Ergodic Theorems for Continuous-time Quantum Walks on Crystal Lattices and the Torus

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Ergodic theorems

Time average = Space average.

If T is ergodic on (Ω, μ),

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=1}^{n} f(T^k x) = \frac{1}{\mu(\Omega)} \int_\Omega f(y)\,\mathrm{d}\mu(y)$$

Mean value of f over a trajectory starting at x is equal to the mean value over the whole space.

$\rightsquigarrow$ the orbit of x covers Ω uniformly.

Kronecker-Weyl theorem

For any $x_0 \in \mathbb{T}^d$ and a.e. y_0,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T a(x_0 + t y_0)\,\mathrm{d}t = \int_{\mathbb{T}^d} a(x)\,\mathrm{d}x\,.$$

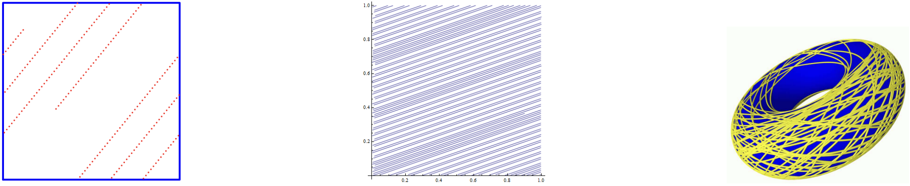


Figure – The trajectory from x_0 equidistributes along a.e. direction y_0 - Wikipedia and O. Knill (Harvard).

Case of the Sphere

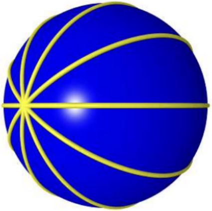


Figure – Trajectories of a free particle on the sphere (O. Knill).

Quantum analogs

Point $v \in \Omega$ $\longrightarrow$ Dirac mass $\delta_v \in \mathscr{H}$.

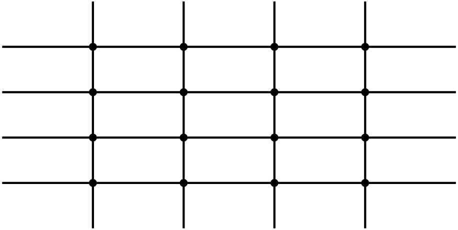
Classical trajectory $\{\phi_t(v)\}_{t \geq 0}$ $\longrightarrow$ Semigroup evolution $\mathrm{e}^{\mathrm{i}t\Delta}\delta_v$.

Mean of a over trajectory $\longrightarrow$ Mean of a over probability measure $\frac{1}{T}\int_0^T |(\mathrm{e}^{\mathrm{i}t\Delta}\delta_v)(u)|^2 \, \mathrm{d}t$

Continuous-time quantum walk

Case of $\mathbb{Z}^d$

Consider $\Lambda_N = [\![0, N-1]\!]^d$ and A_N, the adjacency matrix with periodic conditions.



Case of $\mathbb{Z}^d$

Theorem (BdM-S., AHP 24)

For any $v \in \Lambda_N$, we have for a large class of observables a_N,

$$\lim_{N\to\infty} \left| \lim_{T\to\infty} \frac{1}{T} \int_0^T \langle \mathrm{e}^{-\mathrm{i}tA_N}\delta_v, a_N \mathrm{e}^{-\mathrm{i}tA_N}\delta_v \rangle \, \mathrm{d}t - \langle a_N \rangle \right| = 0 \,,$$

where $\langle a \rangle = \frac{1}{N^d} \sum_{u\in\Lambda_N} a(u)$.

$$\sum_{u\in\Lambda_N} a(u)\mu_{v,T}^N(u) \approx \frac{1}{N^d} \sum_{u\in\Lambda_N} a(u)$$

for $\mu_{v,T}^N(u) = \frac{1}{T}\int_0^T |(\mathrm{e}^{-\mathrm{i}tA_N}\delta_v)(u)|^2 \, \mathrm{d}t$.

Case of $\mathbb{Z}^d$

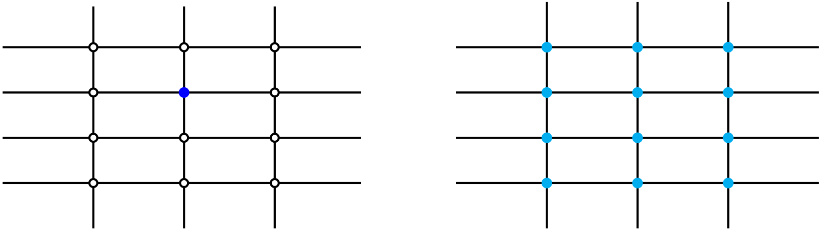


Figure – Left : point mass δ_v at time zero. Right : the density $\mu_{v,T}^N$ for $T, N \gg 0$. Qubits spread out uniformly. Very strong form of delocalization.

Here v is arbitrary. "Evolution forgets its initial state."

Note : In quantum walks literature, if $\mu_t(v) = |\mathrm{e}^{-\mathrm{i}t\mathcal{A}_{\mathbb{Z}^d}}\psi(x)|^2$ for normalized ψ, it is known that $\mu_t \xrightarrow{w} 0$. People studied limits of the process per unit time. That is, if X_t is a random vector with distribution μ_t, the limiting distribution of $\frac{X_t}{t}$.
(Konno 05 and Japanese school. See also Boutet de Monvel-Sabri 23).

Figure – Asymptotics of rescaled process for $(\mathcal{A}_{\mathbb{Z}}, \delta_0)$, $(-\Delta_{\mathbb{R}}, \chi_{[-2,2]})$.

This is not what we do here : we have a finite box with periodic conditions and consider μ_t^N itself, showing that it goes to zero with the same mass everywhere. Finiteness (and periodicity ?) are somewhat important here.

Case of $\mathbb{Z}^d$

Theorem (BdM-S., AHP 24)

For the same class of a_N, we also have for $v \neq w$,

$$\lim_{N\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_0^T \langle \mathrm{e}^{-\mathrm{i}tA_N} \delta_w, a_N \mathrm{e}^{-\mathrm{i}tA_N} \delta_v \rangle \, \mathrm{d}t = 0 \, .$$

More generally, for any ϕ, ψ of compact support, we have

$$\lim_{N\to\infty} \left| \lim_{T\to\infty} \frac{1}{T} \int_0^T \langle \mathrm{e}^{-\mathrm{i}tA_N} \phi, a_N \mathrm{e}^{-\mathrm{i}tA_N} \psi \rangle \, \mathrm{d}t - \langle a_N \rangle \langle \phi, \psi \rangle \right| = 0 \, .$$

Case of $\mathbb{Z}^d$

Proposition

There exists a sequence of observables a_N on Λ_N such that

$$\liminf_{N\to\infty} \left(\langle \mathrm{e}^{-\mathrm{i}tA_N}\delta_v, a_N \mathrm{e}^{-\mathrm{i}tA_N}\delta_v\rangle - \langle a_N\rangle\right) \geq \frac{1}{2}$$

for all time. The same statement holds for the averaged dynamics $\frac{1}{T}\int_0^T$.

Proposition

There exists a sequence of observables a_N on Λ_N such that $\langle \mathrm{e}^{-\mathrm{i}tA_N}\delta_v, a_N \mathrm{e}^{-\mathrm{i}tA_N}\delta_v\rangle$ has no limit as $t \to \infty$.

Crystal lattices

Theorem (BdM-S., AHP 24)

The theorems hold true more generally for periodic Schrödinger operators on $\mathbb{Z}^d$*-periodic graphs, provided they satisfy a certain Floquet condition.*

This condition is satisfied in particular for the adjacency matrix on infinite strips, on the honeycomb lattice, and for Schödinger operators with periodic potentials on the triangular lattice and on $\mathbb{Z}^d$*, for any* d*.*

The average $\langle a_N \rangle$ *may not be the uniform average of* a_N *in general, but a certain weighted average.*

Crystal lattices

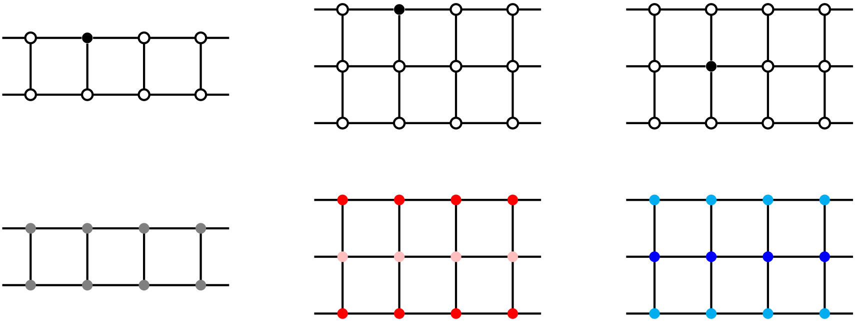


Figure – A point mass on the ladder (left) eventually equidistributes.
On the strip of width 3, if the initial point mass lies in the top layer, it eventually (center) puts $\frac{3}{8}$ of its mass over the top and bottom layers and $\frac{1}{4}$ on the middle. If the point mass was in the middle layer, it eventually (right) puts $\frac{1}{4}$ on the top and bottom layers and $\frac{1}{2}$ in the middle layer.

Crystal lattices

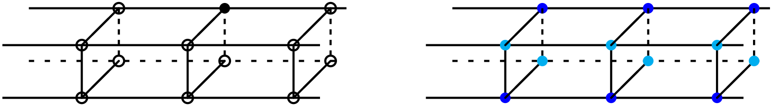


Figure – A point mass (left) will spread $\frac{3}{8}$ of its mass over both its line and the line diagonally opposite to it, and only $\frac{1}{8}$ of its mass on each of the other two lines (right). If the cyclinder has size $4N$, this means that each dark blue vertex carries a mass $\frac{3}{8N}$ and each light blue vertex carries a mass $\frac{1}{8N}$.

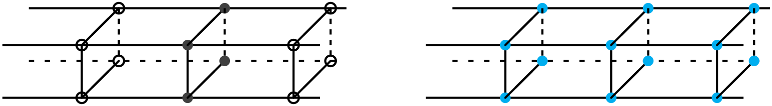


Figure – A uniform mass on V_f spreads uniformly. Not true for 3-strips.

Crystal lattices

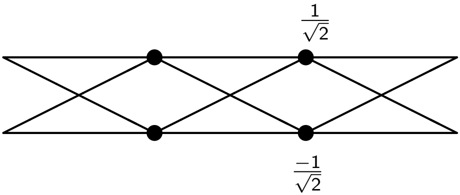


Figure – An initial state with the given weights (and zero on the remaining vertices) stays frozen and does not spread under the action of e^{-itA_N}. This graph has a flat band $\lambda = 0$.

Torus dynamics

We now work in the *continuum* $\mathbb{T}_*^d = [0,1)^d$. Our starting point (initial state) will be $y \in [0,1)^d$.

δ_y is singular. Bad for a probability density. Evolution of an L^2 state ?

We can use $\delta_y^E := \frac{1}{\sqrt{N_E}} \mathbf{1}_{\leq E}(-\Delta)\delta_y \quad$ as $E \to \infty$

or $\phi_y^\varepsilon := \frac{1}{\sqrt{\varepsilon_1 \varepsilon_2 \cdots \varepsilon_d}} \mathbf{1}_{\times_{i=1}^d [y_i, y_i+\varepsilon_i]} \quad$ as $\varepsilon \downarrow 0$

as approximations (momentum and position truncation, respectively).

Torus dynamics

Theorem (BdM-S., AHP 24)

We have for any $T > 0$,

1. *For any* $y \in \mathbb{T}_*^d$, *any* $a \in H^s(\mathbb{T}_*^d)$, $s > d/2$,

$$\lim_{E\to\infty} \frac{1}{T}\int_0^T \langle \mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E, a\mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E\rangle \,\mathrm{d}t = \int_{\mathbb{T}_*^d} a(x)\,\mathrm{d}x\,.$$

2. *If* $x \neq y$, *then for* $a \in H^s(\mathbb{T}_*^d)$, $s > d/2$,

$$\lim_{E\to\infty} \frac{1}{T}\int_0^T \langle \mathrm{e}^{\mathrm{i}t\Delta}\delta_x^E, a\mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E\rangle \,\mathrm{d}t = 0\,.$$

Torus dynamics

Theorem

3. *Result (1) remains true if* $a = a^E$ *depends on the semiclassical parameter* E*, as long as all partial derivatives of order* $\le s$ *are uniformly bounded by* cE^r *for some* $r < \frac{1}{4}$*. More precisely,* $\lim_{E\to\infty} |\frac{1}{T}\int_0^T \langle \mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E, a^E \mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E\rangle\,\mathrm{d}t - \int_{\mathbb{T}_*^d} a^E(x)\,\mathrm{d}x| = 0.$

4. *The probability measure* $\mathrm{d}\mu_{y,T}^E(x) = (\frac{1}{T}\int_0^T |\mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E(x)|^2\,\mathrm{d}t)\mathrm{d}x$ *on* $\mathbb{T}_*^d$ *converges weakly to the uniform measure* $\mathrm{d}x$ *as* $E \to \infty$*.*

$$\int_{T_*^d} a(x)\mathrm{d}\mu_{y,T}^E(x) \approx \int_{\mathbb{T}_*^d} a(x)\,\mathrm{d}x\,.$$

Torus dynamics

Figure – Left : point mass at time zero. Right : Equidistribution as soon as $T > 0$.

Lemma

Time averaging is necessary, even when $\lim_{E\to\infty}\langle \mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E, a\mathrm{e}^{\mathrm{i}t\Delta}\delta_y^E\rangle$ *exists, it generally depends on the value of* t *and it may not be equal to* $\int a(x)\,\mathrm{d}x$*.*

Theorem (BdM-S., AHP 24)

Fix any $y \in \mathbb{T}_*^d$ *and consider* $\phi_y^\varepsilon = \frac{1}{\sqrt{\varepsilon_1\varepsilon_2\cdots\varepsilon_d}}\mathbf{1}_{\times_{i=1}^d[y_i, y_i+\varepsilon_i]}$. *Then for any* $a \in H^s(\mathbb{T}_*^d)$, $s > d/2$, $T > 0$,

$$\lim_{\varepsilon\downarrow 0}\frac{1}{T}\int_0^T \langle \mathrm{e}^{\mathrm{i}t\Delta}\phi_y^\varepsilon, a\mathrm{e}^{\mathrm{i}t\Delta}\phi_y^\varepsilon\rangle\,\mathrm{d}t = \int_{\mathbb{T}_*^d} a(x)\,\mathrm{d}x\,,$$

where $\varepsilon \downarrow 0$ *means more precisely that* $\varepsilon_i \downarrow 0$ *for each* i. *If* $x \neq y$, *then*

$$\lim_{\varepsilon\downarrow 0}\frac{1}{T}\int_0^T \langle \mathrm{e}^{\mathrm{i}t\Delta}\phi_x^\varepsilon, a\mathrm{e}^{\mathrm{i}t\Delta}\phi_y^\varepsilon\rangle\,\mathrm{d}t = 0\,.$$

Furthermore, the probability measure $\mathrm{d}\mu_{y,T}^\varepsilon(x) = (\frac{1}{T}\int_0^T |\mathrm{e}^{\mathrm{i}t\Delta}\phi_y^\varepsilon(x)|^2\,\mathrm{d}t)\mathrm{d}x$ *on* $\mathbb{T}_*^d$ *converges weakly to the uniform measure* $\mathrm{d}x$ *as* $\varepsilon \downarrow 0$.

Sphere dynamics

Theorem (BdM-S., AHP 24)

Fix $\xi \in \mathbb{S}^{d-1}$*. There exists a normalized* δ_ξ*-sequence* $S_\xi^{(n)}$ *such that* $\lim_{T\to\infty} \frac{1}{T}\int_0^T |\mathrm{e}^{\mathrm{i}t\Delta} S_\xi^{(n)}(\eta)|^2 \,\mathrm{d}t$ *is not equidistributed on the sphere as* $n \to \infty$ *and actually diverges for* $\eta = \xi$*.*

If $d = 3$*, there exists an observable* a *such that its mean over* $\frac{1}{T}\int_0^T |\mathrm{e}^{\mathrm{i}t\Delta} S_\xi^{(n)}(\eta)|^2 \,\mathrm{d}t$ *does not equidistribute (even after large* T *and* n*).*

Earlier literature

- Quantum ergodicity of eigenvectors (a lot).
- Physics heuristics - uses simplicity of eigenvalues - here large multiplicity.
- Macià 2010 and Anantharaman-Macià 2014 - Schrödinger dynamics on the torus.
- Anantharaman-Rivière 2012 - dynamics on Anosov manifolds.
- Schubert 2005 - evolution of Lagrangian states.

Perspectives

- Apply the result for more examples of periodic lattices. Requires calculation of Floquet projections.
- Which discrete time quantum walks exhibit the same phenomenon ?

Remarks

The convergence of $\frac{1}{T}\int_0^T |(e^{itH}\psi)(x)|^2 \mathrm{d}t$ is quite trivial. In fact

$$|(e^{itH}\psi)(x)|^2 = \Big|\sum_{k=1}^{m} e^{itE_k}(P_k\psi)(x)\Big|^2,$$

so

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T |(e^{itH}\psi)(x)|^2 \mathrm{d}t = \sum_{k=1}^{n} |(P_k\psi)(x)|^2$$

and $\sum_x (RHS) = \|\psi\|^2$.

The difficulty is to prove the ergodicity of the map, i.e. constancy in x, not the convergence.

Physics Heuristics - From eigenfunctions to dynamics

$$
\begin{aligned}
&\langle \mathrm{e}^{-\mathrm{i}tH_N}\phi, a_N \mathrm{e}^{-\mathrm{i}tH_N}\phi\rangle \\
&\quad = \Big\langle \sum_{m=1}^{N} \langle \psi_m^{(N)}, \phi\rangle \mathrm{e}^{-\mathrm{i}t\lambda_m^{(N)}} \psi_m^{(N)}, a_N \sum_{n=1}^{N} \langle \psi_n^{(N)}, \phi\rangle \mathrm{e}^{-\mathrm{i}t\lambda_n^{(N)}} \psi_n^{(N)} \Big\rangle \\
&\quad = \sum_{n=1}^{N} |\langle \psi_n^{(N)}, \phi\rangle|^2 \langle \psi_n^{(N)}, a_N \psi_n^{(N)}\rangle \\
&\qquad + \sum_{\substack{m,n\le N \\ m\neq n}} \mathrm{e}^{\mathrm{i}t(\lambda_m^{(N)}-\lambda_n^{(N)})} \overline{\langle \psi_m^{(N)}, \phi\rangle} \langle \psi_n^{(N)}, \phi\rangle \langle \psi_m^{(N)}, a_N \psi_n^{(N)}\rangle
\end{aligned}
$$

Proof Sketch - case of $\mathbb{Z}^d$

We expand functions in the Fourier basis $e_m^{(N)}(n) = \frac{1}{N^{d/2}} \mathrm{e}^{2\pi \mathrm{i} m\cdot n/N}$.
If $\psi = \sum_{\ell \in \Lambda_N} \psi_\ell^{(N)} e_\ell^{(N)}$ then

$$(\mathrm{e}^{\mathrm{i}tA_N} a \mathrm{e}^{-\mathrm{i}tA_N} \psi)(n) = \sum_{\ell, m \in \Lambda_N} \psi_\ell^{(N)} \mathrm{e}^{\mathrm{i}t(\lambda_{\ell+m}^{(N)} - \lambda_\ell^{(N)})} a_m^{(N)} e_m^{(N)}(n) e_\ell^{(N)}(n) \,.$$

Hence,

$$\begin{aligned} \langle \mathrm{e}^{-\mathrm{i}tA_N} \delta_v, a \mathrm{e}^{-\mathrm{i}tA_N} \delta_v \rangle &= (\mathrm{e}^{\mathrm{i}tA_N} a \mathrm{e}^{-\mathrm{i}tA_N} \delta_v)(v) \\ &= \frac{1}{N^d} \sum_{w \in \Lambda_N} a(w) + \frac{1}{N^d} \sum_{\substack{m \in \Lambda_N \\ m \neq 0}} a_m^{(N)} e_m^{(N)}(v) \sum_{\ell \in \Lambda_N} \mathrm{e}^{\mathrm{i}t(\lambda_{\ell+m}^{(N)} - \lambda_\ell^{(N)})} \end{aligned}$$

Proof Sketch - Case of $\mathbb{Z}^d$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \langle \mathrm{e}^{-\mathrm{i}tA_N}\delta_v, a\mathrm{e}^{-\mathrm{i}tA_N}\delta_v\rangle \,\mathrm{d}t - \langle a\rangle$$

$$= \frac{1}{N^d}\sum_{\substack{m\in\Lambda_N\\ m\neq 0}} a_m^{(N)} e_m^{(N)}(v)\cdot \#\{\ell\in\Lambda_N : \lambda_{\ell+m}^{(N)} = \lambda_\ell^{(N)}\}\,.$$

the set in the RHS is $\approx$ a hyperplane with N^{d-1} points.

Proof Sketch

The periodic case uses Floquet theory and some analysis from McKenzie-S. 23.

The first torus theorem follows a similar strategy, but has an added T-error term. We use here that $\lambda_{\ell+m} - \lambda_\ell \to \infty$ as $|\ell| \to \infty$.

The second torus theorem is a bit different.

The sphere calculations take some efforts.

Postdoc offer

Figure – 2075 undergraduates from 120+ countries, faculty from 50+ nationalities.

Postdoc wanted !

(Unrelated : instructor also wanted, exercise sessions, no research).