Sharp Polynomial Decay Bounds for Multidimensional Periodic Schrödinger Operators

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Discrete periodic Schrödinger operators

- Setting: discrete in d dimensions $\mathcal{H} = \ell^2(\mathbb{Z}^d)$; standard basis $\{\delta_k\}_{k\in\mathbb{Z}^d}$.
- Discrete Laplacian: $\Delta : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)$, $(\Delta f)(n) = \sum_{k=1}^{d}[f(n+e_k) + f(n-e_k)]$.
- Let $V : \mathbb{Z}^d \to \mathbb{R}$ be a bounded, real-valued potential.
- Moreover, assume V is periodic with period $p = (p_1, p_2, \ldots, p_d)$, i.e. we have $V(n+p_j) = V(n)$ for $n \in \mathbb{Z}, j = 1, 2, \ldots, d$.
- $V : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)$ - multiplication operator by the potential V:

$$(Vf)(n) = V(n)f(n)\,.$$

- Hamiltonian: $H_\mu := \Delta + \mu V$, where $\mu > 0$.

Schrödinger's equation

The solution of

$$\begin{cases} i\partial_t\psi &= H_\mu\psi \\ \psi(0) &= \psi_0 \end{cases}$$

is given by

$$\psi(t) = \exp(-iH_\mu t)\psi_0.$$

Unitary time evolution:

$$\|\psi(t)\| = \|\exp(-iH_\mu t)\psi_0\| = \|\psi_0\| \quad \forall t \in \mathbb{R}.$$

We are interested in finding estimates for the following quantity:

$$|\langle\delta_k, \exp(-iH_\mu t)\delta_j\rangle|.$$

Dynamics of observables; position operator

- Dynamics of observables: $A(t) = \exp(iH_\mu t) A \exp(-iH_\mu t)$.
- Position operator: X_j, $j = 1, \ldots, d$:

$$X_j : \quad \mathrm{dom}(X_j) = \left\{ f \in \ell^2(\mathbb{Z}^d) \,\middle|\, \sum_{n \in \mathbb{Z}^d} n_j^2 |f(n)|^2 < \infty \right\}$$

$$(X_j f)(n) = n_j f(n)$$

- $X = (X_1, \ldots, X_d) : \mathrm{dom}(X) \to (\ell(\mathbb{Z}^d))^d$.

Delocalized behavior: qualitative

- $\sigma(H_\mu)$ is purely absolutely continuous.

$\Rightarrow$ Riemann-Lebesgue:

- For any $j, k \in \mathbb{Z}^d$:

$$\langle \delta_k, \exp(-iH_\mu t)\delta_j \rangle = \int_{\mathbb{R}} e^{-i\lambda t} d\mu_{k,j}(\lambda) = \int_{\mathbb{R}} e^{-i\lambda t} f_{k,j}(\lambda) d\lambda \overset{t\to\infty}{\longrightarrow} 0 \,.$$

- Consequently, for any bounded subset $R \subset \mathbb{Z}^d$, we get

$$\|\chi_R \delta_j(t)\| \overset{t\to\infty}{\longrightarrow} 0 \,.$$

- In contrast, let ψ be an eigenfunction of some selfadjoint $H : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)$, i.e. $H\psi = \lambda\psi$:

$$\|\chi_R \psi(t)\| = \|\chi_R e^{-iHt}\psi\| = \|\chi_R e^{-i\lambda t}\psi\| = \|\chi_R \psi\| \,.$$

Delocalized behavior: ballistic transport

- Asch-Knauf, Damanik-Lukic-Yessen, Fillman

Theorem (Damanik/Lukic/Yessen, Fillman)

Let X be the position operator and H a periodic Jacobi operator. Then there is a bounded selfadjoint operator Q with $\ker(Q) = \{0\}$ such that

$$s - \lim_{t\to\infty} \frac{e^{iHt}Xe^{-iHt}}{t} = Q \qquad \text{“asymptotic velocity”} .$$

- This implies that there exists $c > 0$ such that if t is large enough, one has
$$\|X(t)\delta_0\| = \|X\delta_0(t)\| \geq tc.$$
In particular, the probability of observing a particle (initially at site 0 with prob. one) at distance ct at time t is non-zero (ballistic transport).

Previous work: decay of Lieb-Robinson velocity

Theorem (Abdul-Rahman/Darras/CF/Stolz, 2024)

Let $d = 1$ and assume V is a non-degenerate periodic potential with $p \geq 2$. Then for any $\eta_0 > 0$, there are $C_1 = C_1(\eta_0, V)$, $C_2 = C_2(\eta_0, V)$, and $\mu_0 = \mu_0(\eta_0, V)$ such that

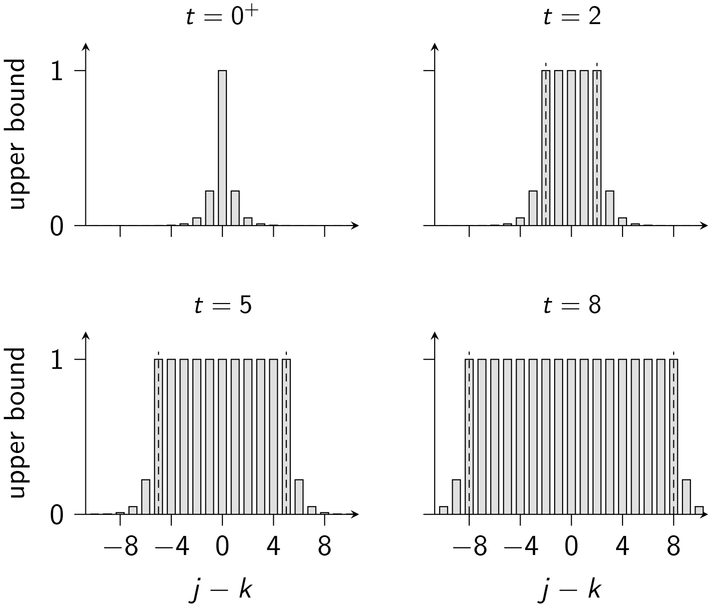
$$|\langle \delta_j, e^{-iH_\mu t} \delta_k \rangle| \leq C_1 \exp\left[-\eta_0 \left(|j-k| - \frac{C_2}{\mu}|t|\right)\right]$$

for all $t \in \mathbb{R}$, $j, k \in \mathbb{Z}$, and all $\mu \geq \mu_0$.

- C_2/μ – upper bound for "Lieb-Robinson velocity"; can be made arbitrarily small by choosing μ sufficiently large, behaves like μ^{-1}.
- If $|t| < (1-\varepsilon)\frac{|j-k|\mu}{C_2}$, we get

$$|\langle \delta_j, e^{-iH_\mu t} \delta_k \rangle| \leq C_1 e^{-\varepsilon\eta_0|j-k|}\ .$$

Visualization



Lieb-Robinson velocity vs. asymptotic velocity

Theorem Abdul-Rahman/Darras/CF/Stolz, 2024

Let $H : \ell^2(\mathbb{Z}^d) \to \ell^2(\mathbb{Z}^d)$ be a selfadjoint operator. Assume that there are constants $C < \infty, \eta > 0$ and $v > 0$ such that

$$|\langle \delta_j, e^{-iHt} \delta_k \rangle| \leq C e^{-\eta(|j-k|_1 - v|t|)}$$

for all $j, k \in \mathbb{Z}^d$ and all $t \in \mathbb{R}$. Then,

$$\limsup_{t \to \infty} \frac{1}{t} \| X e^{-itH} \delta_0 \| \leq v \,.$$

Applying this to H_μ yields

Corollary

If $\mu \geq \mu_0$, then

$$v_{asy}^{(\mu)}(\delta_0) := \limsup_{t \to \infty} \frac{1}{t} \| X e^{-itH_\mu} \delta_0 \| \leq \frac{C_2}{\mu} \,.$$

A better bound on the asymptotic velocity

Let $\gamma(V) := \min_{1\leq i<j\leq p} |V(j) - V(i)| > 0$.

Theorem (Abdul-Rahman/Darras/CF/Stolz, 2024)

Let $d = 1$ and V be non-degenerate with period p. Then, for all $\mu \geq \mu_0$, where μ_0 as in the previous theorem:

$$v_{asy}^{(\mu)}(\delta_0) \leq \frac{2^{p+1}\pi p^2}{\gamma^{p-1}} \cdot \frac{1}{\mu^{p-1}}$$

- Both upper bounds have different decay rates $\Rightarrow$ room for improvement?
- Corollary of a result by Last: $|\sigma(H_\mu)| = \mathcal{O}(1/\mu^{p-1})$.
- Additional question: higher dimensions?

Main new results: upper bound LR velocity

Theorem (Abdul-Rahman/Fillman/CF/Liu, 2025)

Suppose $V : \mathbb{Z}^d \to \mathbb{R}$ is p-periodic and non-degenerate with $p_0 := \min\{p_i : i = 1, 2, \ldots, d\}$. Then, for *any* $\eta_0 > 0$, there are constants $C, C_1, \mu_0 > 0$ depending on d, p, $\gamma(V)$, and η_0 such that for all $n, m \in \mathbb{Z}^d$ and all $\mu \geq \mu_0$, one has

$$|\langle \delta_n, e^{-itH_\mu} \delta_m \rangle| \leq C_1 e^{-\eta_0(|n-m|_1 - C_2 \mu^{-p_0+1}|t|)}$$

for all $t \in \mathbb{R}$.

Remarks:

- Improved: arbitrary dimension, decay rate
- Fly in the ointment (?): decay rate dictated by direction with smallest period

Asymptotic velocity - definitions

- $$v_{asy,j}^{(\mu)}(\psi) := \limsup_{t\to\infty} \frac{1}{t}\|X_j e^{itH_\mu}\psi\|$$
- $$v_{asy}^{(\mu)}(\psi) := \limsup_{t\to\infty} \frac{1}{t}\|X e^{itH_\mu}\psi\|$$
- $$v_{asy,j}^{(\mu)} := \sup_{\psi:\|\psi\|=1} v_{asy,j}^{(\mu)}(\psi)$$
- $$v_{asy}^{(\mu)} := \sup_{\psi:\|\psi\|=1} v_{asy}^{(\mu)}(\psi)$$

Main new results: scaling of asymptotic velocity

Theorem (Abdul-Rahman/Fillman/CF/Liu, 2025)

Suppose $V : \mathbb{Z}^d \to \mathbb{R}$ is p-periodic and non-degenerate with $p_0 := \min\{p_i : i = 1, 2, \ldots, d\}$. Then, as $\mu \to \infty$, one has

$$v_{asy,j}^{(\mu)} = C_j \mu^{-p_j+1} + \mathcal{O}(\mu^{-p_j}),$$

where $C_j > 0$ is a constant depending on V, j, and p. Moreover,

$$v_{asy,j}^{(\mu)}(\delta_0) = c_j \mu^{-p_j+1} + \mathcal{O}(\mu^{-p_j})$$

for a constant $c_j > 0$ depending on V, j, and p.

Corollary

$$v_{asy}^{(\mu)} = C\mu^{-p_0+1} + \mathcal{O}(\mu^{-p_0})$$
$$v_{asy}^{(\mu)}(\delta_0) = c\mu^{-p_0+1} + \mathcal{O}(\mu^{-p_0})$$

Main new results: lower bound LR velocity

The bound on the Lieb-Robinson velocity is optimal in the following sense:

Theorem (Abdul-Rahman/Fillman/CF/Liu, 2025)

Suppose we have a bound of the form

$$|\langle \delta_n, e^{-itH_\mu}\delta_m\rangle| \lesssim e^{-\eta_0(|n-m|_1 - v_{LR}(\mu)|t|)}, \quad \text{for all } n, m \in \mathbb{Z}^d, \; t \in \mathbb{R},$$

holds for all μ large, then $v_{LR}(\mu) \geq c\mu^{-p_0+1}$ for a constant $c > 0$.

- Follows immediately from the result on $v_{asy}^{(\mu)}(\delta_0)$ and the bound on the asymptotic velocity in terms of the LR-velocity.

On the proof

- To begin with, consider $H(\varepsilon) = \varepsilon\Delta + V$ instead of H_μ. Since $H(\varepsilon) = \varepsilon H_{1/\varepsilon}$, and thus $\exp(itH(\varepsilon)) = \exp(i\varepsilon t H_{1/\varepsilon})$, showing bounds involving μ^{-p_0+1} for the LR and asymptotic velocity of H_μ (as $\mu \to \infty$) is equivalent to showing bounds of the form ε^{p_0} for $H(\varepsilon)$ as $\varepsilon \downarrow 0$.
- Floquet-Bloch:

$$
\begin{aligned}
&|\langle \delta_j, e^{-itH(\varepsilon)}\delta_k\rangle| \\
&\doteq \left\| \int_{\mathbb{T}^d} \exp\left(-itA_\varepsilon(e^{i\theta_1}, \dots, e^{i\theta_d})\right) \exp(-i\langle j-k, \theta\rangle) \frac{d\theta}{|\mathbb{T}^d|} \right\| ,
\end{aligned}
$$

where A_ε is the associated Floquet matrix. E.g., if $d = 1$, then

$$
A_\varepsilon(e^{i\theta}) = \begin{pmatrix} V_1 & \varepsilon & & & \varepsilon e^{i\theta} \\ \varepsilon & V_2 & & & \\ & & \ddots & & \\ & & & & \varepsilon \\ \varepsilon e^{-i\theta} & & & \varepsilon & V_d \end{pmatrix}
$$

On the proof

- $$\int_{\mathbb{T}^d} \exp\left(-itA_\varepsilon(e^{i\theta_1}, \dots, e^{i\theta_d})\right) \exp(-i\langle j-k, \theta\rangle) \frac{d\theta}{|\mathbb{T}^d|}$$
$$= \frac{1}{i^d|\mathbb{T}^d|} \oint_{|z_1|=1} \cdots \oint_{|z_d|=1} e^{-itA_\varepsilon(z)} z_1^{-(j_1-k_1+1)} \cdots z_d^{-(j_d-k_d+1)}\, dz$$
- Lemma: for every (poly)annulus $\mathcal{A}$, there is ε such that for $|\varepsilon| < \varepsilon_0$ and $z \in \mathcal{A}$, the spectrum of $A_\varepsilon(z)$ is simple.
- Let $\lambda_1(\varepsilon, z), \lambda_2(\varepsilon, z), \dots, \lambda_m(\varepsilon, z)$ denote the eigenvalues of $A_\varepsilon(z)$, where $m = p_1 p_2 \cdots p_d$. Each eigenvalue $\lambda_k(\varepsilon, z)$ is an analytic function of $(\varepsilon, z) \in (-\varepsilon_0, \varepsilon_0) \times \mathcal{A}$.
- Diagonalize and deform contour:

$$\cdots = \frac{1}{i^d|\mathbb{T}^d|} \oint_{|z_1|=\rho^\pm} \cdots \oint_{|z_d|=\rho^\pm} Q_\varepsilon(z)^* \, e^{-it\mathrm{diag}(\lambda_1(\varepsilon,z),\dots,\lambda_d(\varepsilon,z))} Q_\varepsilon(z) z_1^{-(j_1-k_1+1)} \cdots z_d^{-(j_d-k_d+1)}\, dz$$

Estimate the norm:

-
$$\|\cdots\| \leq \frac{1}{|\mathbb{T}^d|}\oint_{|z_1|=\rho^\pm}\cdots\oint_{|z_d|=\rho^\pm}$$
$$\|Q(z)\|\|\mathrm{diag}(e^{-it\lambda_n(\varepsilon,z)})\|\|Q(z)^*\||z_1|^{-(j_1-k_1+1)}\cdot\cdot|z_d|^{-(j_d-k_d+1)}\,dz_1\dots dz_d$$
$$\leq C_1\exp\left(t\max_{n,z}|\mathrm{Im}\lambda_n(\varepsilon,z)|\right)\prod_{n=1}^{d}e^{-\rho_0|j_n-k_n|}.$$

Rayleigh-Schrödinger Perturbation theory

By standard Rayleigh-Schrödinger perturbation theory:

- Write $A_\varepsilon(z) = V + \varepsilon B$, where $B = B(z)$ and $B_{jj} = 0$.
- Expansion: $\lambda_n(\varepsilon, z) = \sum_{r=0}^{\infty} \lambda_n^{(r)}(z)\varepsilon^r$
- $\lambda_n^{(0)}(z) = V_n$
- $\lambda_n^{(1)}(z) = 0$
- $$\lambda_n^{(2)}(z) = \sum_{m \neq n} \frac{B_{nm}(z)B_{mn}(z)}{V_n - V_m}$$
- $$\lambda_n^{(3)}(z) = \sum_{m \neq n, m' \neq n} \frac{B_{nm}(z)B_{mm'}(z)B_{m'n}(z)}{(V_n - V_m)(V_n - V_{m'})}$$

In general:

$$\lambda_n^{(k)}(z) = \sum_{\gamma : n \to n; |\gamma| = k} f(\gamma, V)B_\gamma$$

In general:

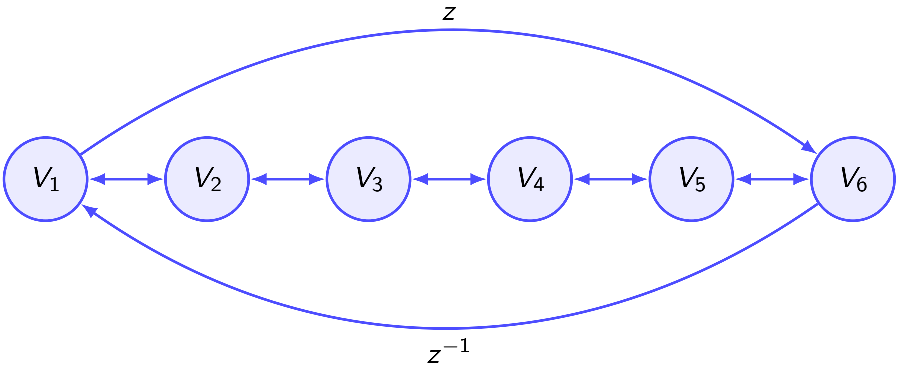
$$\lambda_n^{(k)}(z) = \sum_{\gamma: n \to n; |\gamma| = k} f(\gamma, V) B_\gamma(z)\,,$$

where for a loop $\gamma = (n, m_1, \ldots, m_{k-1}, n)$, we define

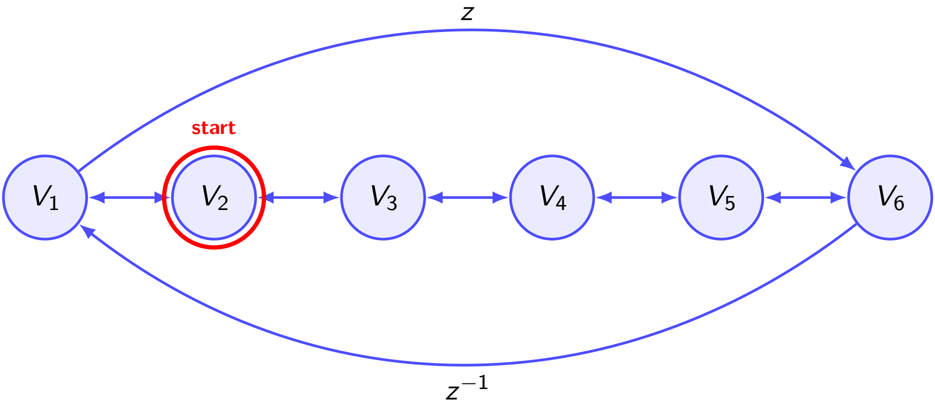
$$B_\gamma(z) = B_{nm_1}(z) B_{m_1 m_2}(z) \ldots B_{m_{k-1} n}(z)\,.$$

Note that $f(\gamma, V) \in \mathbb{R}$ for any n, k, and Z.

Example: $d = 1$, $p = 6$

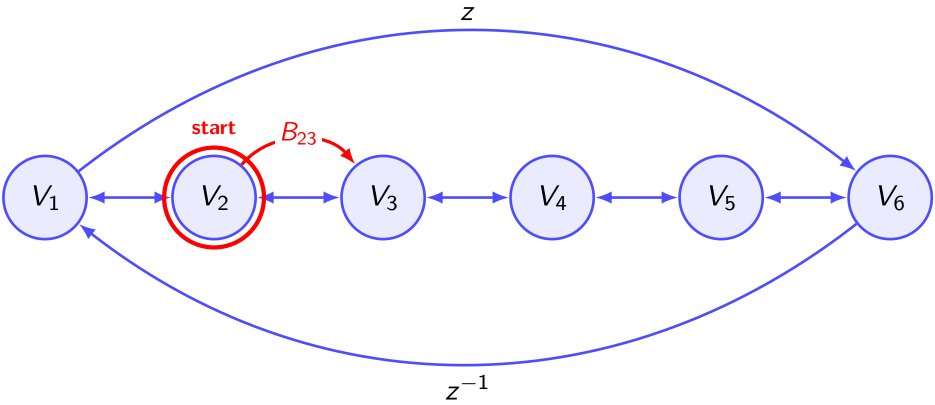


Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 3, 4, 3, 2)$



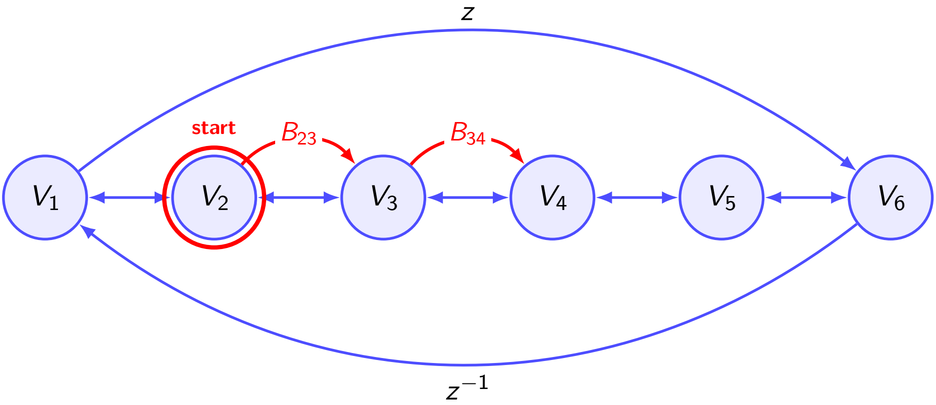
$B_\gamma =$ $\qquad\qquad =$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 3, 4, 3, 2)$



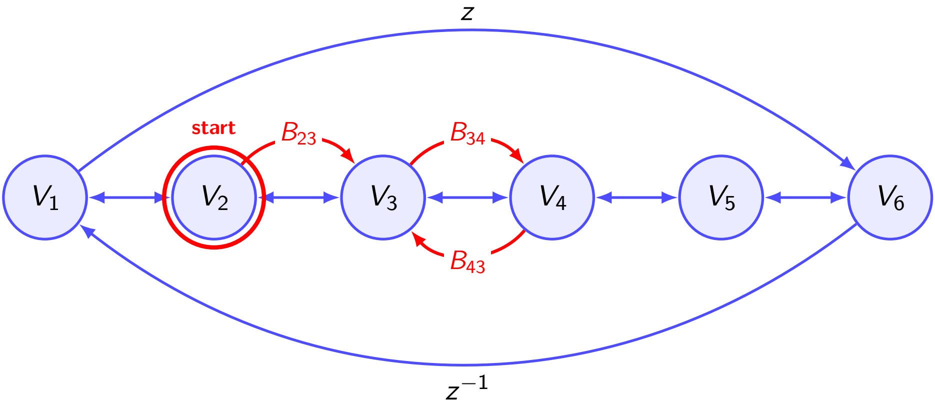
$$B_\gamma = B_{23} \qquad = 1$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 3, 4, 3, 2)$



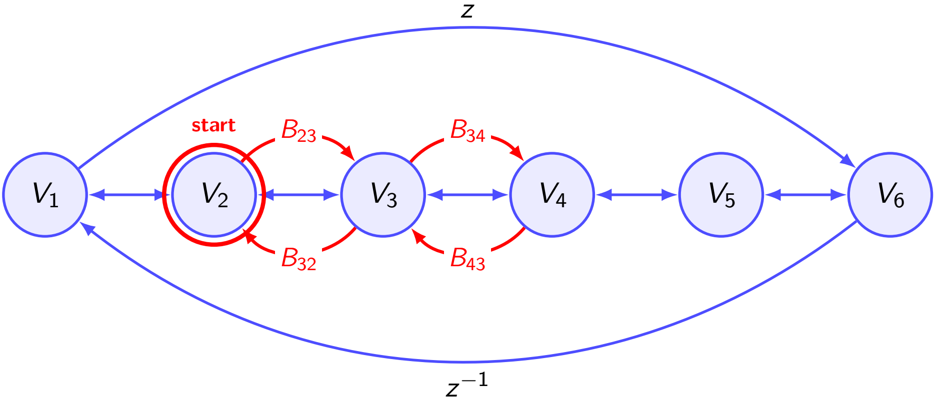
$$B_\gamma = B_{23} B_{34} \qquad = 1 \cdot 1$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 3, 4, 3, 2)$



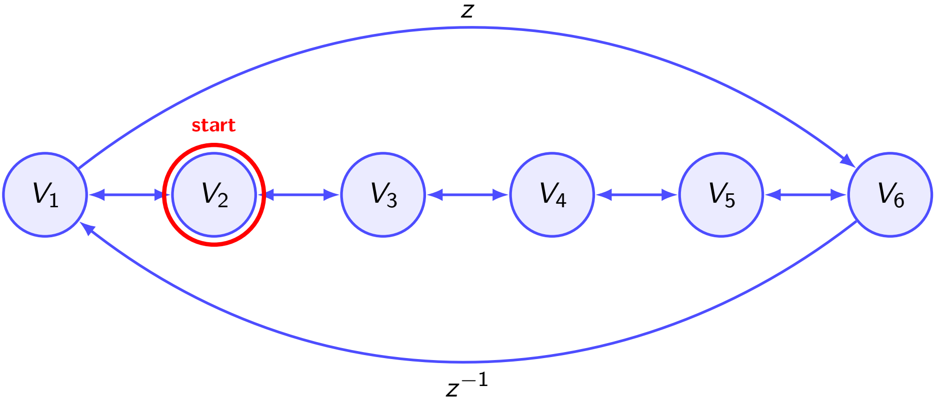
$$B_\gamma = B_{23}B_{34}B_{43} \qquad = 1 \cdot 1 \cdot 1$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 3, 4, 3, 2)$



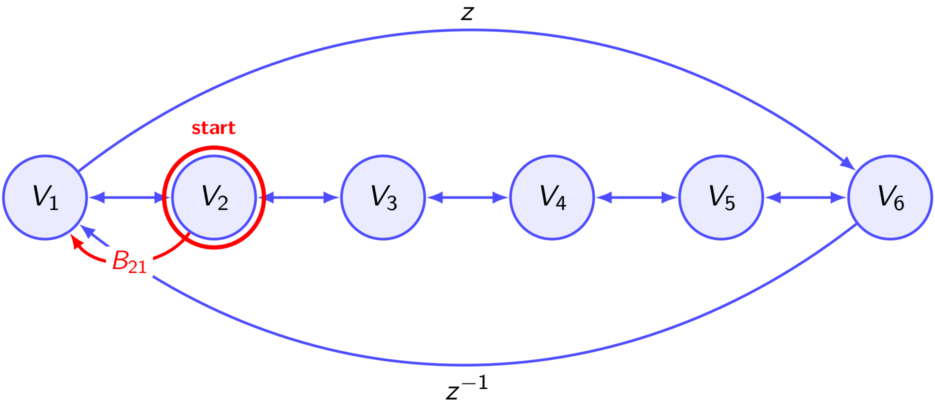
$$B_\gamma = B_{23}B_{34}B_{43}B_{32} = 1 \cdot 1 \cdot 1 \cdot 1 = 1 \in \mathbb{R}.$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 1, 6, 1, 2)$



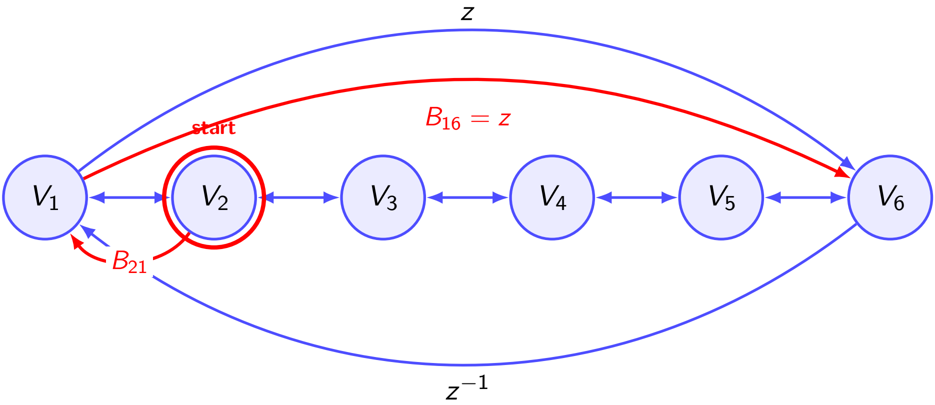
$$B_\gamma = \qquad\qquad =$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 1, 6, 1, 2)$



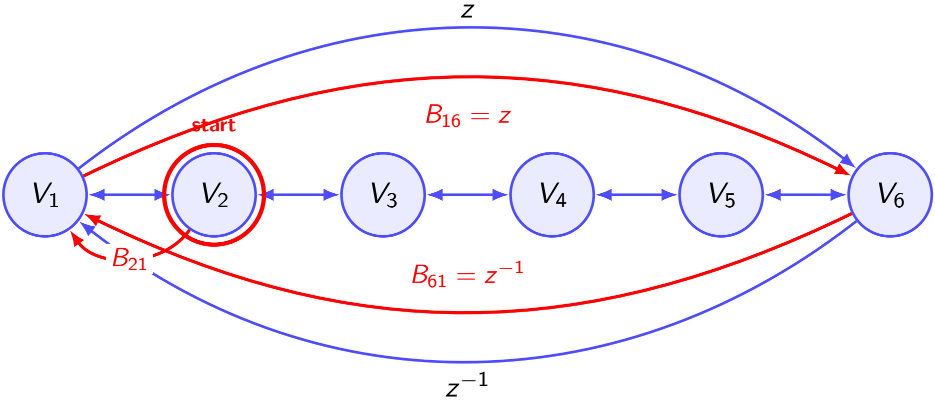
$$B_\gamma = B_{21} \qquad = 1$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 1, 6, 1, 2)$



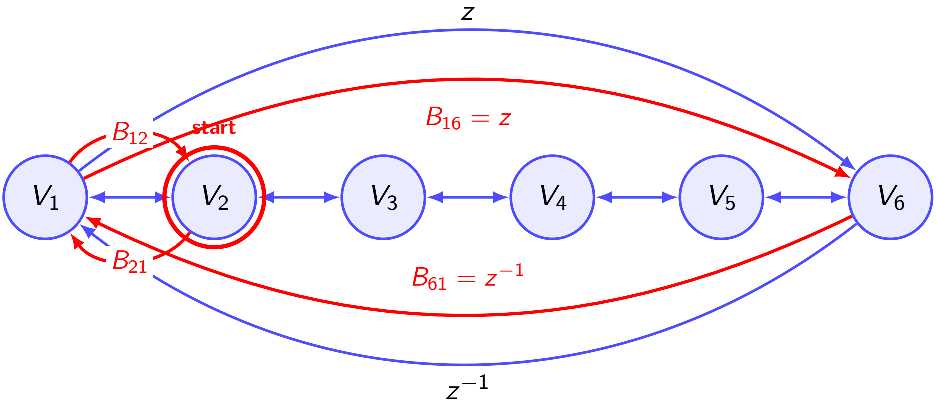
$$B_\gamma = B_{21} B_{16} \qquad = 1 \cdot z$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 1, 6, 1, 2)$



$$B_\gamma = B_{21} B_{16} B_{61} \qquad = 1 \cdot z \cdot z^{-1}$$

Example: $d = 1$, $p = 6$ – building the loop $\gamma = (2, 1, 6, 1, 2)$



$$B_\gamma = B_{21} B_{16} B_{61} B_{12} = 1 \cdot z \cdot z^{-1} \cdot 1 = 1 \in \mathbb{R}.$$

In this example, all loops γ of length 4 starting at 2 and ending at 2 will only add a real, z-independent contribution. Thus,

$$\lambda_2^{(4)}(z) = \sum_{\gamma:2\to 2;|\gamma|=4} f(\gamma, V)B_\gamma \in \mathbb{R}$$

independent of z.

First non-real and z-dependent contribution: loops of length 6

- Precisely two loops from 2 to 2 of length 6:

$$\gamma_1 = (2,3,4,5,6,1,2) \text{ and } \gamma_2 = (2,1,6,5,4,3,2)$$

  with $B_{\gamma_1} = z$, $B_{\gamma_2} = z^{-1}$, and $f(\gamma_1, V) = f(\gamma_2, V)$.
- first z-dependent contribution in the expansion of λ_2:

$$\lambda_2(\varepsilon, z) = V_2 + \varepsilon^2 \lambda_2^{(2)} + \varepsilon^4 \lambda_2^{(4)} + \varepsilon^6 f(\gamma_1, V)(z + z^{-1}) + \dots$$

Lemma

Assume V is p-periodic and non-degenerate; let $p_0 = \min\{p_1, \ldots, p_d\}$. We have:

1. If $r < p_0$, then $\lambda_n^{(r)}(z)$ is real and independent of z.
2. For $r = p_0$, $\lambda_n^{(r)}(z)$ is of the form

$$\lambda_n^{(p_0)}(z) = \sum_{j:p_j=p_0} c_{j,n}(z_j + z_j^{-1}) + \Phi_n$$

   where the $c_{j,n}$'s are nonzero real constants independent of z and Φ_n is a real constant.

If $p_0 = 1$, then $\Phi_n = 0$ and $c_{j,n} = 1$ for each j such that $p_j = p_0$.

Remarks:

- The first non-zero contribution to $|\mathrm{Im}\lambda_n(\varepsilon, z)|$ comes from the term $r = p_0$ in the series expansion $\Rightarrow$ LR-type estimate.

Last step LR-velocity

Shown before:

$$|\langle \delta_j, e^{-itH(\varepsilon)}\delta_k\rangle| \leq C_1 \exp\left(t \max_{n,z} |\mathrm{Im}\lambda_n(\varepsilon, z)|\right) \prod_{n=1}^{d} e^{-\rho_0|j_n-k_n|}$$

Last step LR-velocity

Shown before:

$$|\langle \delta_j, e^{-itH(\varepsilon)}\delta_k\rangle| \leq C_1 \exp\left(t \max_{n,z} |\mathrm{Im}\lambda_n(\varepsilon, z)|\right) \prod_{n=1}^{d} e^{-\rho_0|j_n-k_n|}$$
$$\leq C_1' e^{-\rho_0(|j-k|_1 - C_2\varepsilon^{p_0} t)}$$

$\square$

A little on the asymptotic velocity

- $$v_{asy}^{(\varepsilon)} = \max_{n,\theta,i} p_i \left| \frac{\partial \lambda_n}{\partial \theta_i}(\varepsilon, e^{\theta}) \right|$$
- By the Rayleigh-Schrödinger series lemma:

$$\max_{n,\theta,i} p_i \left| \frac{\partial \lambda_n}{\partial \theta_i}(\varepsilon, e^{i\theta}) \right| = \max_{n,\theta} \left| c_n \sin(\theta_{\hat{i}})\varepsilon^{p_0} + \mathcal{O}(\varepsilon^{p_0+1}) \right| = C\varepsilon^{p_0} + \mathcal{O}(\varepsilon^{p_0+1}).$$

- A marginally more technical but otherwise completely analogous argument yields the estimates for $v_{asy}^{\varepsilon}(\delta_0)$.

Thanks for your attention!