



Quantum Ergodicity for Periodic Graphs

Theo McKenzie^{1,4} , Mostafa Sabri^{2,3}

¹ Harvard University, Cambridge, MA, USA. E-mail: theom@stanford.edu

² Cairo University, Giza, Egypt

³ New York University Abu Dhabi, Abu Dhabi, UAE. E-mail: mostafa.sabri@nyu.edu

⁴ Stanford University, Stanford, CA, USA

Received: 3 December 2022 / Accepted: 2 August 2023

Published online: 19 September 2023 – © The Author(s), under exclusive licence to Springer-Verlag GmbH Germany, part of Springer Nature 2023

Abstract: This article shows that for a large class of discrete periodic Schrödinger operators, most wavefunctions resemble Bloch states. More precisely, we prove quantum ergodicity for a family of periodic Schrödinger operators H on periodic graphs. This means that most eigenfunctions of H on large finite periodic graphs are equidistributed in some sense, hence delocalized. Our results cover the adjacency matrix on $\mathbb{Z}^d$, the triangular lattice, the honeycomb lattice, Cartesian products, and periodic Schrödinger operators on $\mathbb{Z}^d$. The theorem applies more generally to any periodic Schrödinger operator satisfying an assumption on the Floquet eigenvalues.

1. Introduction

We consider a sequence of finite graphs Γ_N that converges (in the sense of Benjamini-Schramm) to some infinite graph Γ . If we take the Schrödinger operator $H_N = \mathcal{A}_N + \mathcal{Q}_N$ on $\ell^2(\Gamma_N)$, then quantum ergodicity is a *spatial delocalization* criterion stating that, in a weak sense, most eigenvectors of H_N are equidistributed on the graph Γ_N .

The terminology comes from [10, 20, 24], where the ergodicity of the geodesic flow on a compact manifold M of unit volume (meaning the classical particle’s free motion covers the manifold uniformly) is shown to imply a quantum counterpart of ergodicity, namely, the Laplacian wavefunctions ψ_λ are equally likely to be anywhere on M (more precisely $|\psi_\lambda(x)|^2 \, d\text{Vol}(x)$ approaches the uniform measure $d\text{Vol}(x)$, when λ gets large). In that setting, quantum ergodicity is regarded as a quantum chaos phenomenon. In the large graph limit however, quantum ergodicity should be regarded instead as providing rich information on the spectral structure of the limiting operator H_Γ on the infinite graph. As such, it is important to control *all* eigenbases of the approximating operators H_N , or at least *generic* eigenbases. In fact, periodic operators always have “one” delocalized basis, namely Bloch states, but this occurs even in scenarios of strong localization for H_Γ .

T. McKenzie: Supported by NSF GRFP Grant DGE-1752814 and NSF Grant DMS-2212881.

Quantum ergodicity for large regular graphs that are spectral expanders with few cycles was first proved in [3], for the adjacency matrix $H_N = \mathcal{A}_N$. In this case the limiting graph Γ is the regular tree. Further results established that this is true in the more general setting where the limiting graph is an infinite tree which is not necessarily regular and $H_N = \mathcal{A}_N + Q_N$, assuming H_Γ has absolutely continuous spectrum [4]. This includes regimes of the Anderson model [5], as well as “periodic trees with periodic potentials,” more precisely universal covers of finite graphs [6].

Note that all of these results require the Benjamini-Schramm limit to be a tree. Proofs of quantum ergodicity, such as [3, 8] and the four proofs in [1], fundamentally use the orthogonality of different powers of the non-backtracking walk or a similar operator on these trees, and the contribution of cycles is treated as an error term that can be shown to be negligible. This tree condition is also a requirement for the quantum ergodicity result in quantum graphs [2].

Along with this line of work, the first author of the present paper gave examples showing that quantum ergodicity does not necessarily hold if one only requires the graphs to be expanders, i.e. if the requirement of being tree-like is removed [16]. This is still the case if we have the requirement that the Benjamini Schramm limit H_Γ has absolutely continuous spectrum. Nevertheless, it remained open whether more specific families of graphs satisfy quantum ergodicity.

In this paper we show that quantum ergodicity is in fact satisfied for a large family of non-tree graphs Γ , namely graphs which are periodic with respect to a basis of $\mathbb{Z}^d$. The simplest example is the adjacency matrix on $\mathbb{Z}^d$, but the results apply to large classes of Schrödinger operators with periodic potentials on various lattices. These graphs do not satisfy the expansion or tree properties of previous proofs. Therefore we need new, different techniques to solve the problem in this case. To our knowledge, Theorems 1.1 and 1.2 are the first positive results establishing quantum ergodicity for a general family of graphs Γ having cycles.

By virtue of their homogeneity, it is quite intuitive to expect delocalization on periodic lattices. Indeed, the spectrum is generally absolutely continuous, though flat bands (infinitely degenerate eigenvalues) can appear [15]. The dynamics are also ballistic [7], meaning the waves spread at maximum speed with time. Here we show that from a spatial point of view, the behavior is quite rich:

- There is a simple family of periodic graphs which is quantum ergodic, i.e. the probability measure $\sum_{x \in \Gamma_N} |\psi_u^{(N)}(x)|^2 \delta_x$ is close to the uniform measure $\frac{1}{|\Gamma_N|} \sum_{x \in \Gamma_N} \delta_x$, for most $u \in [N]$. See Theorem 1.1. Here $(\psi_1^{(N)}, \dots, \psi_N^{(N)})$ is any orthonormal eigenbasis.
- In another class of periodic Schrödinger operators, we have partial quantum ergodicity, in the sense that we no longer have $|\psi_u^{(N)}(x)|^2 \approx \frac{1}{|\Gamma_N|}$, but the sum of $|\psi_u^{(N)}(x)|^2$ over any periodic block $V_f + n_a$ is approximately the same (Theorem 1.2, Proposition 1.4). This means that $\psi_u^{(N)}$ does not favor any particular block, but the mass of $\psi_u^{(N)}$ may not be uniform within the block.
- In other classes of periodic graphs, quantum ergodicity fails completely (Sects. 3.3 and 3.4).

Examples of these three types are $\mathcal{A}$ on $\mathbb{Z}^d$, on an infinite cylinder (Fig. 6), and on the graph in Fig. 4, respectively.

If we focus attention to $\mathbb{Z}^d$, the adjacency matrix on a sub-cube Γ_N of sidelength N with periodic boundary conditions has the eigenbasis $e_r^{(N)}(k) = \frac{1}{N^{d/2}} e^{2\pi i k \cdot r/N}$. We

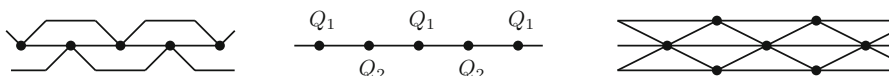


Fig. 1. 1d crystals. Left: $Q = 0$, $V_f = \{(0, 0)\}$, $v = 1$, $\mathbf{a}_1 = (1, 0)$. Center: $Q = \{Q_1, Q_2\}$, $V_f = \{0, 1\}$, $v = 2$, $\mathbf{a}_1 = 2\mathbf{e}_1 = 2$. Right: $Q = 0$, $V_f = \{(0, 0), (0.5, 1), (0.5, -1)\}$, $v = 3$, $\mathbf{a}_1 = (1, 0)$

note that $|e_r^{(N)}(k)|^2 = \frac{1}{N^d}$ is perfectly uniformly distributed on Γ_N . Similarly, for a periodic Schrödinger operator H on a periodic lattice, the Bloch theorem ensures that for any $\lambda \in \sigma(H_N)$, we can find an eigenfunction Ψ_λ such that $|\Psi_\lambda(x)|^2$ is a periodic function (see Sect. 5.2 for a discussion and a proof of this result in our context). In this paper, we study whether such eigenvector delocalization is satisfied for any eigenbasis of the Schrödinger operator. The question is highly nontrivial as the multiplicity $m_{\lambda_k^{(N)}}$ of eigenvalues can grow with N . For example, for $\Gamma = \mathbb{Z}^2$ and N even, the multiplicity of $\lambda_k^{(N)} = 0$ is the set of all (k_1, k_2) such that $2 \cos \frac{2\pi k_1}{N} + 2 \cos \frac{2\pi k_2}{N} = 0$. This contains all $k_2 = \frac{N}{2} \pm k_1$, where $k_1 = 0, \dots, \frac{N}{2} - 1$ is arbitrary. So here, $m_{\lambda_k^{(N)}} \gtrsim N$.

1.1. Main results. Let Γ be a connected, locally finite graph in some Euclidean space. We assume Γ is invariant under translations of some linearly independent vectors $\mathbf{a}_1, \dots, \mathbf{a}_d$.

If we let

$$V_f = \{v_1, \dots, v_v\}$$

be a fundamental cell containing v vertices, then the graph Γ consists of periodic V_f blocks of size v . More precisely, if for $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ we denote $x_{\mathbf{a}} = \sum_{i=1}^d x_i \mathbf{a}_i$, then

$$V(\Gamma) = \mathbb{Z}_{\mathbf{a}}^d + V_f, \quad (1.1)$$

where $\mathbb{Z}_{\mathbf{a}}^d = \{n_{\mathbf{a}} : n \in \mathbb{Z}^d\}$. By “periodic blocks” we will mean sets of the form $V_f + n_{\mathbf{a}}$. Any $u \in V(\Gamma)$ takes the form $u = [u]_{\mathbf{a}} + \{u\}_{\mathbf{a}}$, where $[u]_{\mathbf{a}} \in \mathbb{Z}_{\mathbf{a}}^d$ and $\{u\}_{\mathbf{a}} \in V_f$ represent the integer and fractional parts of u , respectively.

In the case of the simple lattice $\Gamma = \mathbb{Z}^d$ we may take $\mathbf{a}_j = \mathbf{e}_j$ the standard basis and $V_f = \{0\}$. In general one can view (1.1) as expressing the vertex set $V(\Gamma)$ as v copies of the sub-lattices $\mathbb{Z}_{\mathbf{a}}^d$, shifted by vertices $v_n \in V_f$.

Having fixed V_f , we consider a Schrödinger operator $H = \mathcal{A} + Q$ on Γ , where $\mathcal{A}$ is the adjacency matrix and Q satisfies

$$Q(v_n + \mathbf{a}_i) = Q(v_n)$$

for $v_n \in V_f$ and $i = 1, \dots, d$. The potential Q is thus periodic with at most v values.

Let $\Gamma_N = \cup_{n \in \llbracket 0, N-1 \rrbracket^d} (V_f + n_{\mathbf{a}})$ and H_N be the Schrödinger operator defined analogously on Γ_N , considered with periodic boundary conditions: if $\psi \in \ell^2(\Gamma_N)$, then $\psi(v \pm N\mathbf{a}_j) := \psi(v)$. Our first result is the following.

Theorem 1.1 (Case $v = 1$). *Let $\psi_u^{(N)}$ be an orthonormal basis of $\ell^2(\Gamma_N)$ consisting of eigenvectors of H_N . Suppose the fundamental cell has only one vertex, $V_f = \{o\}$. Then for any observable $a = a_N : \Gamma_N \rightarrow \mathbb{C}$ such that $|a_N(v)| \leq 1$ for all v and N , we have*

$$\lim_{N \rightarrow \infty} \frac{1}{|\Gamma_N|} \sum_{u \in \Gamma_N} \left| \langle \psi_u^{(N)}, a \psi_u^{(N)} \rangle - \langle a \rangle \right|^2 = 0, \quad (1.2)$$

where $\langle \psi_u^{(N)}, a\psi_u^{(N)} \rangle = \sum_{v \in \Gamma_N} |\psi_u^{(N)}(v)|^2 a(v)$ and $\langle a \rangle = \frac{1}{|\Gamma_N|} \sum_{v \in \Gamma_N} a(v)$ is the uniform average.

This means that in a weak sense, we have $|\psi_u^{(N)}(v)|^2 \approx \frac{1}{|\Gamma_N|}$ when N is large enough. That is, the eigenvectors $\psi_u^{(N)}$ are uniformly distributed. This theorem applies to the adjacency matrix on $\mathbb{Z}^d$ and the triangular lattice, see Sect. 4.1 for more graphs.

This statement is generally false for higher v , quantum ergodicity can be completely violated for $v = 2$ without further assumptions, see Sect. 3.4.1. For general v , we make an assumption on the Floquet eigenvalues and relax the conclusion. Let $\mathbf{b}_1, \dots, \mathbf{b}_d$ be the dual basis, satisfying $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{i,j}$. We similarly denote $\theta_{\mathbf{b}} = \sum_{i=1}^d \theta_i \mathbf{b}_i$. Then we have:

Theorem 1.2 (General case). *Let $\psi_u^{(N)}$ be an orthonormal basis of $\ell^2(\Gamma_N)$ consisting of eigenvectors of H_N . Let $H(\theta_{\mathbf{b}})$ be the $v \times v$ matrix arising in the Floquet decomposition, with eigenvalues $E_1(\theta_{\mathbf{b}}), \dots, E_v(\theta_{\mathbf{b}})$. Suppose that for any $s, w \in \{1, \dots, v\}$, we have*

$$\lim_{N \rightarrow \infty} \sup_{\substack{m \in \mathbb{L}_N^d \\ m \neq 0}} \frac{\#\{r \in \mathbb{L}_N^d : E_s(\frac{r_{\mathbf{b}} + m_{\mathbf{b}}}{N}) - E_w(\frac{r_{\mathbf{b}}}{N}) = 0\}}{N^d} = 0, \quad (1.3)$$

where $\mathbb{L}_N = \{0, 1, \dots, N-1\}$. Then,

(i) *For any observable $a_N : \Gamma_N \rightarrow \mathbb{C}$ such that $|a_N(v)| \leq 1$ for all v and N , we have*

$$\lim_{N \rightarrow \infty} \frac{1}{|\Gamma_N|} \sum_{u \in \Gamma_N} \left| \langle \psi_u^{(N)}, a\psi_u^{(N)} \rangle - \langle \psi_u^{(N)}, \text{Op}_N(\bar{a})\psi_u^{(N)} \rangle \right|^2 = 0, \quad (1.4)$$

where $\text{Op}_N(\bar{a})$ is an explicit operator (see (2.12)).

If $a = a_N$ is real-valued, we have

$$\min_{v_q \in V_f} \langle a(\cdot + v_q) \rangle \leq \langle \psi_u^{(N)}, \text{Op}_N(\bar{a})\psi_u^{(N)} \rangle \leq \max_{v_q \in V_f} \langle a(\cdot + v_q) \rangle, \quad (1.5)$$

where $\langle a(\cdot + v_q) \rangle = \frac{1}{N^d} \sum_{k \in \mathbb{L}_N^d} a(k_{\mathbf{a}} + v_q)$.

(ii) *If a is locally constant, in the sense that it takes a constant value on each periodic block, $a(v_n + k_{\mathbf{a}}) = a(v_1 + k_{\mathbf{a}}) \forall n$, then*

$$\langle \psi_u^{(N)}, \text{Op}_N(\bar{a})\psi_u^{(N)} \rangle = \langle a \rangle := \frac{1}{|\Gamma_N|} \sum_{v \in \Gamma_N} a(v). \quad (1.6)$$

Specifically, this is true if $v = 1$.

Point (ii) holds more generally if $\langle a(\cdot + v_q) \rangle = \langle a(\cdot + v_1) \rangle \forall q$, i.e. the average of a over each sublattice $\mathbb{L}_N^d + v_q$ of Γ_N is the same.

This theorem applies, for example, to the adjacency matrix on the honeycomb lattice (Sect. 4.2) and to periodic Schrödinger operators on $\mathbb{Z}$ (Sect. 4.4). As we discuss later, it actually applies to periodic operators on $\mathbb{Z}^d$ for all d , this relies on a separate work.

Assumption (1.3) says in particular that the Floquet eigenvalues should not have a short period and should not “hesitate” while tracing the band, going back and forth too often at exactly the same speed. More precisely, for any nonzero α and any s , the set

$$A_{\alpha,s} := \{\theta \in [0, 1)^d : E_s(\theta_{\mathbf{b}} + \alpha_{\mathbf{b}}) = E_s(\theta_{\mathbf{b}})\} \quad (1.7)$$

should be of zero measure. For example, for $d = 1$, we should not have $E_s(\theta_b) = \cos 4\pi\theta$, as then for $\alpha = \frac{1}{2}$, we get $E_s(\theta_b + \alpha_b) = E_s(\theta_b)$ for all θ . Assumption (1.3) can only hold if there is no point spectrum: if a flat band exists, it corresponds to a constant E_s for some s , so $\{r \in \mathbb{L}_N^d : E_s(\frac{r_b + m_b}{N}) - E_s(\frac{r_b}{N}) = 0\} = \mathbb{L}_N^d$, violating (1.3).

In order to prove Theorem 1.2, we average the test function a by considering

$$\frac{1}{T} \int_0^T e^{itH_N} a e^{-itH_N} dt. \quad (1.8)$$

In [1], this is done for the treelike case by considering $\lim_{T \rightarrow \infty} \lim_N \rightarrow \infty$ of (1.8). However, local analysis of this limit becomes difficult in the case that there are many cycles. Instead, in our case, we take the time limit first, taking advantage of the periodicity of our operator. We show that in the limit $T \rightarrow \infty$, (1.8) converges to 0 outside of the subspace of phase space given on the left hand side of 1.3.

In an earlier version of the manuscript we left as an open problem whether assumption (1.3) is satisfied for Schrödinger operators on $\mathbb{Z}^d$ with a periodic potential. This has since been solved by Wencai Liu [23] using algebraic and analytic properties of Bloch varieties. See Sect. 5.3 for background and further criteria. In particular, [23] and Theorem 1.2 imply the following.

Corollary 1.3. *Schrödinger operators with periodic potentials on the triangular lattice and on $\mathbb{Z}^d$ are quantum ergodic for any d .*

Theorem 1.1 only applies to the adjacency matrix on regular graphs of even degree (as follows from the assumption $v = 1$, see Sect. 3.1). The following proposition uses Theorem 1.2 to provide concrete applications to non-regular graphs endowed with a periodic potential.

Proposition 1.4 (Cartesian products). *Suppose that Γ is a $\mathbb{Z}_\alpha^d$ -periodic graph with $v = 1$, and let G_F be any finite graph, endowed with some potential Q . Then the Cartesian product $\Gamma \square G_F$ is a periodic graph with fundamental cell $V_f = G_F$ and periodic potential Q copied across the G_F layers. Moreover, assumption (1.3) is satisfied, so (1.4) holds true.*

If for $\Gamma \square G_F$, the orthonormal basis is of the form $\psi_{n,j} = \phi_n \otimes w_j$, where (ϕ_n) is an orthonormal eigenbasis for H_{Γ_N} , and (w_j) is an orthonormal eigenbasis for H_{G_F} , then

$$\langle \psi_{n,j}, \text{Op}_N(\bar{a}) \psi_{n,j} \rangle = \sum_{v_q \in G_F} \langle a(\cdot + v_q) \rangle |w_j(v_q)|^2, \quad (1.9)$$

where $\langle a(\cdot + v_q) \rangle = \frac{1}{N^d} \sum_{k \in \mathbb{L}_N^d} a(k_\alpha + v_q)$.

Theorem 1.2(ii) shows that for most u , $|\psi_u^{(N)}|^2$ behaves as a periodic function across the blocks, but the distribution of its mass within each block may be non-uniform. Loosely speaking, one has the picture that most eigenfunctions behave like Bloch functions. More precisely, for most u , $\sum_{v_q \in V_f} |\psi_u^{(N)}(k_\alpha + v_q)|^2 \approx \frac{1}{N^d}$, for any k .

On the other hand, (1.9) shows that the mass distribution within each block is not universal and can depend on the eigenbasis in general (see Sect. 4.5 for a concrete example). Such basis-dependence never appeared in the tree models of [1, 4]. There, the theorems

established that $|\psi_u^{(N)}(v)|^2 \approx \frac{\text{Im } \tilde{g}_N^{\lambda_j}(\bar{v}, \bar{v})}{\sum_{v \in \Gamma_N} \text{Im } \tilde{g}_N^{\lambda_j}(\bar{v}, \bar{v})}$, where $\tilde{g}_N^z$ is the Green's function of the

universal cover of Γ_N . In particular, it is certainly independent of $\psi_{\lambda_j}^{(N)}$. Here we have a different phenomenon which can be regarded as partial quantum ergodicity.

Such partial quantum ergodicity can be violated even in dimension one :

Proposition 1.5. *There exist $\mathbb{Z}$ -periodic graphs which violate (1.4).*

We give examples in Sects. 3.3 and 3.4. These graphs have point spectrum and (1.3) is not satisfied. It is natural to ask if assumption (1.3) can be dropped if we simply assume that H_Γ has pure ac spectrum. We construct a counterexample in Sect. 3.4:

Proposition 1.6. *There exist periodic graphs with purely absolutely continuous spectrum which are not quantum ergodic.*

Remark 1.7. Instead of considering the whole spectrum in Theorem 1.2, we can instead suppose that (1.3) is satisfied in some interval I , then the conclusion (1.4) now holds if we average over $\lambda_u^{(N)} \in I$ instead of $u \in \Gamma_N$. This is similar to what is done in [4] for the high girth regime. In other words, if part of the spectrum is well-behaved, then the corresponding eigenfunctions are quantum ergodic. This is helpful for example for graphs having flat bands but satisfying (1.3) away from the degenerate eigenvalue. Then our theorem applies to these regions. For the technical details, see Remark 2.5.

This remark applies in particular to Schrödinger operators with periodic potentials on the Lieb lattice and decorated lattice, recently studied in [12]. These models have flat bands in general. The characteristic polynomial of the Floquet matrix thus takes the form $p(z; \lambda) = s(\lambda)q(z; \lambda)$, where $z_j = e^{2\pi i \theta_j}$, $s(\lambda) = \prod_{j=1}^m (\lambda - \lambda_j)$ and λ_j are all the flat bands. The results of [12] show that for each fixed λ , q is irreducible as a Laurent polynomial in z , except for finitely many λ . The argument in [22, Th. 2.4] then implies that, after removing the flat bands, the Bloch variety is irreducible. This allows to verify the assumptions of [23] to conclude that quantum ergodicity holds in any spectral interval avoiding the flat bands.

Remark 1.8 (Convergence rate). The proof shows that the variance on the LHS of (1.4) is essentially bounded from above by the fraction in (1.3). For $v = 1$, we bound the latter by $\frac{C}{N}$ in Sect. 3.1, so the speed of convergence is at least $\frac{1}{N}$ in Theorem 1.1, which is significantly faster than the logarithmic rate $\frac{1}{\log N}$ of the tree case [1, 3, 4].

Remark 1.9. The fact that a perfectly homogeneous graph like the one in Fig. 4 supports localized eigenfunctions is quite counterintuitive. This topic is further analyzed in [18]. Based on physics literature, it is expected that such “flat bands” disappear after adding a generic periodic potential/edge weight and the spectrum becomes purely absolutely continuous. In this spirit, we show that the graph in Fig. 4 becomes quantum ergodic once we add any potential (Q_1) with $Q_1 \neq Q_2$, copied across the layers.

1.2. Stronger statements. The following two paragraphs illustrate that one cannot obtain much stronger results than the ones we provide.

1.2.1. Quantum unique ergodicity In [3], it was suggested to check whether

$$\lim_{N \rightarrow \infty} \sup_{1 \leq j \leq |\Gamma_N|} |\langle \psi_j^{(N)}, a_N \psi_j^{(N)} \rangle - \langle a_N \rangle| = 0 \quad (1.10)$$

as an indication of *quantum unique ergodicity (QUE)*. This would mean that we can avoid the Cesàro average in (1.2). This criterion is too strong however, at least in our context, in fact it is already violated for the adjacency matrix on $\mathbb{Z}^d$. See Sect. 5.1.

1.2.2. Eigenvector correlators In [1], instead of taking observables $a_N(n)$ which are functions on Γ_N , a quantum ergodicity theorem was proved more generally for band matrix observables, that is, $K_N(n, m)$, where $K_N(n, m) = 0$ if $d(n, m) > R$. It was shown (in Cesàro sense) that $\langle \psi_j^{(N)}, K_N \psi_j^{(N)} \rangle \approx \langle K_N \rangle_{\lambda_j}$, where $\langle K_N \rangle_{\lambda} = \frac{1}{|\Gamma_N|} \sum_{n,m} K_N(n, m) \Phi_{\lambda}(d(x, y))$ and Φ_{λ} is the spherical function of the tree; it has an explicit form in terms of Chebyshev polynomials. Since $\langle \psi_j^{(N)}, K_N \psi_j^{(N)} \rangle = \sum_{n,m} K_N(n, m) \overline{\psi_j^{(N)}(n)} \psi_j^{(N)}(m)$, this shows that the eigenfunction correlator $\overline{\psi_j^{(N)}(n)} \psi_j^{(N)}(m) \approx \frac{1}{|\Gamma_N|} \Phi_{\lambda}(d(n, m))$, a universal quantity; this generalizes the statement that $|\psi_j^{(N)}(n)|^2 \approx \frac{1}{|\Gamma_N|}$.

This stronger statement fails in our case; $\overline{\psi_j^{(N)}(n)} \psi_j^{(N)}(m)$ is not universal, it depends on the basis, even for $\mathcal{A}_{\mathbb{Z}^d}$. See Sect. 5.1.

Still, our proof can be generalized to matrix observables K_N . If $\nu = 1$, we show that

$$\frac{1}{N^d} \sum_{j \in \mathbb{L}_N^d} |\langle \psi_j^{(N)}, K \psi_j^{(N)} \rangle - \langle K \rangle_{\psi_j^{(N)}}|^2 \rightarrow 0,$$

where $\langle K \rangle_{\psi} = \frac{1}{N^d} \sum_{n \in \mathbb{L}_N^d} \sum_{|\tau| \leq R} K(n_a, n_a + \tau_a) \langle \psi, \psi(\cdot + \tau_a) \rangle$, and R is the width of the band matrix. So in a weak sense, $\overline{\psi_j^{(N)}(n_a)} \psi_j^{(N)}(n_a + \tau_a) \approx \frac{1}{N^d} \langle \psi_j^{(N)}, \psi_j^{(N)}(\cdot + \tau_a) \rangle$ for any $n \in \mathbb{Z}^d$.

1.3. Structure of the paper. We prove the general Theorem 1.2 in Sect. 2. In Sect. 3.1, we prove that (1.3) is satisfied for $\nu = 1$, thereby proving Theorem 1.1. We then discuss Cartesian products in Sect. 3.2 and prove Proposition 1.4. In Sects. 3.3 and 3.4, we discuss graph decorations, tensor products and strong products of graphs, giving examples of graphs violating quantum ergodicity. In Sect. 4, we give more specific examples satisfying quantum ergodicity. Finally in Sect. 5, we discuss complementary results such as quantum unique ergodicity, eigenvector correlators, the Bloch theorem, as well as further criteria for checking (1.3) based on Bloch varieties considerations.

2. Proof of the General Criterion

Here we prove Theorem 1.2. The argument is very different than the proof for trees [1, 3, 4]. We will use some ideas from [14] where ergodic averages for the continuous Laplacian $-\Delta$ on the torus $\mathbb{R}^d / \mathbb{Z}^d$ are studied in the high frequency limit.

Throughout, $N \gg 1$ is larger than the maximum adjacency range.

2.1. Step 1. Since $e^{-itH_N} \psi_u^{(N)} = e^{-it\lambda_u^{(N)}} \psi_u^{(N)}$, $\langle \psi_u^{(N)}, e^{itH_N} a e^{-itH_N} \psi_u^{(N)} \rangle = \langle \psi_u^{(N)}, a \psi_u^{(N)} \rangle$ and we have

$$\langle \psi_u^{(N)}, a \psi_u^{(N)} \rangle = \left\langle \psi_u^{(N)}, \frac{1}{T} \int_0^T e^{itH_N} a e^{-itH_N} dt \psi_u^{(N)} \right\rangle. \quad (2.1)$$

In the spirit of Egorov's theorem, we show the sandwich $e^{itH_N} a e^{-itH_N}$ can be expressed as a kind of phase space operator.

Let $\mathbb{L}_N^d = \llbracket 0, N-1 \rrbracket^d$ and define $U : \ell^2(\Gamma_N) \rightarrow \oplus_{j \in \mathbb{L}_N^d} \ell^2(V_f)$ by

$$(U\psi)_j(v_n) = \frac{1}{N^{d/2}} \sum_{k \in \mathbb{L}_N^d} e^{-\frac{ij_b}{N} \cdot k_a} \psi(v_n + k_a). \quad (2.2)$$

Lemma 2.1. *The operator U is unitary and*

$$U H_N U^{-1} = \oplus_{j \in \mathbb{L}_N^d} H\left(\frac{j_b}{N}\right), \quad (2.3)$$

where $H(\theta_b)$ acts on $\ell^2(V_f)$ by

$$H(\theta_b)f(v_n) = \sum_{u \sim v_n} e^{i\theta_b \cdot \lfloor u \rfloor_a} f(\{u\}_a) + Q(v_n)f(v_n). \quad (2.4)$$

The sum is over the vertices u connected to v_n in the whole graph Γ (not just V_f) and we have $u = \lfloor u \rfloor_a + \{u\}_a$, with $\lfloor u \rfloor_a \in \mathbb{Z}_a^d$ and $\{u\}_a \in V_f$, cf. (1.1).

Proof. We have $\|U\psi\|^2 = \|\psi\|^2$ (expand and use $\sum_{j \in \mathbb{L}_N^d} e^{\frac{2\pi i j \cdot (k' - k)}{N}} = N^d \delta_{k, k'}$ and $k_a \cdot j_b = 2\pi k \cdot j$). Next, $U^{-1}((g_j)_{j \in \mathbb{L}_N^d}) = \psi$, where $\psi(k_a + v_n) = \frac{1}{N^{d/2}} \sum_{r \in \mathbb{L}_N^d} g_r(v_n) e^{ik_a \cdot \frac{r_b}{N}}$. In fact, $(\frac{1}{N^{d/2}} e^{-ik_a \cdot j_b/N})_{j \in \mathbb{L}_N^d}$ is an orthonormal basis of $\ell^2(\mathbb{L}_N^d)$. So for such ψ we have $(U\psi)_j(v_n) = \frac{1}{N^d} \sum_{k, r \in \mathbb{L}_N^d} e^{-\frac{ij_b}{N} \cdot k_a} g_r(v_n) e^{ik_a \cdot \frac{r_b}{N}} = \sum_{k \in \mathbb{L}_N^d} \langle \frac{1}{N^{d/2}} e^{-\frac{2\pi i k}{N} \cdot \bullet}, g_\bullet(v_n) \rangle_{\ell^2(\mathbb{L}_N^d)} (\frac{1}{N^{d/2}} e^{-\frac{ij_b}{N} \cdot k_a}) = g_j(v_n)$. This proves unitarity.

Next, for $\psi \in D(H_N)$, $U H_N \psi = U A_N \psi + U Q \psi$, with $U Q \psi = Q U \psi$ since $(Q\psi)(v_n + k_a) = Q(v_n)\psi(v_n + k_a)$ by definition of the periodic potential. On the other hand,

$$\begin{aligned} (U A_N \psi)_j(v_n) &= \frac{1}{N^{d/2}} \sum_{k \in \mathbb{L}_N^d} e^{-\frac{ij_b}{N} \cdot k_a} \sum_{w \sim v_n + k_a} \psi(w) \\ &= \frac{1}{N^{d/2}} \sum_{k \in \mathbb{L}_N^d} e^{-\frac{ij_b}{N} \cdot k_a} \sum_{u \sim v_n} \psi(u + k_a) \\ &= \sum_{u \sim v_n} e^{\frac{ij_b \cdot \lfloor u \rfloor_a}{N}} \cdot \frac{1}{N^{d/2}} \sum_{k \in \mathbb{L}_N^d} e^{-\frac{ij_b \cdot (k_a + \lfloor u \rfloor_a)}{N}} \psi(k_a + \lfloor u \rfloor_a + \{u\}_a). \end{aligned}$$

We claim the inner sum is simply $(U\psi)_j(\{u\}_a)$. In fact, for fixed u , denote $r = \lfloor u \rfloor \in \mathbb{Z}^d$. Then the second sum has the form $\sum_{k \in \mathbb{L}_N^d} f(k+r)$. We partition $\mathbb{L}_N^d$ into $\leq 2^d$ rectangles A_i such that $A_i + r + \ell^{(N,i)} = B_i$, $B_i \subset \mathbb{L}_N^d$ and $\ell_j^{(N,i)} \in \{0, \pm N\}$. Roughly speaking, this says that $A_i + r = B_i \bmod N\mathbb{Z}^d$. For example, if $r = (3, -2, 0)$, we may take $A_1 = \llbracket 0, N-4 \rrbracket \times \llbracket 2, N-1 \rrbracket \times \llbracket 0, N-1 \rrbracket$, $A_2 = \llbracket N-3, N-1 \rrbracket \times \llbracket 2, N-1 \rrbracket \times \llbracket 0, N-1 \rrbracket$, $A_3 = \llbracket 0, N-4 \rrbracket \times \llbracket 0, 1 \rrbracket \times \llbracket 0, N-1 \rrbracket$, $A_4 = \llbracket N-3, N-1 \rrbracket \times \llbracket 0, 1 \rrbracket \times \llbracket 0, N-1 \rrbracket$ and $\ell^{(N,1)} = 0$, $\ell^{(N,2)} = (-N, 0, 0)$, $\ell^{(N,3)} = (0, N, 0)$, $\ell^{(N,4)} = (-N, N, 0)$. Clearly (B_i) partitions $\mathbb{L}_N^d$.

Since ψ is chosen to satisfy periodic conditions, $\sum_{k \in A_i} f(k+r) = \sum_{k \in B_i} f(k)$ for each i , hence $\sum_{k \in \mathbb{L}_N^d} f(k+r) = \sum_{k \in \mathbb{L}_N^d} f(k)$. As r is arbitrary, we have shown that $(U A_N \psi)_j(v_n) = \sum_{u \sim v_n} e^{\frac{ij_b \cdot \{u\} a}{N}} (U \psi)_j(\{u\}_a)$. Thus, $(U H_N \psi)_j = H(\frac{j_b}{N})(U \psi)_j$. This completes the proof. $\square$

Note that $H(\theta_b)$ is a $v \times v$ matrix with orthonormal eigenbasis $f_s^{\theta_b}$ and eigenvalues $E_s(\theta_b)$, $s = 1 \dots, v$. Let $P_s(\theta_b) = \langle f_s^{\theta_b}, \cdot \rangle f_s^{\theta_b}$ be the corresponding eigenprojections.

Let $e_r^{(N)}(k) := \frac{1}{N^{d/2}} e^{2\pi i k \cdot r / N}$. Given $F \in \ell^2(\mathbb{L}_N^{2d} \times V_f^2)$, we now let

$$\text{Op}_N(F)\psi(k_a + v_n) := \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v (U\psi)_r(v_\ell) F(k, r; v_n, v_\ell) e_r^{(N)}(k), \quad (2.5)$$

The “quantization” (2.5) is such that if $F(k, r; v_n, v_\ell) = F(k_a + v_n) \delta_{v_n, v_\ell}$, then $\text{Op}_N(F)\psi = F\psi$. The presence of δ_{v_n, v_ℓ} may seem unusual; indeed it would not be here if we were dealing with just the adjacency matrix on $\mathbb{Z}^d$. The presence of δ_{v_n, v_ℓ} is related to the fact that the Floquet transform (2.2) is only a partial transform in the sense that it keeps v_n fixed.

Define

$$\begin{aligned} F_T(k, r; v_n, v_\ell) &:= \sum_{m \in \mathbb{L}_N^d} \sum_{q, s, w=1}^v \frac{1}{T} \int_0^T e^{it[E_s(\frac{r_b + m_b}{N}) - E_w(\frac{r_b}{N})]} dt \\ &\times P_s\left(\frac{r_b + m_b}{N}\right)(v_n, v_q) a_m^{(N)}(v_q) P_w\left(\frac{r_b}{N}\right)(v_q, v_\ell) e_m^{(N)}(k), \end{aligned} \quad (2.6)$$

where $a_m^{(N)}(v_q) := \langle \frac{e^{\frac{im_b \cdot \bullet a}{N}}}{N^{d/2}}, a(v_q + \bullet a) \rangle_{\ell^2(\mathbb{L}_N^d)}$ are the Fourier coefficients of a .

Lemma 2.2. *We have*

$$\frac{1}{T} \int_0^T e^{itH_N} a e^{-itH_N} dt = \text{Op}_N(F_T).$$

Although the definitions are somewhat long, the meaning is straightforward: this sandwich can be expressed in phase space. F_T “smooths” the function over different eigenvalues of the phase space operator, and Op_N gives the averaging under which this occurs.

Proof. First, we expand ψ in order to relate it to the form of $\text{Op}_N(F_T)$.

$$\psi(k_a + v_n) = (U^{-1} U \psi)(k_a + v_n) = \sum_{r \in \mathbb{L}_N^d} (U \psi)_r(v_n) e_r^{(N)}(k).$$

Recalling (2.3), we obtain

$$(H_N \psi)(k_a + v_n) = \sum_{r \in \mathbb{L}_N^d} \left[H\left(\frac{r_b}{N}\right) (U \psi)_r \right](v_n) e_r^{(N)}(k).$$

Knowing this, we can now examine the operator $e^{itH_N} a e^{-itH_N}$ and expand over the various (v_n, v_q) . This yields

$$(e^{itH_N} a e^{-itH_N} \psi)(k_a + v_n) = \sum_{r \in \mathbb{L}_N^d} \sum_{q=1}^v e^{itH(\frac{r_b}{N})}(v_n, v_q) (U a e^{-itH_N} \psi)_r(v_q) e_r^{(N)}(k).$$

Expanding $a(v_q + n_a) = \frac{1}{N^{d/2}} \sum_{m \in \mathbb{L}_N^d} a_m^{(N)}(v_q) e^{\frac{im_b \cdot n_a}{N}}$, we have

$$\begin{aligned} (U a e^{-itH_N} \psi)_r(v_q) &= \frac{1}{N^d} \sum_{n \in \mathbb{L}_N^d} \sum_{m \in \mathbb{L}_N^d} e^{\frac{-ir_b \cdot n_a}{N}} a_m^{(N)}(v_q) e^{\frac{im_b \cdot n_a}{N}} (e^{-itH_N} \psi)(v_q + n_a) \\ &= \frac{1}{N^{d/2}} \sum_{m \in \mathbb{L}_N^d} a_m^{(N)}(v_q) (U e^{-itH_N} \psi)_{r-m}(v_q). \end{aligned}$$

Here, $r - m$ is understood in $(\mathbb{Z}/N\mathbb{Z})^d$. More precisely, if $r_i - m_i$ is negative for some i , it is replaced by $N + r_i - m_i$ (this uses $e^{-2\pi i j \cdot k} = 1$). The last term expands as

$$\begin{aligned} (U e^{-itH_N} \psi)_{r-m}(v_q) &= [e^{-itH(\frac{r_b - m_b}{N})} (U \psi)_{r-m}](v_q) \\ &= \sum_{\ell=1}^v e^{-itH(\frac{r_b - m_b}{N})}(v_q, v_\ell) (U \psi)_{r-m}(v_\ell). \end{aligned}$$

Moreover, we can write $e^{\pm itH(\theta_b)} = \sum_{s=1}^v e^{\pm itE_s(\theta_b)} P_s(\theta_b)$ through its eigendecomposition. Applying this gives us

$$\begin{aligned} (e^{itH_N} a e^{-itH_N} \psi)(k_a + v_n) &= \frac{1}{N^{d/2}} \sum_{r, m \in \mathbb{L}_N^d} \sum_{q, \ell, s, w=1}^v e^{itE_s(\frac{r_b}{N})} P_s\left(\frac{r_b}{N}\right)(v_n, v_q) \\ &\quad \times a_m^{(N)}(v_q) e^{-itE_w(\frac{r_b - m_b}{N})} \\ &\quad P_w\left(\frac{r_b - m_b}{N}\right)(v_q, v_\ell) (U \psi)_{r-m}(v_\ell) e_r^{(N)}(k) \\ &= \frac{1}{N^{d/2}} \sum_{r, m \in \mathbb{L}_N^d} \sum_{q, \ell, s, w=1}^v e^{it[E_s(\frac{r_b + m_b}{N}) - E_w(\frac{r_b}{N})]} \\ &\quad P_s\left(\frac{r_b + m_b}{N}\right)(v_n, v_q) \\ &\quad \times a_m^{(N)}(v_q) P_w\left(\frac{r_b}{N}\right)(v_q, v_\ell) (U \psi)_r(v_\ell) e_{r+m}^{(N)}(k) \end{aligned}$$

with $r + m$ again understood in $(\mathbb{Z}/N\mathbb{Z})^d$. Since $\frac{1}{N^{d/2}} e_r^{(N)}(k) = e_r^{(N)}(k) e_m^{(N)}(k)$, we get

$$\frac{1}{T} \int_0^T e^{itH} a e^{-itH} dt \psi(k_a + v_n) = \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v (U \psi)_r(v_\ell) F_T(k, r; v_n, v_\ell) e_r^{(N)}(k),$$

with F_T in (2.6). Therefore, according to (2.5), $\frac{1}{T} \int_0^T e^{itH_N} a e^{-itH_N} dt = \text{Op}_N(F_T)$. $\square$

2.2. *Step 2.* Now we observe that if $E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N}) \neq 0$ for some $m \in \mathbb{L}_N^d$ and $s, w \in \{1, \dots, v\}$, then the corresponding term in F_T vanishes as $T \rightarrow \infty$. So define

$$b(k, r, v_n, v_\ell) = \sum_{m \in \mathbb{L}_N^d} \sum_{q, s, w=1}^v \mathbf{1}_{S_r}(m, s, w) P_s\left(\frac{r_b + m_b}{N}\right)(v_n, v_q) \\ \times a_m^{(N)}(v_q) P_w\left(\frac{r_b}{N}\right)(v_q, v_\ell) e_m^{(N)}(k), \quad (2.7)$$

where $S_r = \{(m, s, w) : E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N}) = 0\}$.

Lemma 2.3. *We have convergence in norm,¹*

$$\lim_{T \rightarrow \infty} \|\text{Op}_N(F_T) - \text{Op}_N(b)\|_{HS}^2 = 0.$$

Proof. We use the special basis $\phi_{r, v_\ell}^{(N)} = e_r^{(N)} \otimes \delta_{v_\ell}$ of $\ell^2(V_N)$. That is, $\phi_{r, v_\ell}^{(N)}(k_a + v_q) = e_r^{(N)}(k) \delta_{v_\ell}(v_q) = \frac{e^{2\pi i r \cdot k/N}}{N^{d/2}} \delta_{v_\ell}(v_q)$. By (2.2), $\langle U \phi_{r, v_\ell} \rangle_j(v_q) = \langle e_j^{(N)}, e_r^{(N)} \rangle_{\ell^2(\mathbb{L}_N^d)} \delta_{v_\ell}(v_q) = \delta_{j, r} \delta_{v_\ell}(v_q)$. By definition (2.5), this implies $\text{Op}_N(F) \phi_{r, v_\ell}^{(N)}(k_a + v_n) = F(k, r, v_n, v_\ell) e_r^{(N)}(k)$.

Note that $\|F(\cdot, r, \star, v_\ell) e_n^{(N)}(\cdot)\|_{\ell^2(\Gamma_N)}^2 = \frac{1}{N^d} \|F(\cdot, r, \star, v_\ell)\|_{\ell^2(\Gamma_N)}^2$, where $\cdot$ runs over $k \in \mathbb{L}_N^d$ and $\star$ runs over $v_n \in V_f$. Therefore,

$$\|\text{Op}_N(F)\|_{HS}^2 = \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \|\text{Op}_N(F) \phi_{r, v_\ell}^{(N)}\|^2 = \frac{1}{N^d} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \|F(\cdot, r, \star, v_\ell)\|^2 \quad (2.8)$$

To prove the lemma, we should thus examine the norm of the symbols,

$$\|F_T(\cdot, r, \star, v_\ell) - b(\cdot, r, \star, v_\ell)\|^2 \\ = \left\| \sum_{m \in \mathbb{L}_N^d} \sum_{q, s, w=1}^v \mathbf{1}_{S_r^c}(m, s, w) \frac{e^{iT[E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N})]} - 1}{T[E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N})]} \right. \\ \left. \times P_s\left(\frac{r_b + m_b}{N}\right)(\star, v_q) a_m^{(N)}(v_q) P_w\left(\frac{r_b}{N}\right)(v_q, v_\ell) e_m^{(N)}(\cdot) \right\|^2.$$

This implies that

$$\|\text{Op}_N(F_T) - \text{Op}_N(b)\|_{HS}^2 = \frac{1}{T^2 N^d} \sum_{r, m \in \mathbb{L}_N^d} \sum_{\ell=1}^v \\ \left\| \sum_{q, s, w=1}^v \mathbf{1}_{S_r^c}(m, s, w) \frac{e^{iT[E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N})]} - 1}{E_s(\frac{r_b+m_b}{N}) - E_w(\frac{r_b}{N})} \right. \\ \left. \times P_s\left(\frac{r_b + m_b}{N}\right)(\star, v_q) a_m^{(N)}(v_q) P_w\left(\frac{r_b}{N}\right)(v_q, v_\ell) \right\|_{\mathbb{C}^v}^2 \\ \leq \frac{C_{N,a}}{T^2},$$

¹ It is worthwhile to note that in the case of trees [1, 3, 4], we usually evolve the dynamical system in time T , essentially up to the girth of the graph, take the size of the graph $N \rightarrow \infty$, then finally take $T \rightarrow \infty$. Here we first consider the equilibrium limit in T , then take $N \rightarrow \infty$ in the end of the proof.

where $C_{N,a}$ is finite for any N and is independent of T . Taking $T \rightarrow \infty$ yields that $\text{Op}_N(F_T) \rightarrow \text{Op}_N(b)$ in HS norm. $\square$

2.3. Step 3. We are thus reduced to studying $\text{Op}_N(b)$ with b given in (2.7).

Note that $\sum_{p=1}^v P_p(\theta) = \text{id}$, so $\sum_{p=1}^v P_p(\theta)(v_i, v_j) = \delta_{v_i, v_j}$. Therefore, if we remove the $\mathbf{1}_{S_r}$ term, (2.7) becomes

$$\sum_{m \in \mathbb{L}_N^d} a_m^{(N)}(v_n) e_m^{(N)}(k) \delta_{v_n, v_\ell} = a(k_a + v_n) \delta_{v_n, v_\ell}$$

and the corresponding Op_N applied to ψ simply gives $a(k_a + v_n)\psi(k_a + v_n)$. Hence, $\text{Op}_N(b)\psi$ is just $a\psi$ but with many suppressed Floquet modes.

Let $\bar{a}$ be the part of b corresponding to $m = 0$. Let $\tilde{a} = a - \text{Op}_N(\bar{a})$ and $c = b - \bar{a}$. Then collecting the previous steps, we have

$$\begin{aligned} \sum_{u \in \Gamma_N} |\langle \psi_u^{(N)}, \tilde{a} \psi_u^{(N)} \rangle|^2 &= \sum_{u \in \Gamma_N} \lim_{T \rightarrow \infty} |\langle \psi_u^{(N)}, \text{Op}_N(F_T - \bar{a}) \psi_u^{(N)} \rangle|^2 \\ &\leq \sum_{u \in \Gamma_N} \lim_{T \rightarrow \infty} 2(\|\text{Op}_N(c) \psi_u^{(N)}\|^2 + \|\text{Op}_N(F_T - b) \psi_u^{(N)}\|^2) \\ &= 2\|\text{Op}_N(c)\|_{HS}^2. \end{aligned}$$

Proof of (1.4). It now suffices to show that $\lim_{N \rightarrow \infty} \frac{1}{|\Gamma_N|} \|\text{Op}_N(c)\|_{HS}^2 = 0$. Using (2.8), we have $\frac{1}{|\Gamma_N|} \|\text{Op}_N(c)\|_{HS}^2 = \frac{1}{vN^{2d}} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \|c(\cdot, r, \star, v_\ell)\|_{\ell^2(V_N)}^2$.

We thus consider

$$\begin{aligned} &\frac{1}{N^{2d}} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \left\| \sum_{m \neq 0} \sum_{q, s, w=1}^v \mathbf{1}_{S_r}(m, s, w) \right. \\ &\quad \left. P_s\left(\frac{r_{\mathbf{b}} + m_{\mathbf{b}}}{N}\right)(\star, v_q) a_m^{(N)}(v_q) P_w\left(\frac{r_{\mathbf{b}}}{N}\right)(v_q, v_\ell) e_m^{(N)}(\cdot) \right\|^2 \\ &= \frac{1}{N^{2d}} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \sum_{m \neq 0} \sum_{n=1}^v \left| \sum_{q, s, w=1}^v \mathbf{1}_{S_r}(m, s, w) \right. \\ &\quad \left. P_s\left(\frac{r_{\mathbf{b}} + m_{\mathbf{b}}}{N}\right)(v_n, v_q) a_m^{(N)}(v_q) P_w\left(\frac{r_{\mathbf{b}}}{N}\right)(v_q, v_\ell) \right|^2 \end{aligned}$$

Denote $P_s := P_s(\frac{r_{\mathbf{b}} + m_{\mathbf{b}}}{N})$, $P_w := P_w(\frac{r_{\mathbf{b}}}{N})$ and expand the square modulus to get

$$\begin{aligned} &\frac{1}{N^{2d}} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \sum_{m \neq 0} \sum_{n=1}^v \sum_{q, s, w, q', s', w'=1}^v \mathbf{1}_{S_r}(m, s, w) P_s(v_n, v_q) a_m^{(N)}(v_q) P_w(v_q, v_\ell) \\ &\quad \times \overline{\mathbf{1}_{S_r}(m, s', w') P_{s'}(v_n, v_{q'}) a_m^{(N)}(v_{q'}) P_{w'}(v_{q'}, v_\ell)}. \end{aligned} \tag{2.9}$$

But

$$\sum_{n=1}^v P_s(v_n, v_q) \overline{P_{s'}(v_n, v_{q'})} = \sum_{n=1}^v (P_s \delta_{v_q})(v_n) \overline{(P_{s'} \delta_{v_{q'}})(v_n)} = \langle P_{s'} \delta_{v_{q'}}, P_s \delta_{v_q} \rangle.$$

Similarly, $\sum_{\ell=1}^v P_w(v_q, v_\ell) \overline{P_{w'}(v_{q'}, v_\ell)} = \langle P_w \delta_{v_q}, P_{w'} \delta_{v_{q'}} \rangle$. If $E_s \neq E_{s'}$ or $E_w \neq E_{w'}$, these scalar products vanish. So (2.9) is concentrated on the s', w' for which $E_{s'} = E_s$ and $E_{w'} = E_w$, in which case $\mathbf{1}_{S_r}(m, s, w) = \mathbf{1}_{S_r}(m, s', w')$ and we obtain

$$\begin{aligned} & \frac{1}{N^{2d}} \sum_{r \in \mathbb{L}_N^d} \sum_{m \neq 0} \sum_{q, s, w, q', s', w'=1}^v \mathbf{1}_{S_r}(m, s, w) \langle P_{s'} \delta_{v_{q'}}, P_s \delta_{v_q} \rangle a_m^{(N)}(v_q) \overline{\langle P_w \delta_{v_q}, P_{w'} \delta_{v_{q'}} \rangle a_m^{(N)}(v_{q'})} \\ &= \frac{1}{N^{2d}} \sum_{\substack{m \in \mathbb{L}_N^d \\ m \neq 0}} \sum_{q, q'=1}^v \overline{a_m^{(N)}(v_{q'})} a_m^{(N)}(v_q) \sum_{r \in \mathbb{L}_N^d} \\ & \quad \sum_{s, w, s', w'=1}^v \mathbf{1}_{A_m}(r, s, w) \langle P_{s'} \delta_{v_{q'}}, P_s \delta_{v_q} \rangle \langle P_w \delta_{v_q}, P_{w'} \delta_{v_{q'}} \rangle, \end{aligned}$$

where $A_m = \{(r, s, w) : E_s(\frac{r_{\mathbf{b}} + m_{\mathbf{b}}}{N}) - E_w(\frac{r_{\mathbf{b}}}{N}) = 0\}$ and we used that $(m, s, w) \in S_r \iff (r, s, w) \in A_m$. By hypothesis (1.3), we know that

$$\lim_{N \rightarrow \infty} \sup_{\substack{m \in \mathbb{L}_N^d \\ m \neq 0}} \frac{|A_m|}{N^d} = 0. \quad (2.10)$$

Since $|\langle P_{s'} \delta_{v_{q'}}, P_s \delta_{v_q} \rangle| \leq 1$, it follows that the above is

$$\begin{aligned} & o_N(1) \frac{1}{N^d} \sum_m \sum_{q, q'=1}^v \overline{a_m^{(N)}(v_{q'})} a_m^{(N)}(v_q) \\ &= o_N(1) \frac{1}{N^d} \sum_{q, q'=1}^v \langle a(\cdot + v_{q'}), a(\cdot + v_q) \rangle_{\ell^2(\mathbb{L}_N^d)} = o_N(1) \end{aligned}$$

using $|a(n_{\mathbf{a}} + v_p)| \leq 1$. This completes the proof of (1.4). $\square$

2.4. Step 4. Let us now explore the main term $\bar{a}$. Recall that it corresponds to $m = 0$ in (2.7). Having $(0, s, w) \in S_r$ means that $E_s(\frac{r_{\mathbf{b}}}{N}) = E_w(\frac{r_{\mathbf{b}}}{N})$. This is automatically true for $w = s$. Thus,

$$\begin{aligned} \bar{a} &= \sum_{q, s=1}^v a_0^{(N)}(v_q) e_0^{(N)}(k) P_s\left(\frac{r_{\mathbf{b}}}{N}\right)(v_n, v_q) \left(P_s\left(\frac{r_{\mathbf{b}}}{N}\right)(v_q, v_\ell) + \sum_{\substack{w \neq s \\ E_s = E_w}} P_w\left(\frac{r_{\mathbf{b}}}{N}\right)(v_q, v_\ell) \right) \\ &= \sum_{q=1}^v \langle a(\cdot + v_q) \rangle \sum_{s=1}^{v'} P_{E_s}\left(\frac{r_{\mathbf{b}}}{N}\right)(v_n, v_q) P_{E_s}\left(\frac{r_{\mathbf{b}}}{N}\right)(v_q, v_\ell), \end{aligned} \quad (2.11)$$

where $\langle a(\cdot + v_q) \rangle = \frac{1}{N^d} \sum_{n \in \mathbb{L}_N^d} a(n_{\mathbf{a}} + v_q)$, $v' \leq v$ is the number of *distinct* eigenvalues of $H(\theta_{\mathbf{b}})$ and $P_{E_s}(\theta_{\mathbf{b}}) = \sum_{E_w = E_s} P_w(\theta_{\mathbf{b}})$ is the orthogonal projection onto the eigenspace corresponding to $E_s(\theta_{\mathbf{b}})$. In general, v' is independent of $\theta_{\mathbf{b}}$, except perhaps on a subvariety of dimension $\leq d - 1$, hence of measure zero, as follows from [19, Th. 3.5.3].

Proof of (1.5)–(1.6). By the definition of Op_N , we can write out

$$\begin{aligned} \langle \psi, \text{Op}_N(\bar{a})\psi \rangle &= \sum_{k \in \mathbb{L}_N^d} \sum_{v_n \in V_f} \overline{\psi(k_{\mathbf{a}} + v_n)} [\text{Op}_N(\bar{a})\psi](k_{\mathbf{a}} + v_n) \\ &= \sum_{v_n \in V_f} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v (U\psi)_r(v_{\ell}) \bar{a}(r, v_n, v_{\ell}) \sum_{k \in \mathbb{L}_N^d} \overline{\psi(k_{\mathbf{a}} + v_n)} e_r^{(N)}(k). \end{aligned}$$

But $\sum_k \overline{\psi(k_{\mathbf{a}} + v_n)} e_r^{(N)}(k) = \overline{(U\psi)_r(v_n)}$. Thus,

$$\begin{aligned} \langle \psi, \text{Op}_N(\bar{a})\psi \rangle &= \sum_{v_n \in V_f} \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v (U\psi)_r(v_{\ell}) \overline{(U\psi)_r(v_n)} \bar{a}(r, v_n, v_{\ell}) \\ &= \sum_{q=1}^v \sum_{r \in \mathbb{L}_N^d} \sum_{\ell=1}^v \sum_{s=1}^{v'} P_{E_s}(v_q, v_{\ell}) (U\psi)_r(v_{\ell}) \\ &\quad \sum_{n=1}^v \overline{P_{E_s}(v_q, v_n)} \overline{(U\psi)_r(v_n)} \langle a(\cdot + v_q) \rangle \\ &= \sum_{q=1}^v \langle a(\cdot + v_q) \rangle \sum_{r \in \mathbb{L}_N^d} \sum_{s=1}^{v'} [P_{E_s}(U\psi)_r](v_q) \overline{[P_{E_s}(U\psi)_r](v_q)}. \end{aligned}$$

where $P_s = P_s(\frac{r_{\mathbf{b}}}{N})$. We have shown that

$$\langle \psi, \text{Op}_N(\bar{a})\psi \rangle = \sum_{q=1}^v \langle a(\cdot + v_q) \rangle \sum_{r \in \mathbb{L}_N^d} \sum_{s=1}^{v'} \left| \left[P_{E_s}\left(\frac{r_{\mathbf{b}}}{N}\right) (U\psi)_r \right](v_q) \right|^2. \quad (2.12)$$

In the special case where $\langle a(\cdot + v_q) \rangle = \langle a(\cdot + v_1) \rangle$ for $q = 1, \dots, v$, the above reduces to

$$\langle a(\cdot + v_1) \rangle \sum_{r \in \mathbb{L}_N^d} \sum_{s=1}^{v'} \|P_{E_s}(U\psi)_r\|_{\mathbb{C}^v}^2 = \langle a(\cdot + v_1) \rangle \sum_{r \in \mathbb{L}_N^d} \|(U\psi)_r\|_{\mathbb{C}^v}^2 = \langle a(\cdot + v_1) \rangle \|\psi\|^2.$$

In particular, $\psi = \psi_u^{(N)}$ gives the uniform average $\langle a(\cdot + v_1) \rangle = \frac{1}{N^d} \sum_{n \in \mathbb{L}_N^d} a(n_{\mathbf{a}} + v_1) = \frac{1}{|\Gamma_N|} \sum_{v \in \Gamma_N} a(v)$. This proves (1.6). In the same way, if a is real-valued, we deduce (1.5) from (2.12). $\square$

Remark 2.4. (Necessity of the assumptions) In the previous proof, the only inequality that we used is in Step 3, when bounding the variance by the Hilbert-Schmidt norm of the evolved observable. This bound is standard in proofs of quantum ergodicity, it seems unlikely that we can avoid it. On the other hand, the decay of the Hilbert-Schmidt norm almost necessitates (1.3). In fact, if we can choose the normalized eigenvectors $f_s^{\theta_b}$ corresponding to $E_s(\theta_b)$ such that for some v_ℓ , we have $f_s^{\theta_b}(v_\ell) \neq 0$ for all s, θ , then by taking $a(k_a + v_q) = e^{\frac{i\bar{m}_b \cdot k_a}{N}} \delta_{v_\ell}(v_q)$ in the calculation preceding (2.10), we see that $\frac{|A_m|}{N^d} = o_N(1)$ must hold $\forall m \neq 0$ for the HS norm to go to zero.

Remark 2.5. The main theorem holds more generally if instead of summing over the whole spectrum in (1.4), we sum over eigenvalues in some interval I , in which case we only need (1.3) to hold on I . To see this, we slightly modify the proof as follows: in (2.1), we insert a spectral projection $\chi_I(H_N)$, so the operator is now $\frac{1}{T} \int_0^T e^{itH_N} a e^{-itH_N} \chi_I(H_N) dt$. In (2.6), we replace the sum over all w by the sum over $E_w(\frac{r_b}{N}) \in I$. In fact, by adding the spectral projection through the proof of Lemma 2.2, we now get $(U e^{-itH} \chi_I(H) \psi)_{r-m} = e^{-itH(\frac{r_b-m_b}{N})} \chi_I(H(\frac{r_b-m_b}{N})) (U \psi)_{r-m}$. Consequently, the limiting symbol b now also sums over $E_w(\frac{r_b}{N}) \in I$ instead. The proofs carry over *mutatis mutandis*.

In the end, the symbol $\bar{a}$ in (2.11) now sums over $E_s(\frac{r_b}{N}) \in I$. This gives the illusory impression that the weighted average changes, which of course makes no sense as the term $\langle \psi_u^{(N)}, a \psi_u^{(N)} \rangle$ should approach a fixed quantity whether the Cesàro mean is over the whole spectrum or not. However the quantity $\langle \psi_u^{(N)}, \text{Op}_N(\bar{a}) \psi_u^{(N)} \rangle$ is indeed the same as before. In fact, if we know that $\lambda_u^{(N)} \in I$, we may again insert a projector so that $(U \psi_u^{(N)})_r$ in (2.12) becomes $(U \chi_I(H_N) \psi_u^{(N)})_r = \chi_I(H(\frac{r_b}{N})) (U \psi_u^{(N)})_r$, so the sum over all E_s in (2.12) reduces to the sum over $E_s(\frac{r_b}{N}) \in I$, which is what we obtained when averaging over I .

Remark 2.6. In this paper we always take H_N with periodic conditions. We believe these to be the most natural conditions to approximate the infinite model, avoiding boundary effects from finite truncations. However, it is also interesting to ask if the result remains true if we consider H_N with Dirichlet conditions instead. In this case our Schrödinger operator H_N on Γ_N is the operator on the induced subgraph $\Gamma_N \subset \Gamma$. This has been studied e.g. in [9].

In the proof, we use the periodic conditions to diagonalize H_N in Lemma 2.1. This property no longer holds for Dirichlet conditions if we take the same U . A natural candidate is to consider a discrete sine transform. For simplicity, consider $H = \mathcal{A}$ on $\Gamma = \mathbb{Z}^d$. If $s_k^{(N)}(n) = \prod_{i=1}^d s_{k_i}(n_i)$, with $s_\ell(r) = \sqrt{\frac{2}{N+1}} \sin \pi \frac{(r+1)(\ell+1)}{N+1}$ for $\ell, r = 0, \dots, N-1$, consider for $j \in \mathbb{L}_N^d$,

$$(\mathcal{S}\psi)_j = \langle s_j^{(N)}, \psi \rangle_{\mathbb{L}_N^d} = \sum_{k \in \mathbb{L}_N^d} s_j^{(N)}(k) \psi(k).$$

This operator is unitary. Using that $(s_j^{(N)})$ are eigenfunctions of A_N with eigenvalue $\mu_j^{(N)} = \sum_{i=1}^d 2 \cos \pi \frac{j_i+1}{N+1}$, we see that $(\mathcal{S} A_N \psi)_j = \langle s_j^{(N)}, A_N \psi \rangle = \mu_j^{(N)} (\mathcal{S}\psi)_j$.

However, if we use this sine transform $\mathcal{S}$, we need to replace all later occurrences of $e_r^{(N)}(k)$ by $s_r^{(N)}(k)$. This becomes difficult because these sine functions are not as

well-behaved as the exponentials used in periodic conditions. Namely, $s_{m+n}^{(N)}$ is not a multiple of $s_m^{(N)} s_n^{(N)}$. This creates complications, the proof does not carry over directly, and further work should be done to check whether or not quantum ergodicity holds for H_N .

3. Special Classes of Graphs

In this section we discuss the validity of assumption (1.3) for various classes of graphs. We start with graphs having $\nu = 1$, proving Theorem 1.1. We then discuss Cartesian products, proving Proposition 1.4, and conclude with graph decorations, tensor and strong products, proving Propositions 1.5 and 1.6 along the way.

3.1. Scalar fibers. Step 4 in Sect. 2.4 shows that if $\nu = 1$, then $\langle \psi_u^{(N)}, \text{Op}_N(\bar{a}) \psi_u^{(N)} \rangle = \langle a \rangle$. To prove Theorem 1.1, it remains to establish (1.3) in this context. Here of course $w = s$.

If $\nu = 1$, then the graph is $2D$ -regular for some $D \in \mathbb{N}$. In fact, $V_f = \{o\}$ for some o , and $\Gamma = \mathbb{Z}_a^d + \{o\}$. If $u \sim o$, then $u = \lfloor u \rfloor_a + o$. By translation invariance we have $u - n_a \sim o - n_a$. Applying this to $n_a = \lfloor u \rfloor_a$ gives $o \sim o - \lfloor u \rfloor_a$. We may thus arrange the neighbors of o into $\mathcal{N}_o^+ \cup \mathcal{N}_o^-$, where $\mathcal{N}_o^+ = \{o + n_a\}$ and $\mathcal{N}_o^- = \{o - n_a\}$, for some D nonzero integers $n_a = \sum_{i=1}^d n_i a_i$ with $n_i \in \{0, 1, \dots\}$ depending on the adjacency rule (in case of lattices with only nearest-neighbor adjacency like $\Gamma = \mathbb{Z}^d$, then $n_i \in \{0, 1\}$). Since the rest of the graph is just a periodic copy of the star around o , we see it is $2D$ -regular.

If $\nu = 1$, then the potential Q must be constant. We assume without loss of generality that $Q = 0$.

Proof of Theorem 1.1. The $\nu \times \nu$ matrix $H(\theta_b)$ is now just a scalar given by

$$H(\theta_b) = \sum_{u \sim o} e^{i\theta_b \cdot \lfloor u \rfloor_a} = 2 \sum_{p=1}^D \cos(2\pi \theta \cdot n^{(p)})$$

for some $n^{(1)}, \dots, n^{(D)} \in \{0, 1, \dots\}^d \setminus \{0\}$. We only have one eigenvalue here given by $E(\theta_b) = H(\theta_b)$. So we should show that for any fixed $m \neq 0$, the equation

$$E\left(\frac{r_b + m_b}{N}\right) - E\left(\frac{r_b}{N}\right) = 2 \sum_{p=1}^D \left(\cos\left(2\pi \frac{(r+m) \cdot n^{(p)}}{N}\right) - \cos\left(2\pi \frac{r \cdot n^{(p)}}{N}\right) \right) = 0 \quad (3.1)$$

has $o(N^d)$ solutions in $r \in \mathbb{L}_N^d$. By the sum to product formula, we are led to consider the zeroes of

$$f_m\left(\frac{r}{N}\right) := \sum_{p=1}^D \sin\left(\pi \frac{m \cdot n^{(p)}}{N}\right) \sin\left(\pi \frac{(2r+m) \cdot n^{(p)}}{N}\right). \quad (3.2)$$

For this, we consider the projection of the surface $A_m = \{r \in \mathbb{L}_N^d : f_m(\frac{r}{N}) = 0\}$ onto a vector $\phi \in \mathbb{L}_N^d$ to be specified. More precisely, given $j \in \mathbb{L}_N^d$, we write $j = r + y\phi$, for

$r \in \phi^\perp$ and $y = \frac{\langle \phi, j \rangle}{\|\phi\|^2}$. Note that $y \in [0, N-1]$ since $0 \leq \sum \phi_i j_i \leq (N-1) \sum \phi_i \leq (N-1) \sum \phi_i^2$ for $\phi \in \mathbb{L}_N^d$. We will show that for fixed $r \in \phi^\perp$, there are at most M points y such that $f_m(\frac{j}{N}) = 0$, with M independent of N . By varying $r \in \phi^\perp$, it follows that $|A_m| \leq M|\phi^\perp| \leq MN^{d-1} = o(N^d)$ as required.

We therefore consider the function

$$g_{m,r}(x) = f_m\left(\frac{r}{N} + x\phi\right) = 0$$

for $x \in [0, 1)$. Denote

$$\alpha_p = \sin\left(\pi \frac{m \cdot n^{(p)}}{N}\right), \quad \beta_p = \pi \frac{(2r+m) \cdot n^{(p)}}{N}, \quad \gamma_p = 2\phi \cdot n^{(p)}. \quad (3.3)$$

Then

$$g_{m,r}(x) = \sum_{p=1}^D \alpha_p \sin(\beta_p + \pi \gamma_p x) = \frac{1}{2i} \sum_{p=1}^D \alpha_p (e^{i\beta_p} e^{i\pi \gamma_p x} - e^{-i\beta_p} e^{-i\pi \gamma_p x}).$$

Setting $z = e^{i\pi x}$, this reduces to

$$\tilde{g}_{m,r}(z) = \sum_{p=1}^D (\rho_p z^{\gamma_p} + \rho'_p z^{-\gamma_p})$$

for some $\rho_p, \rho'_p \in \mathbb{C}$. By definition (3.3), $\gamma_p \geq 0$ is an integer. We thus seek the solutions of $\tilde{g}_{m,r}(z)$ on the unit circle. We have $\tilde{g}_{m,r}(z) = 0$ iff $\sum_{p=1}^D (\rho_p z^{\gamma_\star + \gamma_p} + \rho'_p z^{\gamma_\star - \gamma_p}) = 0$, where $\gamma_\star = \max_p \gamma_p$. This is a polynomial in z . By the fundamental theorem of algebra, if this polynomial is nontrivial, it has at most $M = 2 \max_p \gamma_p$ roots. In turn, we have at most M solutions x_j for $g_{m,r}(x) = 0$, and the proof of (2.10) is complete (recall the discussion after (3.2)).

So it remains to check the polynomial $z^{\gamma_\star} \tilde{g}_{m,r}(z) = \sum_{p=1}^D (\rho_p z^{\gamma_\star + \gamma_p} + \rho'_p z^{\gamma_\star - \gamma_p})$ is nontrivial. For this, we check that

1. At least one ρ_p is nonzero.
2. We can choose ϕ such that $\gamma_p \neq 0$ for all p and $\gamma_p \neq \gamma_{p'}$ for $p \neq p'$. This way, no two terms in the sum have the same power, so no cancellation can occur. And since no γ_p is zero, no cancellation can occur from $\rho_{p'} = -\rho_p$.

Proof of 1. Since $m \neq 0$, we have $m_j \neq 0$ for some j . Note that $o + \mathbf{a}_j \in \Gamma$ by translation invariance. Since Γ is connected, some integer combination $o + \sum_{p=1}^D k_p n_{\mathbf{a}}^{(p)}$ of the neighbors of o is $o + \mathbf{a}_j$, where $k_p \in \mathbb{Z}$ is the number of adjacencies of type $n^{(p)}$ traversed on the geodesic from o to $o + \mathbf{a}_j$. It follows that

$$\sin\left(\pi \frac{m}{N} \cdot \sum_{p=1}^D k_p n^{(p)}\right) = \sin\left(\frac{m_{\mathbf{b}}}{2N} \cdot \sum_{p=1}^D k_p n_{\mathbf{a}}^{(p)}\right) = \sin\left(\frac{m_{\mathbf{b}}}{2N} \cdot \mathbf{a}_j\right) = \sin \frac{\pi m_j}{N} \neq 0. \quad (3.4)$$

If we had $\sin(\pi \frac{m \cdot n^{(p)}}{N}) = 0$ for all p , we would have $\frac{m \cdot n^{(p)}}{N} \in \mathbb{Z}$ for all p and thus $\frac{m}{N} \cdot \sum_{p=1}^D k_p n^{(p)} \in \mathbb{Z}$, contradicting (3.4). Thus, $\alpha_p \neq 0$ for at least one p . This completes the proof.

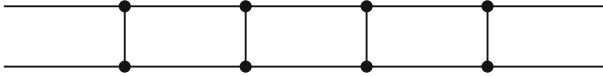


Fig. 2. The ladder graph, $\mathbb{Z} \square P_2$

Proof of 2. We need ϕ to avoid the subspaces $V_p = \{v : v \cdot n^{(p)} = 0\}$ for all $p = 1, \dots, D$ and $V_{p,p'} = \{v : v \cdot n^{(p)} = v \cdot n^{(p')}\}$ for all $D(D-1)$ pairs of $p \neq p'$. Each of these is $d-1$ dimensional, since the $n^{(p)}$ are nonzero and distinct.

It is not difficult to see that such a ϕ exists. However, we give a quite explicit construction below, which in turn gives an explicit bound on M .

Suppose we give a list of $\ell_D = (d-1)D^2 + 1$ vectors in $\mathbb{L}_N^d$ such that any d of them forms a basis. Then each of the subspaces V_p or $V_{p,p'}$ can only contain at most $d-1$ of our vectors, therefore there must be some vector not contained in any of the subspaces and we are done.

A possible list is given by the row vectors

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & 2 & 2^2 & \cdots & 2^{d-1} \\ 1 & 3 & 3^2 & \cdots & 3^{d-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & \ell_D & \ell_D^2 & \cdots & \ell_D^{d-1} \end{bmatrix}.$$

Indeed, any subset of d of these vectors, say the ones from the $x_1, \dots, x_d$ rows, forms a Vandermonde matrix with determinant $\prod_{i < j} (x_i - x_j)$, which is nonzero, meaning any set of d vectors is linearly independent. This finishes the proof. $\square$

We may obtain an upper bound over $M = 2 \max_p \gamma_p$. In fact, the worst case is if the last vector in the list is the first ϕ that avoids all $V_{p,p'}$. In this case, $\gamma_p = 2\phi \cdot n^{(p)} \leq 2d\ell_D^{d-1}q$, where $q = \max_{i,p} n_i^{(p)}$, so $M \leq 4d\ell_D^{d-1}q$.

3.2. The case of Cartesian products. The Cartesian product $\Gamma \square G$ of Γ and G is the graph with vertex set $V(\Gamma) \times V(G)$, in which $(u, v) \sim (u', v')$ if either

- (i) $(u = u' \text{ and } v \sim v')$,
- (ii) or $(u \sim u' \text{ and } v = v')$.

For example, to construct $\mathbb{Z} \square P_2$, where P_2 is the 2-path, replace each vertex of $\mathbb{Z}$ with a 2-path, and connect edges between matching vertices. The result is an infinite ladder.

Similarly, for $\mathbb{Z} \square C_p$, where C_p is a p -cycle, replace each vertex of $\mathbb{Z}$ with a p -cycle, and connect edges between matching vertices (Fig. 6). The graph is 4-regular, naturally embedded in $\mathbb{R}^3$, and is clearly $\mathbb{Z}$ -periodic with fundamental cell $V_f = C_p$. We may endow C_p with a potential Q and copy it in each layer. Then $H(\theta_b)f(u, v) = 2 \cos 2\pi\theta f(u, v) + f(u, v+1) + f(u, v-1) + Q_v f(u, v)$. In other words, $H(\theta_b) = \mathcal{A}_{\mathbb{Z}}(\theta_b) \otimes I + I \otimes H_{G_F}$. The eigenvalues are thus $\{2 \cos 2\pi\theta + \mu_j\}$, where $\{\mu_j\}_{j=1}^p$ are the eigenvalues of the Schrödinger operator of the p -cycle. These observations are general :

Lemma 3.1. *If Γ is a periodic graph with $v = 1$ and G_F is a finite graph endowed a potential Q , then $\Gamma \square G_F$ is a periodic graph with fundamental cell $V_f = G_F$ and*

$$H_{\Gamma \square G_F}(\theta_b) = H_{\Gamma}(\theta_b) \otimes I + I \otimes H_{G_F}. \quad (3.5)$$

Proof. Replace each $u \in \Gamma$ by a copy of G_F . The result has vertex set $V(\Gamma) \times V(G_F)$. According to rules (i)-(ii), we should have $\mathcal{A}_{\Gamma \square G_F} = I \otimes \mathcal{A}_{G_F} + \mathcal{A}_{\Gamma} \otimes I$. This means that if we arrange the vertices of $\Gamma \square G_F$ as successive G_F -layers, then a given (u, v) is connected on the one hand to the neighbors (u, v') in the same layer (rule (i)) and to the neighbors (u', v) outside (rule (ii)). This means that the edges are precisely the old edges of G_F in each layer, as well as bridges between successive layers between the matching vertices. Recalling (2.4), we see that the θ -dependence only arises in the bridges from (u, v) to another layer (the neighbors within G_F have $[u]_{\alpha} = 0$). The bridges occur precisely at the bridges from u to its neighbors in Γ . We conclude that $\mathcal{A}_{\Gamma \square G_F}(\theta_b) = \mathcal{A}_{\Gamma}(\theta_b) \otimes I + I \otimes \mathcal{A}_{G_F}$. If we finally endow G_F a potential and copy it across the layers, then $(Qf)(u, v) = Q_v f(u, v)$, so we obtain (3.5) (note that $\mathcal{A}_{\Gamma}(\theta_b) = H_{\Gamma}(\theta_b)$ as $v = 1$). $\square$

Proof of Proposition 1.4. Since $v = 1$ for Γ , $H_{\Gamma}(\theta_b)$ has just one eigenvalue $E_{\Gamma}(\theta_b)$. So the spectrum of $H_{\Gamma \square G_F}$ is the set $\{E_{\Gamma}(\theta_b) + \mu_j\}$, where μ_j are the eigenvalues of H_{G_F} on the finite graph G_F .

Given nonzero m , we should thus control the quantity

$$E_s\left(\frac{r_b + m_b}{N}\right) - E_w\left(\frac{r_b}{N}\right) = E_{\Gamma}\left(\frac{r_b + m_b}{N}\right) - E_{\Gamma}\left(\frac{r_b}{N}\right) + \mu_s - \mu_w.$$

Here, $E_{\Gamma}(\theta_b) = 2 \sum_{p=1}^D \cos(2\pi \theta \cdot n^{(p)})$ is precisely the quantity we controlled in Sect. 3.1. Following the arguments, we see that the same proof continues to hold here. In fact, $\tilde{g}_{m,r}(z)$ only has an additional term $\mu_s - \mu_w$, and the proof continues to hold, as no γ_p is zero so this term cannot induce cancellations in the polynomial $z^{\gamma_s} \tilde{g}_{m,r}(z)$. Thus, the quantity in (1.3) is $\leq MN^{-1} \rightarrow 0$ as required, with the same $M \leq 4d\ell_D^{d-1}q$ of the case $v = 1$. This shows that the assumption of Theorem 1.2 is satisfied for $\Gamma \square G_F$.

By (3.5), the eigenvectors of $H_{\Gamma \square G_F}(\theta_b)$ are simply the eigenvectors of H_{G_F} (recall that $H_{\Gamma}(\theta_b)$ is just a scalar 1×1 matrix). They are thus independent of θ_b , and so are the eigenprojectors $P_s(\theta_b)$. This makes (2.12) a bit simpler here. If moreover we choose $\psi = \psi_u^{(N)}$ to consist of a tensor basis $\psi_u^{(N)} = \phi_n \otimes w_j$, where (ϕ_n) is an orthonormal eigenbasis of H_{Γ} on Γ and (w_j) is an orthonormal eigenbasis of H_{G_F} , then the expression simplifies further. In fact, recalling (2.2), we have $(U\psi)_r(v_q) = \frac{1}{N^{d/2}} \sum_k e^{-2\pi i r \cdot k/N} \phi_n(k_{\alpha}) w_j(v_q) = \hat{\phi}_n(r) w_j(v_q)$, where $\hat{\phi}_n(r)$ is the Fourier coefficient of ϕ_n in the basis $e_k^{(N)}$ of $\ell^2(\mathbb{L}_N^d)$. Hence, $(P_s(U\psi)_r)(v_q) = \hat{\phi}_n(r)(P_s w_j)(v_q)$. Thus, (2.12) simplifies to

$$\sum_{q=1}^v \langle a(\cdot + v_q) \rangle \sum_r \sum_{s=1}^{v'} |\hat{\phi}_n(r)|^2 |(P_{E_s} w_j)(v_q)|^2 = \sum_{q=1}^v \langle a(\cdot + v_q) \rangle \sum_{s=1}^{v'} |(P_{E_s} w_j)(v_q)|^2,$$

where we used that $\|\phi_n\|^2 = 1$. But w_j is an eigenvector, so $P_{E_s} w_j = w_j$ if $E_s = E_j$ and $P_{E_s} w_j = 0$ otherwise. This completes the proof. $\square$

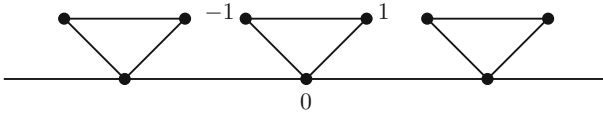


Fig. 3. Decorating $\mathbb{Z}$ with triangles. The values of an eigenfunction are shown (it is then extended by zero)

3.3. Graph decorations. Another way to create a new graph from given infinite and finite graphs Γ and G_F is to simply attach a copy of G_F at each vertex of Γ . More precisely, we identify a special vertex $o_F \in G_F$ to each $v \in \Gamma$. This process is called *graph decoration*. A very simple example is given in Fig. 3. The resulting graph is sometimes denoted by $\Gamma \triangleleft G_F$ (which reflects the procedure).

In contrast to Cartesian products, this process can be problematic for delocalization. For example, as shown in Fig. 3, this can create compactly supported eigenfunctions. The corresponding eigenvalue is a flat band, i.e. an infinitely degenerate eigenvalue. The example in Fig. 3 has the Floquet eigenvalues $\{-1, \frac{2 \cos 2\pi\theta + 1 \pm \sqrt{4 \cos^2 2\pi\theta - 4 \cos 2\pi\theta + 9}}{2}\}$. This generates the spectrum of $H = \mathcal{A}$ consisting of two bands which do not intersect. This spectrum is not very nice as the eigenvalue -1 is embedded in the left band, as can be seen by taking $\theta = \frac{1}{4}$.

It may be interesting to observe that in general, if Γ is a periodic graph having $v = 1$, then $\Gamma, \Gamma \square G_F$ and $\Gamma \triangleleft G_F$ are all “loop graphs” in the sense of Korotyaev and Saburova [15]. This class of graphs was singled out in [15] for being more amenable to spectral analysis. We see that not all graphs in this class are quantum ergodic.

Proof of Proposition 1.5. For the graph in Fig. 3, we have $|\Gamma_N| = 3N$, and on Γ_N , we may construct N localized eigenfunctions f_j , one on each triangle, each supported on only two vertices. Let N be even and take the locally constant observable a which is identically 1 on triangles attached to even vertices, and identically zero on triangles attached to odd vertices. Then $\langle a \rangle = \frac{1}{2}$. On the other hand, if we normalize the eigenfunctions f_j so that their values are $(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}}, 0, 0, \dots, 0)$, then $\langle f_{2j}, af_{2j} \rangle = \sum_v a(v) |f_{2j}(v)|^2 = 1$, while $\langle f_{2j+1}, af_{2j+1} \rangle = 0$ for each j . Hence,

$$\begin{aligned} \frac{1}{|\Gamma_N|} \sum_{u \in \Gamma_N} |\langle \psi_u^{(N)}, a \psi_u^{(N)} \rangle - \langle a \rangle|^2 &\geq \frac{1}{3N} \sum_{j=1}^N |\langle f_j, af_j \rangle - \langle a \rangle|^2 \\ &= \frac{1}{3N} \left[\frac{N}{2} \left(\left| 1 - \frac{1}{2} \right|^2 + \left| 0 - \frac{1}{2} \right|^2 \right) \right] = \frac{1}{12}. \end{aligned}$$

□

3.4. More product operations. Further operations to construct new graphs from old are the *tensor product* and the *strong product* of graphs.

3.4.1. Strong products The strong product $G \boxtimes H$ has vertex set $V(G) \times V(H)$, with $(u, v) \sim (u', v')$ iff $(u = u' \text{ and } v \sim v') \text{ or } (u \sim u' \text{ and } v = v') \text{ or } (u \sim u' \text{ and } v \sim v')$. We thus add more edges to the Cartesian product.

This operation is not as well behaved as the Cartesian one. For example, consider $\mathbb{Z} \boxtimes P_2$, where P_2 is a 2-path. The result (Fig. 4) is an infinite sequence of boxes $\boxtimes$.

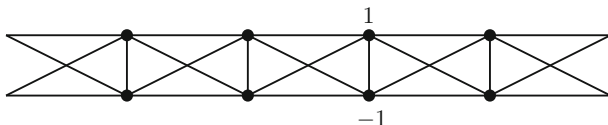


Fig. 4. $\mathbb{Z} \boxtimes P_2$. An eigenfunction localized on two vertices is shown

Unlike the ladder, this graph has some point spectrum. In fact, the Floquet matrix here is $H(\theta_b) = \begin{pmatrix} 2 \cos 2\pi\theta & 1 + 2 \cos 2\pi\theta \\ 2 \cos 2\pi\theta + 1 & 2 \cos 2\pi\theta \end{pmatrix}$, with eigenvalues $\{-1, 1 + 4 \cos 2\pi\theta\}$. Quantum ergodicity is violated (use the eigenfunction shown in Fig. 4 and argue as in Sect. 3.3).

See Sect. 4.6 for a further analysis when we add a potential.

Still, this product sometimes behaves well. For example, $\mathbb{Z} \boxtimes \mathbb{Z}$ gives the king's graph, which is quantum ergodic since it is periodic with $\nu = 1$.

3.4.2. Tensor products Next, the tensor product $G \times H$ has vertex set $V(G) \times V(H)$, with $(u, v) \sim (u', v')$ iff $(u \sim u' \text{ and } v \sim v')$. Equivalently, $\mathcal{A}_{G \times H} = \mathcal{A}_G \otimes \mathcal{A}_H$. The edges of this product are precisely the ones we added to the Cartesian product when discussing strong products.

The product of two connected graphs is not necessarily connected. For example, the tensor product of two path graphs of length 2 $\{a, b\}$ and $\{v, w\}$ gives the union of the two paths $\{(a, v), (b, w)\}$ and $\{(a, w), (b, v)\}$. To consider a product graph of the form $\Gamma \times G_F$ for quantum ergodicity, where Γ is a quantum ergodic graph and G_F is some finite graph, we first need $\Gamma \times G_F$ to be connected. It turns out this is satisfied if and only if either Γ or G_F contains an odd cycle, see [21].

Assume now that we are given a periodic Γ with $\nu = 1$, for simplicity. Just like Cartesian products, the tensor structure of the adjacency matrix translates well into the Floquet fibers. To see this, it is best to first picture the product operation. Geometrically, we simply consider the G_F -layers structure of Cartesian products, but then we remove all edges and add instead the following ones: a given (u, v) in a G_F layer is connected to all vertices (u', v') , where u' is in a different G_F layer and $v' \sim v$ in G_F . Note that $V_f = G_F$ contains no edges. Instead, if we “project” the edges going from a neighboring G_F layer to the starting one, we obtain the finite graph G_F that we started with. We may also endow G_F with some potential Q which is copied across the layers.

By definition (2.4), we have $H(\theta_b)f(u, v) = \sum_{u' \sim u, v' \sim v} e^{i\theta_b \cdot \lfloor u' \rfloor_a} f(u, v') + Q_v f(u, v) = H_\Gamma(\theta_b) \otimes H_{G_F} f(u, v)$, where we used here that $\{(u', v')\}_a = (u, v')$ and $\lfloor u', v' \rfloor_a = \lfloor u' \rfloor_a$ by construction. This shows that $H_{\Gamma \times G_F}(\theta_b) = H_\Gamma(\theta_b) \otimes H_{G_F}$. Consequently,

$$\sigma(H_{\Gamma \times G_F}(\theta_b)) = \{\mu_j E_\Gamma(\theta_b)\}_{j=1}^\nu, \quad (3.6)$$

where μ_j are the eigenvalues of H_{G_F} . Note that if $\mu_j = 0$ for some j , then this creates a flat band $\{0\}$ for $H_{\Gamma \times G_F}$, i.e. an infinitely degenerate eigenvalue.

We now consider the special case of $\mathbb{Z} \times G_F$. So $E_\Gamma(\theta_b) = 2 \cos 2\pi\theta$.

Proof of Proposition 1.6. To construct a counterexample, we take G_F such that

- (i) G_F is not bipartite,
- (ii) $0 \notin \sigma(\mathcal{A}_{G_F})$,

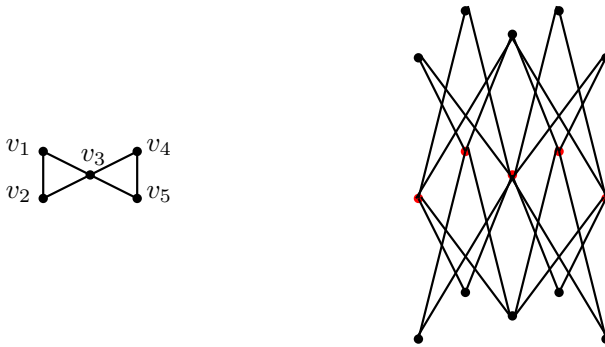


Fig. 5. The butterfly graph G_F (left) and part of the tensor product $\mathbb{Z} \times G_F$ (right). A fundamental set is colored in red

(iii) there exists s such that μ_s and $-\mu_s$ belong to $\sigma(\mathcal{A}_{G_F})$.

Point (i) is necessary to make $\mathbb{Z} \times G_F$ connected, (ii) is necessary to avoid a point spectrum $\{0\}$, and (iii) is what will contradict (1.3).

We take G_F as the butterfly graph, Fig. 5.

Since $\mathcal{A}_{G_F}$ is a 5×5 matrix, we can compute its eigenvalues and eigenvectors explicitly and find the following:

$$\begin{aligned} \mu_1 &= \frac{1 + \sqrt{17}}{2}, & \mu_2 &= \frac{1 - \sqrt{17}}{2}, & \mu_3 &= -1, & \mu_4 &= -1, & \mu_5 &= 1 \\ w_1 &= c_1 \left(1, 1, \frac{-1 + \sqrt{17}}{2}, 1, 1 \right), & w_2 &= c_2 \left(1, 1, \frac{-1 - \sqrt{17}}{2}, 1, 1 \right), \\ w_3 &= \frac{1}{\sqrt{2}} (0, 0, 0, -1, 1), & w_4 &= \frac{1}{\sqrt{2}} (-1, 1, 0, 0, 0), & w_5 &= \frac{1}{2} (-1, -1, 0, 1, 1) \end{aligned}$$

for normalization constants c_1, c_2 . We actually only need w_4, w_5 for the following argument, it is immediate to check that they are eigenvectors for μ_4, μ_5 , respectively.

We see properties (i)–(iii) are satisfied, take e.g. $\mu_s = 1$.

By (3.6), $\sigma(\mathcal{A}_{\mathbb{Z} \times G_F}(\theta_b))$ is just $\{2\mu_j \cos 2\pi\theta\}$, where μ_j runs over the above list of eigenvalues. It follows that $\sigma(\mathcal{A}_{\mathbb{Z} \times G_F})$ is purely absolutely continuous (as each Floquet eigenvalue is analytic and nonconstant, see [17, Th. XIII.86]). The graph $\mathbb{Z} \times G_F$ is also connected, since $\llbracket -n, n \rrbracket \times G_F$ is connected for any n by [21].

If $\mu_s = 1$ and $\mu_w = -1$, we find that

$$\begin{aligned} E_s(\theta_b + \alpha_b) - E_w(\theta_b) &= \mu_s(2 \cos(2\pi(\theta + \alpha)) + 2 \cos 2\pi\theta) \\ &= \mu_s \cos \pi(2\theta + \alpha) \cos \pi\alpha. \end{aligned}$$

This is zero if $\alpha = \frac{1}{2}$, for all θ . This suffices to contradict (1.3). In fact, taking $m = \frac{N}{2} \in \mathbb{L}_N$ assuming N is even, the fraction in (1.3) is equal to 1 and does not vanish.

We now show the tensor product $\mathbb{Z} \times G_F$ is not quantum ergodic. The hint for the choice of the observable comes from Remark 2.4. Namely, consider $a(k + v_q) = e^{2\pi i m k / N} \delta_{v_1}(v_q)$. Then $\langle a(\cdot + v_q) \rangle = 0$ for all v_q , so $\langle \psi, \text{Op}_N(\bar{a})\psi \rangle = 0$ by (2.12). We choose the problematic value of m , namely $m = \frac{N}{2}$, so we take $a(k + v_q) := e^{\pi i k} \delta_{v_1}(v_q)$.

Now, choose $\phi_n(k) = \frac{1}{\sqrt{N}} e^{2\pi i n k / N}$ as an eigenbasis for $\mathcal{A}_{P_N}$ with periodic conditions and consider the orthonormal sequence

$$g_n = \frac{\phi_n \otimes w_4 + \phi_{n+\frac{N}{2}} \otimes w_5}{\sqrt{2}}$$

in $\Gamma_N = P_N \otimes G_F$, for $n = 0, \dots, \frac{N}{2} - 1$, with eigenvalue $-\lambda_n = -2 \cos \frac{2\pi n}{N}$.

Since $\langle \psi, \text{Op}_N(\bar{a})\psi \rangle = 0$, it suffices to show that $\frac{1}{|\Gamma_N|} \sum_{u \in \Gamma_N} |\langle \psi_u, a\psi_u \rangle|^2$ does not converge to zero. We have

$$\begin{aligned} \langle g_n, a g_n \rangle &= \sum_{k=0}^{N-1} \sum_{q=1}^5 a(k+v_q) |g_n(k+v_q)|^2 \\ &= \frac{1}{2} \sum_{k=0}^{N-1} e^{\pi i k} |\phi_n(k) w_4(v_1) + \phi_{n+\frac{N}{2}}(k) w_5(v_1)|^2 \\ &= \frac{1}{2N} \sum_{k=0}^{N-1} e^{\pi i k} \left| \frac{e^{2\pi i n k / N}}{\sqrt{2}} + \frac{e^{2\pi i (n+\frac{N}{2}) k / N}}{2} \right|^2 \\ &= \frac{1}{4N} \sum_{k=0}^{N-1} e^{\pi i k} \left| 1 + \frac{e^{\pi i k}}{\sqrt{2}} \right|^2 \\ &= \frac{1}{4N} \sum_{k=0}^{N-1} e^{\pi i k} \left(\frac{3}{2} + \frac{e^{\pi i k} + e^{-\pi i k}}{\sqrt{2}} \right) = \frac{1}{2\sqrt{2}}. \end{aligned}$$

Thus, by completing the orthonormal family (g_n) to an o.n.b. (ψ_u) , we get

$$\frac{1}{|\Gamma_N|} \sum_{u \in \Gamma_N} |\langle \psi_u, a\psi_u \rangle|^2 \geq \frac{1}{5N} \sum_{n=0}^{\frac{N}{2}-1} |\langle g_n, a g_n \rangle|^2 = \frac{N/2}{5N} \cdot \frac{1}{8} = \frac{1}{80}.$$

This completes the proof. $\square$

4. Concrete Examples

4.1. Graphs with scalar fibers. For the adjacency matrix $H = \mathcal{A}$ on $\mathbb{Z}^d$ or the triangular lattice (sometimes called hexagonal, see [15, Fig. 3]) where each vertex has 6 neighbors, or the king's graph (sometimes called EHM lattice), we have $\nu = 1$ so Theorem 1.1 applies.

The family of periodic graphs having $\nu = 1$ is quite rich. For example, one can consider $\mathbb{Z}$ and add edges up to some fixed distance k from each vertex. More precisely,

$$(\mathcal{A}f)(n) = f(n-k) + f(n-k+1) + \dots + f(n+k-1) + f(n+k).$$

Then $V_f = \{0\}$, $\alpha_1 = \epsilon_1$ and $H(\theta_b) = 2 \cos 2\pi\theta + 2 \cos 4\pi\theta + \dots + 2 \cos 2\pi k\theta$. See Fig. 1 (left) for $k = 2$. Similar variations can be performed on $\mathbb{Z}^d$.

We remark that the connectedness of Γ is important. For example, if we consider $\mathbb{Z}$ with $(\mathcal{A}f)(n) = f(n-2) + f(n+2)$, then the graph is disconnected (there are two copies of $\mathbb{Z}$, for the even and odd vertices, respectively). Here, $V_f = \{0\}$, $\alpha_1 = \epsilon_1$ and $H(\theta_b) = 2 \cos 4\pi\theta$, which does not obey (1.3), since for $\alpha = \frac{1}{2}$, we have $E(\theta_b + \alpha_b) = E(\theta_b)$ for all θ .

4.2. Honeycomb lattice. Consider the honeycomb lattice ([15, Fig. 7], a.k.a graphene or hexagonal lattice) where each vertex has 3 neighbors. Here $v = 2$, $H(\theta_b) = \begin{pmatrix} 0 & \xi(\theta_b) \\ \xi(\theta_b) & 0 \end{pmatrix}$, where $\xi(\theta_b) = 1 + e^{-i\theta_b \cdot a_1} + e^{-i\theta_b \cdot a_2}$ for the crystal basis $a_1 = a(1, 0)$, $a_2 = \frac{a}{2}(1, \sqrt{3})$, $a > 0$. This gives the eigenvalues $\pm|\xi(\theta_b)| = \pm\sqrt{3 + 2\cos 2\pi\theta_1 + 2\cos 2\pi\theta_2 + 2\cos 2\pi(\theta_1 - \theta_2)}$. Assumption (1.3) is clearly satisfied if $w \neq s$ as the bands only meet at 0 (for $(\theta_1, \theta_2) = (\frac{2}{3}, \frac{1}{3})$). On the other hand, we can control the event that $|\xi(\theta_b + \alpha_b)| = |\xi(\theta_b)|$ by squaring, deducing as a special consequence of the arguments in Sect. 3.1 that (1.3) is satisfied. This shows that Theorem 1.2 holds true. Let us investigate (2.12).

The eigenvectors are $w_{\pm}(\theta_b) = \frac{1}{\sqrt{2}}(1, \pm e^{-i\phi(\theta_b)})^T$, where $\phi(\theta_b)$ is the argument of $\xi(\theta_b)$. So $P_{\pm}(\theta_b)f(v_1) = \frac{f(v_1) \pm e^{i\phi(\theta_b)}f(v_2)}{2}$, $P_{\pm}(\theta_b)f(v_2) = \frac{f(v_1) \pm e^{i\phi(\theta_b)}f(v_2)}{2}(\pm e^{-i\phi(\theta_b)})$. It follows that $|P_+f(v_1)|^2 + |P_-f(v_1)|^2 = \frac{|f(v_1) + e^{i\phi(\theta_b)}f(v_2)|^2 + |f(v_1) - e^{i\phi(\theta_b)}f(v_2)|^2}{4} = \frac{|f(v_1)|^2 + |f(v_2)|^2}{2} = \frac{\|f\|^2}{2} = |P_+f(v_2)|^2 + |P_-f(v_2)|^2$.

We showed that for the honeycomb lattice, (2.12) reduces to

$$\sum_{q=1}^2 \sum_{r \in \mathbb{L}_N^d} \frac{\|(U\psi)_r\|_{\mathbb{C}^v}^2}{2} \langle a(\cdot + v_q) \rangle = \frac{\langle a(\cdot + v_1) \rangle + \langle a(\cdot + v_2) \rangle}{2} \|\psi\|^2$$

which is the uniform average.

4.3. Ladder graph. Consider the ladder graph $\mathbb{Z} \square P_2$ in Fig. 2. As a Cartesian product, we already know that Proposition 1.4 holds true, but we show here that we always get the uniform average in this example.

We have $H(\theta_b)f(v_1) = e^{2\pi i\theta}f(v_1) + e^{-2\pi i\theta}f(v_1) + f(v_2)$ and $H(\theta_b)f(v_2) = e^{2\pi i\theta}f(v_2) + e^{-2\pi i\theta}f(v_2) + f(v_1)$. Thus, $H(\theta_b) = \begin{pmatrix} 2\cos 2\pi\theta & 1 \\ 1 & 2\cos 2\pi\theta \end{pmatrix}$. The eigenvalues are $E_{\pm}(\theta_b) = 2\cos 2\pi\theta \pm 1$. Clearly $(1, 1)$ and $(1, -1)$ are eigenvectors. So the eigenprojectors are $P_{\pm}(\theta_b)f = \langle w_{\pm}, f \rangle w_{\pm}$, with $w_{\pm} = \frac{1}{\sqrt{2}}(1, \pm 1)$, independently of θ . Thus, $P_{\pm}f(v_1) = \frac{f(v_1) \pm f(v_2)}{2}$ and $P_{\pm}f(v_2) = -\frac{f(v_1) \pm f(v_2)}{2}$. As in the honeycomb lattice, we deduce that (2.12) reduces to $\frac{\langle a(\cdot + v_1) \rangle + \langle a(\cdot + v_2) \rangle}{2} \|\psi\|^2$.

If we endow P_2 with a potential $Q_{\bullet}, Q_{\circ}$, then we get a ladder with a potential coming in two parallel sheets, the upper sheet only containing $Q_{\bullet}$, the lower only $Q_{\circ}$. The construction can be generalized to $\mathbb{Z} \square P_k$ to create an infinite k -strip. Proposition 1.4 continues to apply, but the average may be non-uniform.

4.4. Periodic potentials on the integer lattice. Consider $\mathbb{Z}$ endowed with a periodic potential taking v values Q_i . We have $V_f = \{1, \dots, v\}$, $a_1 = v\mathbf{e}_1$ and $b_1 = \frac{2\pi}{v}\mathbf{e}_1$.

Now $H(\theta_b)f(1) = Q_1f_1 + f_2 + e^{-2\pi i\theta}f(v)$, $H(\theta_b)f(i) = Q_if_i + f_{i-1} + f_{i+1}$ for $1 < i < v$ and $H(\theta_b)f(v) = Q_vf_v + f_{v-1} + e^{2\pi i\theta}f_1$. We thus have

$$H(\theta_b) = \begin{pmatrix} Q_1 & 1 & 0 & \dots & e^{-2\pi i\theta} \\ 1 & Q_2 & 1 & & 0 \\ & & \ddots & & \\ & & & 1 & \\ e^{2\pi i\theta} & 0 & & 1 & Q_v \end{pmatrix}.$$

Let $z = e^{2\pi i\theta}$. Expanding the determinant of the characteristic polynomial $p(z; \lambda)$ in detail, we see that [13, Lemma 3.1]

$$p(z; \lambda) = \Delta(\lambda) - z - z^{-1} \quad (4.1)$$

for some polynomial $\Delta(\lambda, Q)$. This splitting into pure λ and z parts is specific to one dimension.

Now fix $\alpha \neq 0$, let $\zeta = e^{2\pi i\alpha}$ and suppose that $E_s(\theta_b + \alpha_b) = E_w(\theta_b)$ for some s, w . Then $\lambda = E_s(\theta_b + \alpha_b)$ solves (4.1). On the other hand, $\lambda = E_s(\theta_b + \alpha_b)$ is also a root of the characteristic polynomial of $H(\theta_b + \alpha_b)$, which is

$$p(z\zeta; \lambda) = \Delta(\lambda) - z\zeta - (z\zeta)^{-1}.$$

For this choice of λ we thus have $p(\lambda; z) = p(\lambda; z\zeta) = 0$. So $z + z^{-1} = z\zeta + (z\zeta)^{-1}$. This yields a quadratic expression for z . Hence, for any fixed $\alpha \neq 0$, there are at most two θ such that $E_s(\theta_b + \alpha_b) = E_w(\theta_b)$. This implies (1.3).

The case of $\mathcal{A} + Q$ on $\mathbb{Z}^d$, $d > 1$, with $Q(n + p_j \mathbf{e}_j) = Q(n)$, is more delicate. The criterion has been established in [23] using the point of view of Bloch varieties; see Sect. 5.3 for some background. Here we simply mention that for this model, it is equivalent to study

$$\tilde{H}(\theta) = D_\theta + B_Q,$$

on $\ell^2(V_f)$, where D_θ is a diagonal operator and B_Q is a convolution given by

$$\begin{aligned} (D_\theta f)(u) &= \left(\sum_{j=1}^d 2 \cos 2\pi \left(\frac{u_j + \theta_j}{p_j} \right) \right) f(u), \\ (B_Q f)(u) &= \sum_{v_q \in V_f} \widehat{Q} \left(\frac{u - v_q}{p} \right) f(v_q), \end{aligned}$$

with $\widehat{Q}(\sigma) = \frac{1}{v} \sum_{v_n \in V_f} Q(v_n) e^{-2\pi i \sigma \cdot v_n}$ and $\frac{u}{p} := (\frac{u_1}{p_1}, \dots, \frac{u_d}{p_d})$.

Note that $V_f = \times_{j=1}^d \llbracket 0, p_j - 1 \rrbracket$, so that $v = \prod_{j=1}^d p_j$. It is not difficult to show that our operator $H(\theta_b)$ is unitarily equivalent to $\tilde{H}(\theta)$, with

$$H(\theta_b) = \mathcal{F}_\theta^{-1} \tilde{H}(\theta) \mathcal{F}_\theta,$$

where $\mathcal{F}_\theta : \ell^2(V_f) \rightarrow \ell^2(V_f)$ is given by

$$(\mathcal{F}_\theta f)(u) = \frac{1}{\sqrt{v}} \sum_{v_q \in V_f} e^{-2\pi i (\frac{u+\theta}{p}) \cdot v_q} f(v_q).$$

This equivalence is used in the proof of [23].

Back to $d = 1$, let us examine (2.12) for $\mathbb{Z}$ with a 2-periodic potential $Q_\bullet, Q_\circ$. Here $H(\theta_b) = \begin{pmatrix} Q_\bullet & 1 + e^{-2\pi i \theta} \\ 1 + e^{2\pi i \theta} & Q_\circ \end{pmatrix}$. The eigenvalues solve $(Q_\bullet - \lambda)(Q_\circ - \lambda) - (2 + 2 \cos 2\pi \theta) = 0$, so $E_\pm(\theta_b) = \frac{Q_\bullet + Q_\circ \pm c}{2}$, with $w_\pm = (\frac{Q_\bullet - Q_\circ \pm c}{2(1 + e^{2\pi i \theta})}, 1)$ and $c = \sqrt{(Q_\bullet - Q_\circ)^2 + 16 \cos^2 \pi \theta}$.

After some tedious calculations, we conclude that (2.12) takes the form

$$\begin{aligned} \langle \psi, \text{Op}_N(\bar{a}) \psi \rangle &= \sum_{q=1}^2 \langle a(\cdot + v_q) \rangle \sum_{r=0}^{N-1} \left[|P_+\left(\frac{r_b}{N}\right)(U\psi)_r(v_q)|^2 \right. \\ &\quad \left. + |P_-\left(\frac{r_b}{N}\right)(U\psi)_r(v_q)|^2 \right] \\ &= \langle a(\cdot) \rangle \sum_{r=0}^{N-1} \left[\frac{8 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} |(U\psi)_r(0)|^2 \right. \\ &\quad + \frac{8 \cos^2 \frac{\pi r}{N}}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} |(U\psi)_r(1)|^2 \\ &\quad \left. - \frac{2(Q_\circ - Q_\bullet)}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} \text{Re}(1 + e^{-\frac{2\pi i r}{N}})(U\psi)_r(0) \overline{(U\psi)_r(1)} \right] \\ &\quad + \langle a(\cdot + 1) \rangle \sum_{r=0}^{N-1} \left[\frac{8 \cos^2 \frac{\pi r}{N}}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} |(U\psi)_r(0)|^2 \right. \\ &\quad + \frac{8 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} |(U\psi)_r(1)|^2 \\ &\quad \left. + \frac{2(Q_\circ - Q_\bullet)}{16 \cos^2 \frac{\pi r}{N} + (Q_\circ - Q_\bullet)^2} \text{Re}(1 + e^{-\frac{2\pi i r}{N}})(U\psi)_r(0) \overline{(U\psi)_r(1)} \right]. \end{aligned} \quad (4.2)$$

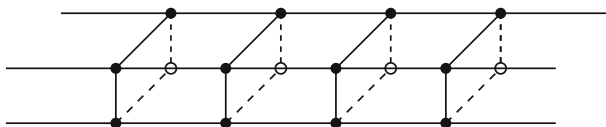
Note that if $\langle a(\cdot) \rangle = \langle a(\cdot + 1) \rangle$, this indeed reduces to $\langle a(\cdot) \rangle \|\psi\|^2$.

Let us study the expression in the limit $|Q_\circ - Q_\bullet| \rightarrow \infty$. We obtain

$$\lim_{|Q_\circ - Q_\bullet| \rightarrow \infty} \langle \psi, \text{Op}_N(\bar{a}) \psi \rangle = \langle a(\cdot) \rangle \sum_{r=0}^{N-1} |(U\psi)_r(0)|^2 + \langle a(\cdot + 1) \rangle \sum_{r=0}^{N-1} |(U\psi)_r(1)|^2.$$

Here, $(U\psi)_r(0) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-\frac{2\pi i r k}{N}} \psi(2k)$ and $(U\psi)_r(1) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{-\frac{2\pi i r k}{N}} \psi(2k+1)$. It follows that

$$\lim_{|Q_\circ - Q_\bullet| \rightarrow \infty} \langle \psi, \text{Op}_N(\bar{a}) \psi \rangle = \langle a(\cdot) \rangle \sum_{k=0}^{N-1} |\psi(2k)|^2 + \langle a(\cdot + 1) \rangle \sum_{k=0}^{N-1} |\psi(2k+1)|^2.$$

Fig. 6. The cylinder, $\mathbb{Z} \square C_4$

4.5. *Cylinders.* Consider the Cartesian product $\Gamma = \mathbb{Z} \square C_4$, where C_4 is the 4-cycle.

Given any o.n.b. (ϕ_n) for $\mathcal{A}$ on the N -path, consider the bases

$$\begin{aligned} w_1 &= \frac{1}{2}(1, 1, -1, -1), & w_2 &= \frac{1}{\sqrt{2}}(0, 1, 0, -1), \\ w_3 &= \frac{1}{\sqrt{2}}(1, 0, -1, 0), & w_4 &= (1, 1, 1, 1) \end{aligned}$$

and

$$\kappa_j = \frac{1}{2}(1, \omega^j, \omega^{2j}, \omega^{3j})$$

for $\mathcal{A}_{C_4}$, where $\omega = e^{\pi i/2}$ and $j = 0, \dots, 3$. By Proposition 1.4, we know that the orthonormal eigenbases of Γ approach some weighted averages.

If we choose the eigenbasis $\psi_{n,j} = \phi_n \otimes w_j$, then by (1.9),

$$\langle \psi_{n,j}, \text{Op}_N(\bar{a}) \psi_{n,j} \rangle = \begin{cases} \frac{1}{4} \sum_{q=1}^4 \langle a(\cdot + v_q) \rangle & \text{if } j = 1, 4 \\ \frac{\langle a(\cdot + v_2) \rangle + \langle a(\cdot + v_4) \rangle}{2} & \text{if } j = 2, \\ \frac{\langle a(\cdot + v_1) \rangle + \langle a(\cdot + v_3) \rangle}{2} & \text{if } j = 3. \end{cases}$$

On the other hand, if $\tilde{\psi}_{n,j} = \phi_n \otimes \kappa_j$, then for $j = 1, \dots, 4$,

$$\langle \tilde{\psi}_{n,j}, \text{Op}_N(\bar{a}) \tilde{\psi}_{n,j} \rangle = \frac{1}{4} \sum_{q=1}^4 \langle a(\cdot + v_q) \rangle.$$

This example shows that $\langle \psi_u^{(N)}, \text{Op}_N(\bar{a}) \psi_u^{(N)} \rangle$ in general depends on the choice of the basis, even for simple regular graphs, and it may or may not be the uniform average. In fact, this gives the uniform average for the basis $\tilde{\psi}_{n,j}$, but not for $\psi_{n,j}$, take for example the observable

$$a(i + v_1) = a(i + v_3) = -1, \quad a(i + v_2) = a(i + v_4) = 1,$$

where we parametrized the vertices of the cylinder $\mathbb{Z} \square C_4$ by $u = i + v_q$, where $i \in \mathbb{Z}$ is the layer's level and $v_q \in C_4 = (v_1, v_2, v_3, v_4)$ are the vertices within it.

The problem with $\psi_{n,j}$ is that it is concentrated on half the cylinder for $j = 2, 3$, while $\tilde{\psi}_{n,j}$ is spread on the whole. The semi-delocalization of $\psi_{n,j}$ is not detected by locally constant observables.

4.6. Boxes again. Back to Fig. 4, let us show that the graph becomes quantum ergodic once we add a potential (Q_1, Q_2) which is copied across the layers, for any $Q_1 \neq Q_2$.

First assume $(Q_1, Q_2) = (Q, -Q)$, $Q > 0$. In this case we get the Floquet eigenvalues

$$E_{\pm}(\theta_b) = 2 \cos 2\pi\theta \pm \sqrt{(1 + 2 \cos 2\pi\theta)^2 + Q^2}.$$

We now use the idea in Sect. 4.4: if for some s, w we have $E_s(\theta_b + \alpha_b) = E_w(\theta_b)$, then $\lambda = E_s(\theta_b + \alpha_b)$ solves both the characteristic polynomial of $H(\theta_b)$ and $H(\theta_b + \alpha_b)$. Denote $c_\theta := 2 \cos 2\pi\theta$. It follows that for such λ ,

$$\lambda^2 - 2c_{\theta+\alpha}\lambda - (1 + Q^2 + 2c_{\theta+\alpha}) = \lambda^2 - 2c_\theta\lambda - (1 + Q^2 + 2c_\theta)$$

In turn, this implies

$$(c_{\theta+\alpha} - c_\theta)(\lambda + 1) = 0.$$

So either $\lambda = -1$ or $c_{\theta+\alpha} - c_\theta = 0$. The case $\lambda = -1$ never happens. In fact, if $\lambda = c + \sqrt{(1+c)^2 + Q^2}$, then one can easily show that there is an M such that $\lambda \geq -1 + \frac{Q}{M} > -1$. Similarly, if $\lambda = c - \sqrt{(1+c)^2 + Q^2}$, then we can find M such that $\lambda \leq -1 - \frac{Q}{M} < -1$.

Thus, the only way the Floquet assumption can be violated is if $c_{\theta+\alpha} - c_\theta = 0$. Clearly, for a given nonzero α , only $\theta = \frac{1-\alpha}{2}$ is possible. In particular, (1.3) is satisfied.

Renumbering $v_1 \leftrightarrow v_2$ in V_f , the previous discussion also applies if $Q < 0$. Finally, any $(Q_1, Q_2) = (Q, -Q) + c_Q \text{Id}$ for $Q = \frac{Q_1 - Q_2}{2}$ and $c_Q = \frac{Q_1 + Q_2}{2}$. If $Q_1 \neq Q_2$, then $\mathcal{A}_\Gamma + (Q, -Q)$ satisfies (1.3), hence so does $\mathcal{A}_\Gamma + (Q_1, Q_2)$.

5. Complementary Results

5.1. QUE and eigenvector correlators.

5.1.1. Quantum unique ergodicity We first investigate QUE for $\mathcal{A}_\mathbb{Z}$ and $\mathcal{A}_{\mathbb{Z}^2}$.

For $\Gamma = \mathbb{Z}$, taking $\mathbb{L}_N$ with periodic conditions amounts to considering N -cycles. On C_{4N} , consider the observable $a_N = (1, 0, 1, 0, \dots, 1, 0)$ and the eigenvector $v^{(N)} = \frac{1}{\sqrt{2N}}(0, 1, 0, -1, \dots, 0, 1, 0, -1)$ with eigenvalue 0, where the string $(0, 1, 0, -1)$ is repeated N times. Then $\langle v^{(N)}, a_N v^{(N)} \rangle = 0$ while $\langle a_N \rangle = \frac{1}{2}$, so (1.10) is violated.

On $\mathbb{Z}^2$, the whole sequence may converge to a nonzero limit. If $e_\ell^{(N)}(k) = \frac{1}{N} e^{2\pi i k \cdot \ell / N}$, take $\phi_{(\ell_1, \ell_1)} = e_{(\ell_1, \ell_1)}$ and $\phi_{(\ell_1, \ell_2)} = \frac{1}{\sqrt{2}} e_{(\ell_1, \ell_2)}^{(N)} + \text{sgn}(\ell_1 - \ell_2) \frac{1}{\sqrt{2}} e_{(\ell_2, \ell_1)}^{(N)}$ if $\ell_1 \neq \ell_2$. This gives an orthonormal eigenbasis with $|\phi_{(\ell_1, \ell_2)}^{(N)}(n)|^2 = \frac{1 \pm \cos 2\pi[(\ell_1 - \ell_2)(n_1 - n_2)/N]}{N^2}$ if $\ell_1 \neq \ell_2$. So $\langle \phi_{(\ell_1, \ell_2)}, a_N \phi_{(\ell_1, \ell_2)} \rangle = \langle a_N \rangle \pm \frac{1}{N^2} \sum_n a_N(n) \cos 2\pi \frac{(\ell_1 - \ell_2)(n_1 - n_2)}{N}$. If $a_N(n) = f(n/N)$, we thus get

$$\langle \phi_{(\ell_1, \ell_2)}^{(N)}, a_N \phi_{(\ell_1, \ell_2)}^{(N)} \rangle - \langle a_N \rangle \rightarrow \pm \int_{[0,1]^2} f(x, y) \cos 2\pi(\ell_1 - \ell_2)(x - y) dx dy.$$

This is nonzero for $f(x, y) = \cos 2\pi(\ell_1 - \ell_2)(x - y)$.

5.1.2. No correlator universality We next consider the question of matrix observables.

On $\mathbb{Z}^2$, consider standard basis $(e_\ell^{(N)})_{\ell \in \mathbb{L}_N^2}$ and the basis $(\phi_\ell^{(N)})_{\ell \in \mathbb{L}_N^2}$ defined in the previous paragraph. Consider

$$K_N(n, m) = \begin{cases} 1 & \text{if } n - m = (\pm 1, 0), \\ 0 & \text{otherwise.} \end{cases}$$

Then $\langle e_\ell^{(N)}, K e_\ell^{(N)} \rangle = 2 \cos(\frac{2\pi \ell_1}{N})$, so $\frac{1}{N^2} \sum_{\ell \in \mathbb{L}_N^2} |\langle e_\ell^{(N)}, K e_\ell^{(N)} \rangle|^2 \rightarrow \int_0^1 4 \cos^2(2\pi x) dx = 2$.

On the other hand, $\langle \phi_\ell^{(N)}, K \phi_\ell^{(N)} \rangle = \cos(\frac{2\pi \ell_1}{N}) + \cos(\frac{2\pi \ell_2}{N})$, so $\frac{1}{N^2} \sum_{\ell \in \mathbb{L}_N^2} |\langle \phi_\ell^{(N)}, K \phi_\ell^{(N)} \rangle|^2 \rightarrow \int_{[0,1]^2} \cos^2(2\pi x_1) + \cos^2(2\pi x_2) + 2 \cos(2\pi x_1) \cos(2\pi x_2) dx = 1$.

This implies there can be no quantity $\langle K_N \rangle_{\lambda_j^{(N)}}$ independent of the basis such that $\frac{1}{N^2} \sum_j |\langle \psi_j^{(N)}, K_N \psi_j^{(N)} \rangle - \langle K_N \rangle_{\lambda_j^{(N)}}|^2 \rightarrow 0$.

5.1.3. Matrix generalization We finally sketch how to generalize quantum ergodicity to matrix observables K . For simplicity we only discuss the case $\nu = 1$. We may assume $V_f = \{0\}$ up to translating coordinates. Here, $H(\theta_b) = E(\theta_b)$.

For Step 1, we note that

$$(e^{itH_N} K e^{-itH_N} \psi)(k_a) = \sum_{r \in \mathbb{L}_N^d} e^{itE(\frac{r_b}{N})} (U K e^{-itH_N} \psi)_r e_r^{(N)}(k).$$

Here, $(U K e^{-itH_N} \psi)_r = \frac{1}{N^{d/2}} \sum_{n \in \mathbb{L}_N^d} e^{-\frac{ir_b}{N} \cdot n_a} (K e^{-itH_N} \psi)(n_a)$. If R is the band width, then $(K e^{-itH_N} \psi)(n_a) = \sum_{|\tau| \leq R} K(n_a, n_a + \tau_a) (e^{-itH_N} \psi)(n_a + \tau_a)$. Denote $K^\tau(n_a) := K(n_a, n_a + \tau_a)$. Next, expand $K^\tau(n_a) = \frac{1}{N^{d/2}} \sum_{m \in \mathbb{L}_N^d} K_m^\tau e^{\frac{im_b \cdot n_a}{N}}$, where $K_m^\tau = \langle e_m^{(N)}, K^\tau(\cdot_a) \rangle_{\ell^2(\mathbb{L}_N^d)}$. Then we obtain

$$\begin{aligned} (U K e^{-itH_N} \psi)_r &= \frac{1}{N^d} \sum_{n, m \in \mathbb{L}_N^d} \sum_{|\tau| \leq R} e^{-\frac{i(r_b - m_b) \cdot n_a}{N}} K_m^\tau (e^{itH_N} \psi)(n_a + \tau_a) \\ &= \frac{1}{N^{d/2}} \sum_{m \in \mathbb{L}_N^d} \sum_{|\tau| \leq R} K_m^\tau e^{\frac{i(r_b - m_b) \cdot \tau_a}{N}} (U e^{-itH_N} \psi)_{r-m}. \end{aligned}$$

From here, we proceed as before, replacing $a_m^{(N)}(v_q)$ by $\sum_{|\tau| \leq R} K_m^\tau e^{\frac{ir_b \cdot \tau_a}{N}}$. There are of course many simplifications because $\nu = 1$. In the end, $\bar{a}$ is replaced by

$$\bar{K} = \sum_{|\tau| \leq R} K_0^\tau e^{\frac{ir_b \cdot \tau_a}{N}} e_0^{(N)}(k) = \sum_{|\tau| \leq R} \langle K^\tau \rangle e^{\frac{ir_b \cdot \tau_a}{N}},$$

where $\langle K^\tau \rangle = \frac{1}{N^d} \sum_{n \in \mathbb{L}_N^d} K(n, n + \tau)$. Hence,

$$\begin{aligned} \langle \psi, \text{Op}_N(\bar{K}) \psi \rangle &= \sum_{k \in \mathbb{L}_N^d} \overline{\psi(k_a)} \sum_{r \in \mathbb{L}_N^d} (U\psi)_r \sum_{|\tau| \leq R} \langle K^\tau \rangle e^{\frac{ir_b \cdot \tau_a}{N}} e_r^{(N)}(k) \\ &= \sum_{|\tau| \leq R} \langle K^\tau \rangle \sum_{k \in \mathbb{L}_N^d} \overline{\psi(k_a)} \psi(k_a + \tau_a) = \sum_{|\tau| \leq R} \langle K^\tau \rangle \langle \psi, \psi(\cdot + \tau_a) \rangle. \end{aligned}$$

This is the same expression we stated in Sect. 1.2.2. Interestingly, by examining the proof, we see that R can be taken to increase with N , like $R \lesssim N^\delta$ with $\delta < \frac{1}{2d}$.

5.2. Bloch's theorem. We prove here a version of the Bloch theorem for discrete periodic operators. This result is well-known in the continuum, but doesn't seem to have been explored in our setting. We also comment on the corresponding eigenfunction average.

Theorem 5.1. *Let H be a periodic Schrödinger operator over the infinite periodic graph Γ , and suppose $\lambda \in \sigma(H)$. Then we may find Ψ_λ on Γ such that $H\Psi_\lambda = \lambda\Psi_\lambda$ and $\Psi_\lambda(k_a + v_n) = e^{i\theta_b \cdot k_a} f(v_n)$, for some $\theta \in [0, 1)^d$ and f on V_f .*

Similarly, if $\lambda \in \sigma(H_N)$, we may find Ψ_λ on Γ_N such that $H_N\Psi_\lambda = \lambda\Psi_\lambda$ and $\Psi_\lambda(k_a + v_n) = e^{i\frac{j_b \cdot k_a}{N}} f(v_n)$, for some $j \in \mathbb{L}_N^d$ and f on V_f .

Proof. H is unitarily equivalent to $\int_{[0,1)^d} H(\theta_b) d\theta$, so $\sigma(H) = \cup_{n=1}^v \sigma_n$, where $\sigma_n = \text{Ran } E_n(\theta_b) = [E_n^-, E_n^+]$, see [7, 15]. Hence, $\lambda \in \sigma(H)$ implies $\lambda = E_r(\theta_b)$ for some r and $\theta \in [0, 1)^d$. Let $\psi_r^{\theta_b}$ be the corresponding eigenvector on V_f and define $\Psi_\lambda(k_a + v_n) := e^{i\theta_b \cdot k_a} \psi_r^{\theta_b}(v_n)$. Then

$$\begin{aligned} H\Psi_\lambda(k_a + v_n) &= \sum_{u \sim k_a + v_n} \Psi_\lambda(u) + Q(v_n)\Psi_\lambda(k_a + v_n) \\ &= \sum_{w \sim v_n} \Psi_\lambda(w + k_a) + Q(v_n)\Psi_\lambda(k_a + v_n) \\ &= \sum_{w \sim v_n} \Psi_\lambda(k_a + \lfloor w \rfloor_a + \{w\}_a) + Q(v_n)\Psi_\lambda(k_a + v_n) \\ &= e^{i\theta_b \cdot k_a} \left(\sum_{w \sim v_n} e^{i\theta_b \cdot \lfloor w \rfloor_a} \psi_r^{\theta_b}(\{w\}_a) + Q(v_n)\psi_r^{\theta_b}(v_n) \right) \\ &= e^{i\theta_b \cdot k_a} (H(\theta_b)\psi_r^{\theta_b})(v_n) = e^{i\theta_b \cdot k_a} E_r(\theta_b)\psi_r^{\theta_b}(v_n) = \lambda\Psi_\lambda(k_a + v_n). \end{aligned}$$

The case of Γ_N is the same since $H_N \equiv \oplus_{j \in \mathbb{L}_N^d} H(\frac{j_b}{N})$. $\square$

Note that on Γ_N , we have $\|\Psi_\lambda\|^2 = \sum_{k \in \mathbb{L}_N^d} \sum_{n=1}^v |f(v_n)|^2 = N^d \|f\|_{\mathbb{C}^v}^2$. If $\tilde{\Psi}_\lambda = \frac{1}{\|\Psi_\lambda\|} \Psi_\lambda$, then $\langle \tilde{\Psi}_\lambda, a\tilde{\Psi}_\lambda \rangle = \frac{1}{N^d \|f\|_{\mathbb{C}^v}^2} \sum_{k \in \mathbb{L}_N^d} \sum_{n=1}^v |f(v_n)|^2 a(k_a + v_n) = \sum_{n=1}^v \langle a(\cdot + v_n) \rangle \frac{|f(v_n)|^2}{\|f\|_{\mathbb{C}^v}^2}$. This average is in general not uniform unless a is locally constant. This is in accord with Theorem 1.2.

Remark 5.2. Note that these Bloch functions exist even in case of flat bands. For example, in Fig. 4, instead of considering the localized functions $(\dots, 0, 0, \begin{pmatrix} 1 \\ -1 \end{pmatrix}, 0, 0, \dots)$, one can consider the Bloch function $e^{2\pi i k \cdot \theta} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, where $k \in \mathbb{Z}$ is the position. We see that this delocalized function is also an eigenvector with the same eigenvalue -1 .

This shows the limitations of this theorem; while there always exist an eigenfunction with periodic modulus (hence well distributed over the crystal and delocalized), there can also exist a lot of localized eigenfunctions for the same energy, which is the phenomenon that quantum ergodicity investigates.

5.3. Bloch varieties and assumption (1.3). Let $p(\theta; \lambda)$ be the characteristic polynomial of $H(\theta_b)$. Let $z_j = e^{2\pi i \theta_j}$. By definition (2.4), we see that $p(z; \lambda)$ is a Laurent polynomial in z and polynomial in λ .

We say that p is *irreducible* if the only way to write it as a product of two Laurent polynomials $p(z; \lambda) = f(z; \lambda)g(z; \lambda)$ is to take f or g to be a Laurent monomial $Cz_1^{a_1} \cdots z_d^{a_d}$, for some $a_j \in \mathbb{Z}$, which are the units of the ring $\mathbb{C}[z, z^{-1}, \lambda]$.

The important point in the previous definition is that the factors f, g should be Laurent polynomials of $(z; \lambda)$. For example, as we saw in (4.1), for Schrödinger operators with a periodic potential on $\mathbb{Z}$, we have $p(z; \lambda) = \Delta(\lambda) - z - z^{-1}$. In this case, studying irreducibility is equivalent to considering the polynomial

$$z^2 - z\Delta(\lambda) + 1. \quad (5.1)$$

In principle one can always write this as a product $(z - g_1(\lambda))(z - g_2(\lambda))$. However, (5.1) is actually regarded as irreducible here because $g_i(\lambda)$ are not polynomials of λ , cf. [13, p.19].

If a flat band $E_r(\theta_b) \equiv c$ exists, then the characteristic polynomial is reducible, since we then have $p(z; \lambda) = (\lambda - c)g(z; \lambda)$ for some Laurent polynomial $g(z; \lambda)$. Thus, irreducibility implies pure ac spectrum.

Irreducibility entails that the Bloch variety of H ,

$$B_H = \{(\theta, \lambda) \in \mathbb{C}^{d+1} : p(z; \lambda) = 0\}$$

cannot be written as the union of two proper analytic subsets, except for periodicity. That is, if Ω_1 and Ω_2 are two components of B_H , then $\Omega_2 = \Omega_1 + (k, 0)$ for some $k \in \mathbb{Z}^d$.

Now, let us write

$$p(z; \lambda) = (-1)^v \prod_{m=1}^K p_m(z; \lambda)$$

for some irreducible Laurent polynomials $p_m(z; \lambda)$. It is proved in [23] that if for all nonzero $\alpha \in [0, 1)^d$ and all m_1, m_2 ,

$$p_{m_1}(z; \lambda) \not\equiv p_{m_2}(\zeta z; \lambda) \quad (5.2)$$

as Laurent polynomials, where $\zeta = (e^{2\pi i \alpha_1}, \dots, e^{2\pi i \alpha_d})$ and $\zeta z := (\zeta_1 z_1, \dots, \zeta_d z_d)$, then (1.3) is satisfied. In particular, if $p(z; \lambda)$ is irreducible and for any $\zeta \neq 1$ with $|\zeta| = 1$, we have $p(z; \lambda) \not\equiv p(\zeta z; \lambda)$ as polynomials, then (1.3) is satisfied. This is a remarkable simplification as we now only need to study the condition for the characteristic polynomial, instead of the eigenvalues which may be difficult to compute or may

have complicated root expressions. This is in fact how (1.3) is established in [23], using [22].

For comparison, to establish the criterion in general, we can always argue as in Sect. 4.4, namely try to show that for *fixed* λ , there are not too many z such that $p(z, \lambda) = p(z\zeta, \lambda)$. In case of irreducibility however, we just need to show that $p(z, \lambda) \not\equiv p(z\zeta, \lambda)$ as polynomials. This can be done for example by comparing the coefficients of λ^k or z^k for some k and showing they can only be equal on a set of zero measure.

In particular, the Bloch variety for periodic Schrödinger operators on the triangular lattice and the EHM lattice is also irreducible [11], so one only needs to verify $p(z; \lambda) \not\equiv p(z\zeta; \lambda)$. The argument used in [23] applies to Schrödinger operators with a periodic potential on the triangular lattice, so they are quantum ergodic as well.

It should be noted that irreducibility is not necessary for (1.3) to hold. For example, the infinite ladder Sect. 4.3 has characteristic polynomial $(z + z^{-1} - \lambda)^2 - 1 = (z + z^{-1} + 1 - \lambda)(z + z^{-1} - 1 - \lambda)$, hence reducible. Still, (1.3) is satisfied.

Even when the characteristic polynomial is reducible, criterion (5.2) applies, and it can be much simpler to check than (1.3) directly.²

Acknowledgments The authors are thankful to Nalini Anantharaman for helpful discussions. M.S. is very thankful to Wencai Liu for discussions concerning his results [11, 12, 22, 23] on irreducibility of Bloch varieties.

Data Availability No data sets were generated during this study.

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.

References

1. Anantharaman, N.: Quantum ergodicity on regular graphs. *Commun. Math. Phys.* **353**, 633–690 (2017)
2. Anantharaman, N., Ingremeau, M., Sabri, M., Winn, B.: Quantum ergodicity for expanding quantum graphs in the regime of spectral delocalization. *Journal de Mathématiques Pures et Appliquées* **151**, 28–98 (2021)
3. Anantharaman, N., Le Masson, E.: Quantum ergodicity on large regular graphs. *Duke Math. J.* **164**, 723–765 (2015)
4. Anantharaman, N., Sabri, M.: Quantum ergodicity on graphs: from spectral to spatial delocalization. *Ann. Math.* **189**, 753–835 (2019)
5. Anantharaman, N., Sabri, M.: Quantum ergodicity for the Anderson model on regular graphs. *J. Math. Phys.* **58**, (2017)
6. Anantharaman, N., Sabri, M.: Recent results of quantum ergodicity on graphs and further investigation. *Ann. Fac. Sci. Toulouse Math.* **28**, 559–592 (2019)
7. de Monvel, A. Boutet, Sabri, M.: Ballistic transport in periodic and random media, [arXiv:2202.00940](https://arxiv.org/abs/2202.00940). Accepted in Operator Theory Advances and Applications
8. Brooks, S., Le Masson, E., Lindenstrauss, E.: Quantum ergodicity and averaging operators on the sphere. *Int. Math. Res. Not.* **2016**(19), 6034–6064 (2016)
9. Chung, F., Yau, S.T.: Discrete Green's functions. *J. Combin. Theory Ser. A* **91**(1–2), 191–214 (2000)
10. Colin de Verdière, Y.: Ergodicité et fonctions propres du laplacien. *Commun. Math. Phys.* **102**, 497–502 (1985)
11. Fillman, J., Liu, W., Matos, R.: Irreducibility of the Bloch variety for finite-range Schrödinger operators. *J. Funct. Anal.* **283**, 109670 (2022)

² Note that we only discussed the (ir)-reducibility of the *Bloch* variety here. The irreducibility of the *Fermi* variety, where λ is fixed, is significantly harder to prove [22], but we do not need it.

12. Fillman, J., Liu, W., Matos, R.: Algebraic properties of the Fermi variety for periodic graph operators. [arXiv:2305.06471](https://arxiv.org/abs/2305.06471)
13. Gieseke, D., Knörrer, H., Trubowitz, E.: The geometry of algebraic Fermi curves, volume 14 of *Perspectives in Mathematics*. Academic Press (1993)
14. Klimek, S., Kondracki, W.: Ergodic Properties of the Quantum Geodesic Flow on Tori. *Math. Phys. Anal. Geom.* **8**, 173–186 (2005)
15. Korotyaev, E., Saburova, N.: Schrödinger operators on periodic discrete graphs. *J. Math. Anal. Appl.* **420**, 576–611 (2014)
16. McKenzie, T.: The necessity of conditions for graph quantum ergodicity and Cartesian products with an infinite graph. *Comptes Rendus. Mathématique* **360**, 399–408 (2022)
17. Reed, M., Simon, B.: *Methods of Modern Mathematical Physics. Vol. 4 : Analysis of Operators*. Academic Press (1978)
18. Sabri, M., Youssef, P.: Flat bands of periodic graphs. *J. Math. Phys.* **64** (2023)
19. Simon, B.: *Basic Complex Analysis, A Comprehensive Course in Analysis, Part 2A*. AMS (2015)
20. Šnirel'man, A.I.: Ergodic properties of eigenfunctions. *Uspehi Mat. Nauk* **29**, 181–182 (1974)
21. Weichsel, P.M.: The Kronecker product of graphs. *Proc. Amer. Math. Soc.* **13**, 47–52 (1962)
22. Liu, W.: Irreducibility of the Fermi variety for discrete periodic Schrödinger operators and embedded eigenvalues. *Geom. Funct. Anal.* **32**, 1–30 (2022)
23. Liu, W.: Bloch varieties and quantum ergodicity for periodic graph operators, [arXiv:2210.10532](https://arxiv.org/abs/2210.10532). To appear in *J. Anal. Math*
24. Zelditch, S.: Uniform distribution of eigenfunctions on compact hyperbolic surfaces. *Duke Math. J.* **55**, 919–941 (1987)

Communicated by J. Ding