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Crystalline conductance and absolutely continuous spectrum of 1D samples

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Abstract. We characterize the absolutely continuous spectrum of half-line one-dimensional Schrödinger operators in terms of the limiting behavior of the Crystaline Landauer-Büttiker conductance of the associated finite samples.

1 Introduction

This note is a direct continuation of [BJLP2] and completes the research program initiated in [BJP]. This program concerns characterization of the absolutely continuous spectrum of half-line discrete Schrödinger operators in terms of the limiting conductances of the associated finite samples and is intimately linked with the celebrated Schrödinger Conjecture/Property of Schrödinger operators [Av, MMG]. In [BJLP2], this characterization was carried out for the well-known Landauer-Büttiker (LB) and the Thouless (Th) conductance. Here we extend these results to the Crystaline Landauer-Büttiker (CLB) conductance introduced in [BJLP1]. The CLB conductance provides a natural link between the LB and Th conductances and is likely to play an important role in future studies of transport properties of 1D samples.

We briefly recall the setup and results of [BJLP1, BJLP2], referring the reader to the introductions of these papers for details and additional information. The starting point is the discrete Schrödinger operator[1]

$$h_{\mathcal{S}} = -\Delta + v,$$

acting on the Hilbert space $\ell^2(\mathbb{Z}_+)$, where $\mathbb{Z}_+$ denotes the set of positive integers.[2] The operator $h_{\mathcal{S}}$ is the one-electron Hamiltonian of the extended sample. The one-electron Hamiltonian $h_{\mathcal{S}_L}$ of the sample of length L is obtained by restricting $h_{\mathcal{S}}$ to $\mathcal{H}_L = \ell^2(\mathbb{Z}_L)$, where $\mathbb{Z}_L = \{1, \cdots, L\}$. In the Electronic Black Box (EBB) model considered in [BJLP1, BJLP2], this finite sample is connected at its end points 1 and L to reservoirs described by the following one-electron data: Hilbert spaces $\mathcal{H}_{l/r}$, where l/r stands for left/right, Hamiltonians $h_{l/r}$, and unit vectors $\psi_{l/r} \in \mathcal{H}_{l/r}$. For latter reference, we introduce the functions

$$F_{l/r}(E) = \langle \psi_{l/r}, (h_{l/r} - E - \mathrm{i}0)^{-1} \psi_{l/r} \rangle, \tag{1.1}$$

and the sets (note that $\operatorname{Im} F_{l/r}(E) \geq 0$)

$$\Sigma_{l/r} = \{E \,:\, \operatorname{Im} F_{l/r}(E) > 0\}.$$

In the absence of coupling, the one-electron Hamiltonian of the joint system sample+reservoirs is

$$h_{0,L} = h_l + h_{\mathcal{S}_L} + h_r,$$

acting on $\mathcal{H} = \mathcal{H}_l \oplus \mathcal{H}_L \oplus \mathcal{H}_r$. The junctions between the sample and the reservoirs are described by

$$h_{T,l} = |\psi_l\rangle\langle\delta_1| + |\delta_1\rangle\langle\psi_l| \qquad \text{and} \qquad h_{T,r} = |\psi_r\rangle\langle\delta_L| + |\delta_L\rangle\langle\psi_r|,$$

and the coupled one-electron Hamiltonian is

$$h_{\kappa,L} = h_{0,L} + \kappa(h_{T,l} + h_{T,r}),$$

where $\kappa \neq 0$ is a coupling constant. The left/right reservoir is initially at equilibrium at zero temperature and chemical potential $\mu_{l/r}$ where $\mu_l < \mu_r$. The voltage differential induces a steady state charge current from the right to the left reservoir across the sample and the corresponding conductance is given by the Landauer-Büttiker formula, see, e.g., [La, BILP, AJPP, CJM, N],

$$G_{\mathrm{LB}}(L, I) = \frac{1}{2\pi|I|} \int_I \mathcal{T}_{\mathrm{LB}}(L, E)\, \mathrm{d}E, \tag{1.2}$$

where $I = (\mu_l, \mu_r)$, $|I| = \mu_r - \mu_l$, and

$$\mathcal{T}_{\mathrm{LB}}(L, E) = 4\kappa^4 |\langle \delta_1, (h_{\kappa,L} - E - \mathrm{i}0)^{-1} \delta_L \rangle|^2 \operatorname{Im} F_l(E) \operatorname{Im} F_r(E), \tag{1.3}$$

is the transmission probability from the right to the left reservoir at energy E. Obviously, only the energies in $\Sigma_l \cap \Sigma_r$ contribute to the integral (1.2). For this reason, in some applications of the LB formula we will need to assume the *transparency condition* that $I \subset \Sigma_l \cap \Sigma_r$ (see Theorems 1.1 and 1.2).

[1] The setup and all our results extend to the case of Jacobi matrices, see [BJLP3]. For notational simplicity we will restrict ourselves here to the physically relevant case of Schrödinger operators.

[2] For our purposes, the choice of boundary condition is irrelevant. For definiteness we shall impose Dirichlet b.c. on the discrete Laplacian Δ.

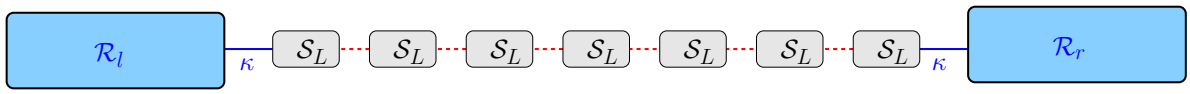

Figure 1: The EBBM described by the Hamiltonian $h_{\kappa,L}^{(N)}$ for $N = 7$.

The Thouless formula is the special case of Landauer-Büttiker formula in which the reservoirs are implemented in such a way that the coupled Hamiltonian is the periodic discrete Schrödinger operator on $\ell^2(\mathbb{Z})$

$$h_{\kappa,L} = h_{\mathrm{per},L} = -\Delta + v_{\mathrm{per},L},$$

where the sample potential $v(n)$ is extended from $\mathbb{Z}_L$ to $\mathbb{Z}$ by setting $v_{\mathrm{per},L}(n+mL) = v(n)$ for $n \in \mathbb{Z}_L$ and $m \in \mathbb{Z}$. We shall refer to the corresponding EBB model as *crystaline* (see [BJLP1] for details). In this case the transport is reflectionless and the Landauer-Büttiker formula coincides with the Thouless formula:

$$G_{\mathrm{Th}}(L, I) = \frac{|\mathrm{sp}(h_{\mathrm{per},L}) \cap I|}{2\pi|I|}, \tag{1.4}$$

where $\mathrm{sp}(h_{\mathrm{per},L})$ denotes the spectrum of $h_{\mathrm{per},L}$.

The CLB conductance has appeared implicitly in early physicists works on Thouless conductance [ET]. The following precise mathematical definition was proposed in [BJLP2]. Consider the Landauer-Büttiker formula $G_{\mathrm{LB}}^{(N)}(L, I)$ for the model in which the sample $\mathcal{S}_L$ is replaced by its N-fold repetition while the reservoirs remain fixed (see Figure 1). The limit $N \to \infty$ then gives the CLB formula. To describe it, let $h_{\mathrm{per},L}^{(l)}$ and $h_{\mathrm{per},L}^{(r)}$ be the restrictions of $h_{\mathrm{per},L}$ to $\ell^2((-\infty, 0] \cap \mathbb{Z})$ and $\ell^2([1, \infty) \cap \mathbb{Z})$ with Dirichlet boundary conditions, and

$$\begin{aligned} m_l(L, E) &= \langle \delta_0, (h_{\mathrm{per},L}^{(l)} - E - \mathrm{i}0)^{-1}\delta_0 \rangle, \\ m_r(L, E) &= \langle \delta_1, (h_{\mathrm{per},L}^{(r)} - E - \mathrm{i}0)^{-1}\delta_1 \rangle. \end{aligned} \tag{1.5}$$

We set $\mathcal{T}_{\mathrm{CLB}}(E) = 0$ for $E \in \mathbb{R} \setminus (\mathrm{sp}(h_{\mathrm{per},L}) \cap \Sigma_l \cap \Sigma_r)$ and

$$\mathcal{T}_{\mathrm{CLB}}(L, E) = \left[1 + \frac{1}{4}\left(\frac{|m_r(L, E) - \kappa^2 F_r(E)|^2}{\mathrm{Im}\,(m_r(L, E))\mathrm{Im}\,(\kappa^2 F_r(E))} + \frac{|m_l(L, E) - \kappa^2 F_l(E)|^2}{\mathrm{Im}\,(m_l(L, E))\mathrm{Im}\,(\kappa^2 F_l(E))}\right)\right]^{-1} \tag{1.6}$$

for $E \in \mathrm{sp}(h_{\mathrm{per},L}) \cap \Sigma_l \cap \Sigma_r$. The Crystaline Landauer-Büttiker conductance is defined as

$$G_{\mathrm{CLB}}(L, I) = \frac{1}{2\pi|I|}\int_I \mathcal{T}_{\mathrm{CLB}}(L, E)\mathrm{d}E.$$

In [BJLP1] it was shown that

$$\lim_{N\to\infty} G_{\mathrm{LB}}^{(N)}(L, I) = G_{\mathrm{CLB}}(L, I),$$

and that

$$G_{\mathrm{Th}}(L, I) = \sup G_{\mathrm{CLB}}(L, I), \tag{1.7}$$

where the supremum is taken over all realizations of the reservoirs. The latter identity clarifies the common heuristics in the physics literature that the Thouless conductance should be considered as an upper bound on the possible conductances of a finite sample. Since the supremum is achieved precisely for the crystaline EBB model [BJLP1], it also identifies the heuristic notion of "optimal feeding" of the sample by reservoirs, needed to reach the Thouless conductance, with the reflectionless electron transport across junctions.

Let $\mathrm{sp}_{\mathrm{ac}}(h_{\mathcal{S}})$ denote the absolutely continuous spectrum of $h_{\mathcal{S}}$. The main result of [BJLP2] is:

Theorem 1.1 *Let (L_k) be a sequence of positive integers satisfying $\lim L_k = \infty$. Consider the following statements:*

(1)
$$I \cap \mathrm{sp}_{\mathrm{ac}}(h_{\mathcal{S}}) = \emptyset.$$

(2)
$$\lim_{k\to\infty} G_{\mathrm{LB}}(L_k, I) = 0.$$

(3)
$$\lim_{k\to\infty} G_{\mathrm{Th}}(L_k, I) = 0.$$

Then $(1) \Rightarrow (2)$ and $(1) \Leftrightarrow (3)$. If the transparency condition $I \subset \Sigma_l \cap \Sigma_r$ holds, then also $(2) \Rightarrow (1)$, and all three statements are equivalent.

Remark. The transparency condition is necessary for the implication $(2) \Rightarrow (1)$, and in our context it should be considered as an assumption on the non-triviality of the setup. The same remark applies to Theorem 1.2 below.

In this note we complete Theorem 1.1 with:

Theorem 1.2 *Let (L_k) be a sequence of positive integers satisfying $\lim L_k = \infty$. Consider the following statements:*

(1)
$$I \cap \mathrm{sp}_{\mathrm{ac}}(h_{\mathcal{S}}) = \emptyset.$$

(2)
$$\lim_{k\to\infty} G_{\mathrm{CLB}}(L_k, I) = 0.$$

Then $(1) \Rightarrow (2)$. If the transparency condition $I \subset \Sigma_l \cap \Sigma_r$ holds, then also $(2) \Rightarrow (1)$.

Theorems 1.1 and 1.2 naturally lead to questions regarding the relative scaling and the rate of convergence to zero of the conductances $G_{\#}(L, I)$, $\# \in \{\mathrm{LB}, \mathrm{Th}, \mathrm{CLB}\}$, in the regime $I \cap \mathrm{sp}_{\mathrm{ac}}(h_{\mathcal{S}}) = \emptyset$. Although these questions played a prominent role in early physicists works on the subject (see, e.g., [AL, CGM])

we are not aware of any mathematically rigorous works on this topic. We plan to address these problems in the continuation of our research program.

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2 Proofs

2.1 Proof of Theorem 1.2

Our proof proceeds by showing that for any sequence (L_k), the vanishing of the CLB conductance is equivalent to the vanishing of the Th conductance. Due to (1.7), it suffices to prove that if $I \subset \Sigma_l \cap \Sigma_r$, then

$$\lim_{k\to\infty} G_{\mathrm{CLB}}(L_k, I) = 0 \quad \Longrightarrow \quad \lim_{k\to\infty} G_{\mathrm{Th}}(L_k, I) = 0. \tag{2.1}$$

Relation (1.6) expresses the CLB conductance in terms of the m-functions m_l and m_r of the periodic operator $h_{\mathrm{per},L}$. The first part of the proof consists in estimating these m-functions in terms of the norm of the transfer matrix

$$T(L,E) = \begin{bmatrix} v(L)-E & -1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} v(1)-E & -1 \\ 1 & 0 \end{bmatrix},$$

of $h_{\mathcal{S}}$ for fixed L; see Proposition 2.4 below.

The connection between the m-functions and the transfer matrix is provided by the following lemma (see [BJLP1, Lemma 3.3]).

Lemma 2.1 *For any $E \in \mathrm{sp}(h_{\mathrm{per},L})$, the eigenvalues of $T(L,E)$ are of the form $\mathrm{e}^{\pm \mathrm{i}\theta(L,E)}$ and*

$$\psi_+(L,E) = \begin{bmatrix} 1 \\ m_r(L,E)^{-1} \end{bmatrix} \quad \textit{and} \quad \psi_-(L,E) = \begin{bmatrix} 1 \\ m_l(L,E) \end{bmatrix},$$

are corresponding eigenvectors.

Remark. The fact that the eigenvalues of $T(L,E)$ are complex conjugate further implies the following relation between the two m-functions: $m_r(L,E)^{-1} = \overline{m_l}(L,E)$, i.e. $m_r\overline{m_l} = 1$.

The following proposition provides a lower bound of the CLB conductance in terms of the transfer matrix $T(L,E)$ and the imaginary part of its eigenvalues.

Proposition 2.2 *If there exists $\delta, M > 0$ such that $\operatorname{Im} F_{l/r}(E+i0) > \delta$ and $|F_{l/r}(E+i0)| \leq M$ for a.e. $E \in I$, then there exists $C > 0$ such that for any L*

$$G_{\mathrm{CLB}}(L,I) \geq \frac{1}{2\pi|I|} \int_{I\cap \mathrm{sp}(h_{\mathrm{per},L})} \left[1 + C\frac{\|T(L,E)\|}{|\sin(\theta(L,E))|}\right]^{-1} \mathrm{d}E. \tag{2.2}$$

Proof. One easily gets from (1.6) that

$$G_{\mathrm{CLB}}(L,I) \geq \frac{1}{2\pi|I|} \int_{I\cap \mathrm{sp}(h_{\mathrm{per},L})} \left[1 + \frac{A+B|m_r(L,E)|^2}{2\mathrm{Im}\,(m_r(L,E))} + \frac{A+B|m_l(L,E)|^2}{2\mathrm{Im}\,(m_l(L,E))}\right]^{-1} \mathrm{d}E,$$

with $A = \frac{\kappa^2 M^2}{\delta}$ and $B = \frac{1}{\kappa^2\delta}$, where we used that $I \subset \Sigma_l \cap \Sigma_r$. Since $m_r\overline{m_l} = 1$,

$$\frac{A+B|m_r(L,E)|^2}{\mathrm{Im}\,(m_r(L,E))} = \frac{A|m_l(L,E)|^2 + B}{\mathrm{Im}\,(m_l(L,E))}.$$

Hence, with $C = \max(A,B)$, we have

$$G_{\mathrm{CLB}}(L,I) \geq \frac{1}{2\pi|I|} \int_{I\cap \mathrm{sp}(h_{\mathrm{per},L})} \left[1 + C\frac{1+|m_l(L,E)|^2}{\mathrm{Im}\,(m_l(L,E))}\right]^{-1} \mathrm{d}E. \tag{2.3}$$

We now relate the integrand on the right-hand side of the last inequality to the transfer matrix $T(L,E)$. Using Lemma 2.1 and $m_r\overline{m_l} = 1$, an easy calculation gives

$$T(L,E) = \frac{1}{\mathrm{Im}\,(m_l(L,E))} \begin{bmatrix} \mathrm{Im}\,(\mathrm{e}^{i\theta(L,E)}m_l(L,E)) & -\sin(\theta(L,E)) \\ |m_l(L,E)|^2\sin(\theta(L,E)) & \mathrm{Im}\,(\mathrm{e}^{-i\theta(L,E)}m_l(L,E)) \end{bmatrix},$$

from which we get the lower bound

$$\|T(L,E)\| \geq C'|\sin(\theta(L,E))|\frac{1+|m_l(L,E)|^2}{\mathrm{Im}\,(m_l(L,E))},$$

for some positive constant C'. Inserting this inequality into (2.3) completes the proof. □

In view of (2.2), to get a lower bound of the CLB conductance in terms of the norm of the transfer matrix, the only issue is when $|\sin(\theta(L,E))|$ gets small. The following shows that this cannot happen too often. In the sequel, $|A|$ denotes the Lebesgue measure of $A \subset \mathbb{R}$.

Lemma 2.3 *For any $\epsilon > 0$ and all L,*

$$|\{E \in \mathrm{sp}(h_{\mathrm{per},L}) \,:\, |\sin(\theta(L,E))| \leq \epsilon\}| \leq 2\pi\epsilon.$$

The proof of this lemma relies on a general estimate on the so-called dispersion curves of the periodic operator $h_{\mathrm{per},L}$ and requires additional notation and facts. We postpone it to Section 2.2.

Combining Proposition 2.2 with Lemma 2.3 and recalling the inequality $\|T(L,E)\| \geq 1$, we get

Proposition 2.4 *If there exists $\delta, M > 0$ such that $\operatorname{Im} F_{l/r}(E+i0) > \delta$ and $|F_{l/r}(E+i0)| \leq M$ for a.e. $E \in I$, then there exists $C > 0$ such that for any $\epsilon > 0$ and all L,*

$$G_{\mathrm{CLB}}(L,I) \geq \frac{1}{2\pi|I|}\left(1+C\epsilon^{-1}\right)^{-1} \int_{I\cap(\mathrm{sp}(h_{\mathrm{per},L})\setminus\Omega_{\epsilon,L})} \|T(L,E)\|^{-1}\mathrm{d}E,$$

with $|\Omega_{\epsilon,L}| \leq 2\pi\epsilon$.

Our last ingredient is the following estimate on the norm of transfer matrices which was proven in [BJLP2, Section 5.3].

Proposition 2.5 *There exists a set $O_{\epsilon,L} \subset \mathrm{sp}(h_{\mathrm{per},L})$ such that $|O_{\epsilon,L}| \leq (1+\pi)\epsilon$ and*

$$\|T(L,E)\| \leq \frac{8\pi}{\epsilon^2}, \qquad \forall E \in \mathrm{sp}(h_{\mathrm{per},L}) \setminus O_{\epsilon,L}.$$

We are now in position to finish the proof of Theorem 1.2. For any $n > 0$, let

$$I_n := \{E \in I \,:\, \operatorname{Im} F_{l/r}(E+i0) > 1/n \text{ and } |F_{l/r}(E+i0)| \leq n\},$$

and $I_n' = I \setminus I_n$. Obviously, since $I \subset \Sigma_l \cap \Sigma_r$, $\lim\limits_{n\to\infty} |I_n'| = 0$.

Using Proposition 2.4 together with Proposition 2.5 on I_n, one gets that for any n and for any $\epsilon > 0$,

$$\begin{aligned}
|I|G_{\mathrm{CLB}}(L,I) &\geq |I_n|G_{\mathrm{CLB}}(L,I_n) \\
&\geq |I_n|\left(1+C_n\epsilon^{-1}\right)^{-1} \int_{I_n\cap(\mathrm{sp}(h_{\mathrm{per},L})\setminus\Omega_{\epsilon,L})} \|T(L,E)\|^{-1}\mathrm{d}E \\
&\geq |I_n|\left(1+C_n\epsilon^{-1}\right)^{-1} \frac{\epsilon^2}{8\pi}\left(|\mathrm{sp}(h_{\mathrm{per},L})\cap I_n| - |\Omega_{\epsilon,L}| - |O_{\epsilon,L}|\right) \\
&\geq |I_n|\left(1+C_n\epsilon^{-1}\right)^{-1} \frac{\epsilon^2}{8\pi}\left(|\mathrm{sp}(h_{\mathrm{per},L})\cap I| - |I_n'| - (1+3\pi)\epsilon\right),
\end{aligned}$$

for some C_n which does not depend on ϵ and L.

Suppose now that the sequence (L_k) is such that $\lim\limits_{k\to\infty} G_{\mathrm{CLB}}(L_k,I) = 0$. It follows that

$$\limsup_{k\to\infty} |\mathrm{sp}(h_{\mathrm{per},L_k})\cap I| \leq |I_n'| + (1+3\pi)\epsilon.$$

Since this holds for any $\epsilon > 0$ and $|I_n'| \to 0$, this proves that $\lim\limits_{k\to\infty} |\mathrm{sp}(h_{\mathrm{per},L_k})\cap I| = 0$, and hence $\lim\limits_{k\to\infty} G_{\mathrm{Th}}(L_k,I) = 0$.

2.2 Proof of Lemma 2.3

We first introduce some notation and recall a few basic facts about periodic operators, referring the reader to [Si, Chapter 5] for proofs and additional information.

For any $k \in \mathbb{R}$ and $m \in \mathbb{Z}$ let

$$H(k,m) = \begin{bmatrix} v_{\mathrm{per}}(m+1) & -1 & \cdots & 0 & -\mathrm{e}^{-\mathrm{i}kL} \\ -1 & v_{\mathrm{per}}(m+2) & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & v_{\mathrm{per}}(m+L-1) & -1 \\ -\mathrm{e}^{\mathrm{i}kL} & 0 & \cdots & -1 & v_{\mathrm{per}}(m+L) \end{bmatrix},$$

and denote by $E_1(k) \leq \cdots \leq E_L(k)$ the repeated eigenvalues of $H(k,0)$. The functions $\mathbb{R} \ni k \mapsto E_\ell(k)$ are called the dispersion curves and will be the key object in the proof of Lemma 2.3. They are $2\pi/L$-periodic and even. They are strictly monotone and real analytic on the interval $(0,\pi/L)$. Moreover, they satisfy

$$E_L(0) > E_L\left(\frac{\pi}{L}\right) \geq E_{L-1}\left(\frac{\pi}{L}\right) > E_{L-1}(0) \geq E_{L-2}(0) > \cdots$$

This implies in particular that each $E_\ell(k)$ is a simple eigenvalue of $H(k,0)$ for $k \in (0,\pi/L)$. It follows that for each $\ell \in \{1,\ldots,L\}$ there is a unique real analytic function

$$(0,\pi/L) \ni k \mapsto \vec{u}_\ell(k) = (u_\ell(k,1),\ldots,u_\ell(k,L))^T \in \mathbb{C}^L,$$

such that $H(k,0)\vec{u}_\ell(k) = E_\ell(k)\vec{u}_\ell(k)$, $u_\ell(k,1) > 0$ and $\|\vec{u}_\ell(k)\| = 1$. A bounded two-sided sequence $u_\ell(k) = (u_\ell(k,m))_{m\in\mathbb{Z}}$ is obtained by setting

$$u_\ell(k,j+nL) = \mathrm{e}^{\mathrm{i}knL} u_\ell(k,j), \tag{2.4}$$

for any $j \in \{1,\ldots,L\}$ and $n \in \mathbb{Z}$. Then, for any $m \in \mathbb{Z}$,

$$\vec{u}_\ell(k,m) = (u_\ell(k,m+1),\ldots,u_\ell(k,m+L))^T,$$

is a normalized eigenvector of $H(k,m)$ for the eigenvalue $E_\ell(k)$.

It follows from Floquet theory that $E \in \mathrm{sp}(h_{\mathrm{per},L})$ iff the eigenvalue equation

$$h_{\mathrm{per},L} u = Eu \tag{2.5}$$

has a non-trivial solution u satisfying $u(n+L) = \mathrm{e}^{\mathrm{i}kL}u(n)$ for some $k \in \mathbb{R}$ and all $n \in \mathbb{Z}$. This solution is called Bloch wave of energy E and u is such a Bloch wave if and only if $E = E_\ell(k)$ for some ℓ and $(u(1),\ldots,u(L))^T$ is an eigenvector of $H(k,0)$ for $E_\ell(k)$. In particular, for any m,

$$\mathrm{sp}(h_{\mathrm{per},L}) = \bigcup_{k\in[0,\pi/L]} \mathrm{sp}(H(k)) = \bigcup_{\ell=1}^{L} B_\ell,$$

where B_ℓ is the closed interval with boundary points $E_\ell(0)$ and $E_\ell(\pi/L)$. The B_ℓ are called spectral bands of $h_{\mathrm{per},L}$ and have pairwise disjoint interiors. E is an interior point of B_ℓ iff $E = E_\ell(k)$ for some $k \in (0,\pi/L)$. Because E_ℓ is monotone such a k is unique and we shall denote it $k(E)$. On each band B_ℓ, the function $k(E)$ is thus a strictly monotone function whose image is $(0,\pi/L)$.

The characteristic polynomial of $H(k,m)$ satisfies

$$\det(H(k,m)-z) = \mathrm{tr}(T(L,z)) - 2\cos(kL).$$

As a consequence, $\mathrm{sp}(h_{\mathrm{per},L}) = \{E : |\mathrm{tr}(T(L,E))| \leq 2\}$ and, for any $E \in \mathrm{sp}(h_{\mathrm{per},L})$, $k(E)$ is determined by the identity

$$\mathrm{tr}(T(L,E)) = 2\cos(k(E)L).$$

Since $\det(T(L,E)) = 1$, one infers that for $E \in \mathrm{sp}(h_{\mathrm{per},L})$ the eigenvalues of $T(L,E)$ actually are $\mathrm{e}^{\pm \mathrm{i}k(E)L}$, i.e., $\theta(L,E) = \pm k(E)L$. The proof of Lemma 2.3 relies of the following general estimate.

Proposition 2.6 *For any $\ell = 1,\dots,L$ and $k \in \left(0, \frac{\pi}{L}\right)$ one has*

$$|E'_\ell(k)| \leq 2.$$

Although not explicitly stated, this result already appears in [BJLP2] (in the proof of Proposition 5.2). For the convenience of the reader we give its proof.

Proof. For any k and m the vector $\vec{u}_\ell(k,m) = (u_\ell(k,m+1),\dots,u_\ell(k,m+L))^T$ is a normalized eigenvector of $H(k,m)$ for $E_\ell(k)$. The Feynman-Hellmann formula gives

$$\begin{aligned} E'_\ell(k) &= \left\langle \vec{u}_\ell(k,m), \frac{\mathrm{d}H(k,m)}{\mathrm{d}k}\vec{u}_\ell(k,m)\right\rangle \\ &= \mathrm{i}L\left(\overline{u_\ell(k,m+1)}\mathrm{e}^{-\mathrm{i}kL}u_\ell(k,m+L) - \overline{u_\ell(k,m+L)}\mathrm{e}^{\mathrm{i}kL}u_\ell(k,m+1)\right), \end{aligned}$$

and the relation (2.4) yields

$$E'_\ell(k) = 2L\,\mathrm{Im}\left(\overline{u_\ell(k,m)}u_\ell(k,m+1)\right),$$

for all m. Summing over $m = 1,\dots,L$, we can write

$$E'_\ell(k) = \sum_{m=1}^{L} 2\,\mathrm{Im}\left(\overline{u_\ell(k,m)}u_\ell(k,m+1)\right).$$

The normalization of u_ℓ yields

$$|E'_\ell(k)| \leq \sum_{m=1}^{L}\left(|u_\ell(k,m)|^2 + |u_\ell(k,m+1)|^2\right) = \|\vec{u}_\ell(k,0)\|^2 + \|\vec{u}_\ell(k,1)\|^2 = 2.$$

□

Proof of Lemma 2.3. Fix $\epsilon > 0$. Since $\theta(L,E) = \pm k(E)L$ is a monotone function in each spectral band B_ℓ and varies between 0 and π, $|\sin(\theta(L,E))| \leq \epsilon$ can only hold near the band edges ($\sin(\theta(L,E))$ vanishes precisely at these edges). From Proposition 2.6 we get that for any $E \in \mathrm{sp}(h_{\mathrm{per},L})$

$$|\theta'(L,E)| \geq \frac{L}{2}. \tag{2.6}$$

Using $\sin(\alpha) \geq \frac{2\alpha}{\pi}$ for $0 \leq \alpha \leq \frac{\pi}{2}$ or $\sin(\alpha) \geq 2 - \frac{2\alpha}{\pi}$ for $\frac{\pi}{2} \leq \alpha \leq \pi$ one has, for any band B_ℓ,

$$|\{E \in B_\ell \,:\, |\sin(\theta(L,E))| \leq \epsilon\}| \leq \left|\left\{E \in B_\ell \,:\, |\theta(L,E)| \leq \frac{\epsilon\pi}{2}\right\}\right| + \left|\left\{E \in B_\ell \,:\, |\pi - \theta(L,E)| \leq \frac{\epsilon\pi}{2}\right\}\right|,$$

which together with (2.6) gives

$$|\{E \in B_\ell \,:\, |\sin(\theta(L,E))| \leq \epsilon\}| \leq \frac{2\epsilon\pi}{L}.$$

Summing these inequalities over the L bands proves the lemma. □

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