\oplus} \Big(\tfrac{1}{2}\big(1 - \tanh(\pi\mathfrak{D}) - i\cosh(\pi\mathfrak{D})^{-1}\tanh(\mathfrak{X})\big)(S^\theta - 1) + \mathfrak{K}^\theta\Big) \tfrac{d\theta}{2\pi} \tag{17}$$

acting in $\mathfrak{H}$, with $\mathfrak{K}^\theta$ as in Theorem 5.

Note that a more precise version of this statement is provided in [9] with the unitary equivalence clearly stated. Let us also emphasize that event though this theorem is the culminating result of this paper, it is also the starting point for subsequent investigations. Indeed, in recent years, similar formulas for the wave operators have been at the root of index theorems in scattering theory. Such results correspond to generalizations and to a topological version of the so-called Levinson's theorem. The index theorems are based on fact that wave operators are partial isometries relating, through the projection on their cokernels, the scattering theory of a system to its bound states. Now, in our situation, due to the direct integral of (17) states which belong to the cokernel of W_- are no more bound states but surface states. Therefore, the relation mentioned at the beginning of this introduction will be an index theorem based on Theorem 6. In fact, a relation of this type has already appeared in [23], and it relates *the total density of surface states* and *the density of the total time delay*, see this reference for more details. Let us mention also [8] which contains a bulk-edge correspondence for two-dimensional topological insulators whose proof is partially based on scattering theory. Four our model, the necessary C^*-algebraic framework will be introduced in the second paper, and the continuity of the scattering matrices and the existence of their limits at thresholds established here will play a crucial role for the choice of the C^*-algebras. The θ-dependence of all the operators appearing in the current paper will also be a key ingredient for the construction. More information on these issues, and the applications of the analytical results obtained here, will be presented in the subsequent paper.

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