Convergence rates for Langevin dynamics

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Outline

General framework (1/3)

Langevin dynamics + nongradient drift term

$$\begin{cases} \mathrm{d}q_t = \frac{p_t}{m}\,\mathrm{d}t, \\ \mathrm{d}p_t = (-\nabla U(q_t) + \tau F)\,\mathrm{d}t - \xi \frac{p_t}{m}\,\mathrm{d}t + \sqrt{\frac{2}{\beta}\xi}\,\mathrm{d}W_t, \end{cases} \qquad (q,p) \in \mathcal{E},$$

- $\mathcal{E} = \mathcal{D} \times \mathbb{R}^d$ phase space, $\mathcal{D} = (2\pi\mathbb{T})^d$ compact position space
  $U : \mathcal{D} \to \mathbb{R}$ smooth periodic potential,
  $F \in \mathbb{R}^d$, $|F| = 1$, $\tau \in \mathbb{R}$, external non-gradient force
  W_t s.t. $W_{t+s} - W_t \sim \mathcal{N}(0,s)$ standard brownian motion
  $m, \xi, \beta > 0$, physical parameters
- Hamiltonian $H(q,p) = \frac{p^2}{2m} + U(q)$ (internal energy)
- Limiting regimes

$$\xi \to 0 \quad \Rightarrow \quad \text{Hamiltonian limit}$$

$$\xi \to \infty \quad \Rightarrow \quad \text{overdamped limit}$$

General framework (2/3)

Langevin dynamics + nongradient drift term

$$\begin{cases} \mathrm{d}q_t = \dfrac{p_t}{m}\,\mathrm{d}t, \\ \mathrm{d}p_t = (-\nabla U(q_t) + \tau F)\,\mathrm{d}t - \xi \dfrac{p_t}{m}\,\mathrm{d}t + \sqrt{\dfrac{2}{\beta}\xi}\,\mathrm{d}W_t, \end{cases} \qquad (q,p) \in \mathcal{E},$$

– $U = 0$: invariant *equilibrium* measure

$$\mu_{\mathrm{OU}}(\mathrm{d}q\,\mathrm{d}p) = Z_{\mu_{\mathrm{OU}}}^{-1}\,\mathrm{e}^{-\beta\frac{(p-\bar{p}_\tau)^2}{2m}}\,\mathrm{d}q\,\mathrm{d}p\,, \qquad \bar{p}_\tau = \tau m F/\xi$$

the variable p is an Ornstein-Uhlenbeck process

– $\tau = 0$: invariant *equilibrium* measure

$$\mu(\mathrm{d}q\,\mathrm{d}p) = Z_\mu^{-1}\mathrm{e}^{-\beta H(q,p)}\,\mathrm{d}q\,\mathrm{d}p$$

– $U \neq 0, \tau \neq 0$: $\exists!$ invariant *nonequilibrium* measure whose explicit form is generally unknown

General framework (3/3)

- Hypoelliptic generator of the dynamics $\underline{\mathcal{L}_{\xi,\tau} = \mathcal{L}_{\text{ham}} + \xi\mathcal{L}_{\text{FD}} + \tau\mathcal{L}_{\text{pert}}}$, with

$$\mathcal{L}_{\text{ham}} = \frac{p}{m}\cdot\nabla_q - \nabla U(q)\cdot\nabla_p, \quad \mathcal{L}_{\text{FD}} = -\frac{p}{m}\cdot\nabla_p + \beta^{-1}\Delta_p, \quad \mathcal{L}_{\text{pert}} = F\cdot\nabla_p$$

- Semigroup $T_t = \mathrm{e}^{t\mathcal{L}_{\xi,\tau}}$ defined as (setting $x = (q,p)$)

$$(T_t\varphi)(x) = \mathbb{E}_x\Big[\varphi(x_t)\Big] = \int_{\mathcal{E}}\varphi(y)\,P_t(x,\mathrm{d}y), \quad x_{t=0} = x$$

- Kolmogorov backward equation for observables $u(x,t) = \mathrm{e}^{t\mathcal{L}_{\xi,\tau}}\varphi(x)$

$$\partial_t u(x,t) = \mathcal{L}_{\xi,\tau}u_0(x)\,, \qquad u_0(x) = u(x,0) = \varphi(x)$$

- Asymptotic convergence to the average

$$u(x,t) = (\mathrm{e}^{t\mathcal{L}_{\xi,\tau}}\varphi)(x) \xrightarrow{t\to+\infty} \int_{\mathcal{E}}\varphi\underline{\psi_\tau}\,, \quad \forall\varphi\in L^2(\mu).$$

- Stationarity condition : $\{\psi_\tau$ stationary measure$\} \Leftrightarrow \Big\{\underline{\int_{\mathcal{E}}(\mathcal{L}\varphi)\,\psi_\tau = 0}\Big\}$

Convergence? How fast?

1. The stationary state

Existence and uniqueness of the stationary state (arbitrary $\tau \in \mathbb{R}$)

Hypotheses : (i) $P_t(x, \mathrm{d}y)$ is irreducible and regular

(ii) $\exists\ W : \mathcal{E} \to [1, +\infty)$ and $a > 0, b \geq 0$ such that

$$(\mathcal{L}_{\xi,\tau} W)(x) \leq -aW(x) + b, \qquad \forall x \in \mathcal{E}$$

Define $L^\infty_{W_n}(\mathcal{E}) = \left\{ \varphi \text{ measurable } \middle| \ \|\varphi\|_{L^\infty_{W_n}} = \left\| \frac{\varphi}{W_n} \right\|_{L^\infty} < +\infty \right\}$, then

Existence and uniqueness of the invariant measure ψ_τ [1]

Given $\tau_* > 0$ and $\xi > 0$, for all $\tau \in [-\tau_*, \tau_*]$, (a) $\exists!\ \psi_\tau \in C^\infty(\mathcal{E})$ stationary measure and (b) for any $n \geq 2$ there exist $C_n(\tau_*), \lambda_n(\tau_*) > 0$ such that

$$\forall t \geq 0\,, \quad \left\| \mathrm{e}^{t\mathcal{L}_{\xi,\tau}} \varphi - \int_{\mathcal{E}} \varphi \psi_\tau \right\|_{L^\infty_{W_n}} \leq C_n \mathrm{e}^{-\lambda_n t} \left\| \varphi - \int_{\mathcal{E}} \varphi \psi_\tau \right\|_{L^\infty_{W_n}}\,,$$

for any $\varphi \in L^\infty_{W_n}(\mathcal{E})$, with $W_n = 1 + |p|^n$ Lyapunov functions.

Convergence rates not quantitative! Consider $\psi_\tau = h_\tau \mu$ and work in $L^2(\mu)$.

[1] Rey-Bellet (2006), Hairer & Mattingly (2011), Lelièvre & Stoltz (2016), ...

Properties of the stationary state

1. *Non-zero average velocity* [stationarity condition with $\varphi = p$]

$$v_\tau = \mathbb{E}_\tau\left(\frac{p}{m}\right) = \frac{1}{\xi}\Big(\tau F - \mathbb{E}_\tau(\nabla U)\Big)$$

2. *Energy conservation of the global system* [stationarity condition with $\varphi = \mathcal{H}$]

$$\tau F \cdot v_\tau = 2\frac{\xi}{m}\left(\mathbb{E}_\tau\left[\frac{p^2}{2m}\right] - \frac{d}{2\beta}\right)$$

3. *Positive entropy production rate* $\left[\mathscr{H}(t) = \int_{\mathcal{E}} f_t \ln f_t \, \mathrm{d}\mu,\ f_t = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f_0\right]$

$$\beta\tau F \cdot v_\tau = \frac{\xi}{\beta}\int_{\mathcal{E}} \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu\,,$$

4. *Bound on the degenerate Fisher information* (from 1. and 3.)

$$\int_{\mathcal{E}} \frac{|\nabla_p h_\tau|^2}{h_\tau}\,\mathrm{d}\mu \leq \left(\frac{\beta\tau}{\xi}\right)^2\left(1 + \frac{\|\nabla U\|_\infty}{\tau}\right),$$

5. *Bound on the energy flow* (from 2. and 3.)

$$\mathbb{E}_\tau\left[\frac{p_i^2}{2m}\right] - \frac{1}{2\beta} \leq \frac{m}{2d}\left(\frac{\tau}{\xi}\right)^2\left(1 + \frac{\|\nabla U\|_\infty}{\tau}\right)$$

Implication of the generic convergence result

Consider the space $\mathscr{B}(E)$ of bounded operators on a generic space E, endowed with the operator norm

$$\|A\|_{\mathscr{B}(E)} = \sup_{\phi \in E \setminus \{0\}} \frac{\|A\phi\|_E}{\|\phi\|_E} .$$

The generic exponential convergence result in E implies

$$\|\mathrm{e}^{t\mathcal{L}}\varphi\|_E \leq C\mathrm{e}^{-\lambda t}\|\varphi\|_E \qquad \Rightarrow \qquad \|\mathrm{e}^{t\mathcal{L}}\|_{\mathscr{B}(E)} \leq C\mathrm{e}^{-\lambda t}$$

This allows the definition of $\mathcal{L}^{-1}$ and an estimation of its upper bound

$\mathcal{L}^{-1}$ bound

If $\|\mathrm{e}^{t\mathcal{L}}\|_{\mathscr{B}(E)} \leq C\mathrm{e}^{-\lambda t}$ holds, then the operator $\mathcal{L}^{-1} = -\int_0^\infty \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$ is a well-defined operator on E and admits the following upper bound:

$$\|\mathcal{L}^{-1}\|_{\mathscr{B}(E)} \leq \frac{C}{\lambda} .$$

Perturbation expansion of the invariant measure

Define $L_0^2(\mu) = \left\{\phi \in L^2(\mu) \;\middle|\; \int_{\mathcal{E}} \phi \, d\mu = 0 \right\}$. Since $\forall \xi > 0$ and $|F| = 1$

$$\|\mathcal{L}_{\xi,0}^{-1}\|_{\mathscr{B}(L_0^2(\mu))} \leq \frac{K}{\min(\xi, \xi^{-1})} \quad \text{and} \quad \|\mathcal{L}_{\text{pert}}\varphi\|^2_{L^2(\mu)} \leq \beta\xi^{-1} \left\langle \varphi, \mathcal{L}_{\xi,0}\varphi \right\rangle_{L^2(\mu)},$$

considering $\varphi = \mathcal{L}_{\xi,0}^{-1}\phi$ we have that

$$\forall \xi > 0, \qquad \left\|\mathcal{L}_{\text{pert}}\mathcal{L}_{\xi,0}^{-1}\right\|_{\mathscr{B}(L_0^2(\mu))} \leq \sqrt{\frac{\beta}{\xi}\left\|\mathcal{L}_{\xi,0}^{-1}\right\|_{\mathscr{B}(L_0^2(\mu))}} \leq \frac{\sqrt{\beta K}}{\min(1, \xi)}.$$

Expansion of h_τ in powers of τ [2]

Given the spectral radius $r \geq \dfrac{\sqrt{\beta K}}{\min(1, \xi)}$ of $(\mathcal{L}_{\text{pert}}\mathcal{L}_{\xi,0}^{-1})^*$, then, for $|\tau| < r^{-1}$, $\psi_\tau = h_\tau \mu$, where $h_\tau \in L^2(\mu)$ admits the following expansion in powers of τ:

$$h_\tau = \left(1 + \tau\left(\mathcal{L}_{\text{pert}}\mathcal{L}_{\xi,0}^{-1}\right)^*\right)^{-1}\mathbf{1} = \left(1 + \sum_{n=1}^{+\infty}(-\tau)^n\left[\left(\mathcal{L}_{\text{pert}}\mathcal{L}_{\xi,0}^{-1}\right)^*\right]^n\right)\mathbf{1}. \qquad (1)$$

In particular, τ can be chosen $\mathcal{O}(1)$ for large ξ.

[2] Lelivre & Stoltz (2016).

2. Exponential convergence of the law of the process

Evolution of the law of the process

[notation: $x = (q, p)$, $x_t = (q_t, p_t)$]

- Take $x_0 \sim \psi_0 = f_0\mu$, $f_0 \geq 0$ and $\int_{\mathcal{E}} f_0\mu = 1$ the (all adjoints on $L^2(\mu)$)

$$\mathbb{E}_{\psi_0}[\varphi(x_t)] = \int_{\mathcal{E}} (T_t\varphi)(x)\psi_0(x)\,\mathrm{d}x = \int_{\mathcal{E}} \varphi(x)(T_t^* f_0)(x)\mu(\mathrm{d}x)$$

- Law at time t : $\psi(t) = f(t)\,\mu$ with $f(t) = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f_0$ where

$$\mathcal{L}^*_{\xi,\tau} = -\mathcal{L}_{\mathrm{ham}} + \xi\mathcal{L}_{\mathrm{FD}} + \tau F \cdot \nabla_p^*\,, \qquad \nabla_p^* = -\nabla_p + \frac{\beta}{m}p.$$

- Fokker-Planck equation

$$\partial_t f = \left[-\left(\frac{p}{m} \cdot \nabla_q - \nabla U(q) \cdot \nabla_p\right) - \xi\beta^{-1}\nabla_p^*\nabla_p + \tau\nabla_p^* \right] f$$

- Stationary solution $h_\tau = \dfrac{\psi_\tau}{\mu}$ such that $\mathcal{L}^*_{\xi,\tau} h_\tau = 0$
- Asymptotically it is expected that

$$f(t) = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f_0 \xrightarrow{t\to+\infty} h_\tau, \quad \forall f_0 \in L^2(\mu).$$

Exponential convergence: standard hypocoercive approach

Consider

$$L^2_1(\mu) = \left\{ f \in L^2(\mu),\ \int_{\mathcal{E}} f \, d\mu = 1 \right\}, \quad \mathcal{H}(\mu) = \left\{ f \in L^2(\mu),\ (\nabla_p + \nabla_q) f \in L^2(\mu) \right\}$$

$$\langle f, g \rangle_a = \langle f, g \rangle_{L^2(\mu)} + a \left\langle (\nabla_p + \nabla_q) f, (\nabla_p + \nabla_q) g \right\rangle_{L^2(\mu)}, \text{ with } a > 0.$$

Theorem (Exponential convergence in $\mathcal{H} \cap L^2_1(\mu) \xrightarrow{\text{hypo. reg.}} L^2(\mu)$)

There exist $\tau_* > 0$ and $a(\xi) \sim \min(\xi, \xi^{-1})$ such that, for all $f \in \mathcal{H}(\mu) \cap L^2_1(\mu)$, all $\xi > 0$ and all $\tau \in [-\tau_* \min(\xi, \xi^{-1}), \tau_* \min(\xi, \xi^{-1})]$

$$\forall t \geq 0, \quad \left\| \mathrm{e}^{t \mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{a(\xi)} \leq \mathrm{e}^{-\overline{\lambda}_\tau \min(\xi, \xi^{-1}) t} \| f - h_\tau \|_{a(\xi)}, \quad \overline{\lambda}_\tau = \overline{\lambda}_0 + \mathrm{O}(\tau).$$

In addition, by hypoelliptic regularisation, $\forall f \in L^2_1(\mu)$

$$\forall t \geq 0, \qquad \left\| \mathrm{e}^{t \mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leq C \mathrm{e}^{-\overline{\lambda}_\tau \min(\xi, \xi^{-1}) t} \| f - h_\tau \|_{L^2(\mu)}.$$

- Equilibrium convergence rate $\overline{\lambda}_0 \min(\xi, \xi^{-1})$ recovered for $\tau = 0$.
- Suboptimal result for large ξ : $\tau \sim \mathcal{O}(\xi^{-1})$, while it should be $\tau \sim \mathcal{O}(1)$

Elements of proof (std hypocoercive approach, 1/2)

1. Poincaré inequality for $\mu(\mathrm{d}q, \mathrm{d}p) = \nu(\mathrm{d}q)\kappa(\mathrm{d}p)$

$$\forall g \in H^1(\mu) \cap L_0^2(\mu), \qquad \|g\|_{L^2(\mu)}^2 \leq \frac{1}{K_\nu^2}\|\nabla_q g\|_{L^2(\mu)}^2 + \frac{1}{K_\kappa^2}\|\nabla_p g\|_{L^2(\mu)}^2.$$

with $K_\kappa = \sqrt{\beta/m}$ and $K_\nu < 2\,(2\pi)^2 \mathrm{e}^{\beta(U_{\max} - U_{\min})}$

2. Define the domain $D(\mathcal{L}_{\xi,\tau}^*) = \{f \in L^2(\mu),\ \mathcal{L}_{\xi,\tau} f \in L^2(\mu)\}$ and

$$f(t) = \mathrm{e}^{t\mathcal{L}_{\xi,\tau}^*} f - h_\tau\,, \quad \Rightarrow \quad \int_{\mathcal{E}} f(t)\mu = 0, \quad \forall t \geq 0$$

3. Formally $\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2}\|f(t)\|_{a(\xi)}^2\right) = \langle f(t), \mathcal{L}_{\xi,\tau}^* f(t)\rangle_{a(\xi)}$ thus we need to prove

$$\forall g \in D(\mathcal{L}_{\xi,\tau}^*) \cap L_0^2(\mu), \qquad \left\langle g, \mathcal{L}_{\xi,\tau}^* g\right\rangle_{a(\xi)} \leq -\lambda(\xi,\tau)\|g\|_{a(\xi)}^2,$$

Elements of proof (std hypocoercive approach, 2/2)

4. Introduce $X^T = \left(\|\nabla_p g\|_{L^2(\mu)} \; \|\nabla_q g\|_{L^2(\mu)} \right)$ then

$$\left\langle g, -\mathcal{L}^*_{\xi,\tau} g \right\rangle_{a(\xi)} \geq X^T \Big(S(\xi) - |\tau| T(\xi) \Big) X \geq \lambda(\xi,\tau) X^T P(\xi) X \geq \lambda(\xi,\tau) \|g\|^2_{a(\xi)}$$

where

$$S = \begin{pmatrix} S_{pp}(\xi) & S_{qp}(\xi) \\ S_{qp}(\xi) & S_{qq}(\xi) \end{pmatrix}, \quad T = \begin{pmatrix} T_{pp}(\xi) & T_{qp}(\xi) \\ T_{qp}(\xi) & T_{qq}(\xi) \end{pmatrix},$$

$$P = \begin{pmatrix} a(\xi) + K_\kappa^{-2} & a(\xi) \\ a(\xi) & a(\xi) + K_\nu^{-2} \end{pmatrix}$$

5. Choose $\lambda(\xi,\tau)$ as the smallest non-zero eigenvalue of

$$\Big(S(\xi) - |\tau| T(\xi) \Big) P(\xi)^{-1}$$

6. Find explicit behavior in ξ in the two limiting regimes by appropriately imposing the condition of positive definiteness of matrix.

Exponential convergence: direct $L^2(\mu)$ estimates

Direct approach to hypocoercivity in $L^2(\mu)$ [3]

Theorem (Exponential convergence in $L^2(\mu)$)

There exist $C, \tau_* > 0$ such that, for all $\tau \in [-\tau^* \min(\xi, 1), \tau^* \min(\xi, 1)]$ and all $\xi \in (0, +\infty)$

$$\forall f \in L^2_1(\mu),\ \forall t \geq 0, \qquad \left\| \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leq C\mathrm{e}^{-\overline{\lambda}_\tau \min(\xi,\xi^{-1})t} \| f - h_\tau \|_{L^2(\mu)}.$$

Moreover, $\overline{\lambda}_\tau = \overline{\lambda}_0 + \mathrm{O}(\tau)$.

Optimal behavior for large ξ :

$\tau \sim \mathcal{O}(1)$ consistently with the well-definiteness of h_τ perturbation expansion.

[3] Dolbeault, Mouhot and Schmeiser, C. R. Math. Acad. Sci. Paris (2009) and Trans. AMS, **367**, 3807–3828 (2015).

Sketch of the proof

1. Projector $\Pi : L^2(\mu) \to L^2(\nu)$ such as $(\Pi g)(q) = \int_{\mathbb{R}^{Nd}} g(q,p)\, \kappa(\mathrm{d}p)$
2. Modified squared norm with $A = -\left(1 - \Pi \mathcal{L}_{\mathrm{ham}}^2 \Pi\right)^{-1} \Pi \mathcal{L}_{\mathrm{ham}}$

$$\mathscr{E}(g) = \frac{1}{2}\|g\|^2_{L^2(\mu)} + a(\xi)\, \langle A\, g, g\rangle_{L^2(\mu)}\,,$$

3. $(-\mathcal{L}^*_{\xi,\tau})$ is **coercive** in $L^2_0(\mu)$ wrt the scalar product $\langle\langle \cdot,\cdot \rangle\rangle$ induced by $\mathscr{E}$

$$\langle\langle -\mathcal{L}^*_{\xi,\tau} g, g \rangle\rangle \geq \lambda \|g\|^2_{L^2(\mu)}, \qquad g \in C^\infty \cap L^2_0(\mu)$$

(ingredients: Poincaré inequality, $\mathcal{L}_{\mathrm{ham}} A^*$ and $\mathcal{L}_{\mathrm{pert}} A^*$ bounded in $L^2_0(\mu)$)

4. Given $\mathscr{E}(f(t)) = \mathscr{H}(t)$ with $f(t) = \mathrm{e}^{t\mathcal{L}^*_{\xi,\tau}} f - h_\tau$ it holds

$$\mathscr{H}'(t) \leq -\frac{2\lambda}{1+a(\xi)} \mathscr{H}(t) \xrightarrow{\text{Gronwall}} \mathscr{H}(t) \leq \mathrm{e}^{-\frac{2\lambda}{1+a(\xi)}\, t} \mathscr{H}(0)$$

5. Conclude by norm equivalence between $\mathscr{E}(g)$ and $\|g\|_{L^2(\mu)}$ (uniform in ξ).

3. Numerical estimation

Galerkin discretization (d=1)

Computation of the spectral gap of $\mathcal{L}_{\xi,\tau}$

$$\gamma(\xi,\tau) \doteq \min\left\{\mathrm{Re}(z),\, z \in \sigma(-\mathcal{L}_{\xi,\tau})\backslash\{0\}\right\}, \quad \gamma(\xi,\tau) \geq \overline{\lambda}_\tau \min(\xi, \xi^{-1}).$$

- Equilibrium measure is a product measure $\mu = \nu \times \kappa$ with

$$\nu(\mathrm{d}q) = Z_\nu^{-1}\, \mathrm{e}^{-\beta U(q)}\, \mathrm{d}q, \quad \kappa(\mathrm{d}p) = \left(\frac{\beta}{2\pi m}\right)^{3N/2} \prod_{i=1}^{3N} \mathrm{e}^{-\frac{\beta}{2m} p_i^2}\, \mathrm{d}p_i.$$

- Discretization basis: Hermite polynomials in p and weighted Fourier modes

$$\psi_{nk}(q,p) = G_k(q) H_n(p), \qquad n \in \{0,\dots,N\}, \quad k \in \{-K,\dots,K\}$$

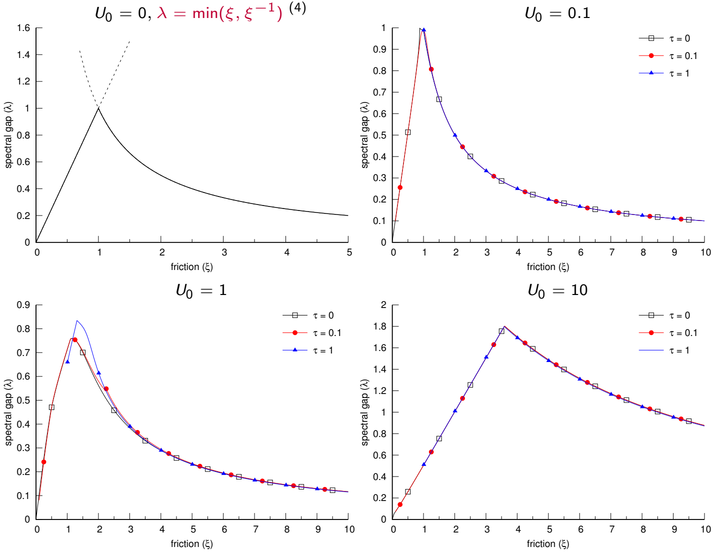
  $\{\psi_{nk}(q,p)\}_{n\in[0,N],k\in[-K,K]}$ orthonormal basis in $L^2(\mu)$, complete for $N, K \to \infty$.

- Matrix representation of $\mathcal{L}_{\xi,\tau}$ as $\left[\hat{L}_{\xi,\tau}\right]_{n'k',nk} = \left\langle \psi_{n'k'}, \mathcal{L}_{\xi,\tau}\psi_{nk}\right\rangle_{L^2(\mu)}$

$$\hat{L} = \begin{pmatrix} \hat{0} & \hat{A}_1 & \hat{0} & \cdots & \cdots & \hat{0} \\ \hat{B}_1 & -\hat{C}_1 & \hat{A}_2 & & & \vdots \\ \hat{0} & \hat{B}_2 & -\hat{C}_2 & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & \ddots & \vdots \\ \vdots & & & \ddots & -\hat{C}_{N-1} & \hat{A}_N \\ \hat{0} & \cdots & \cdots & \cdots & \hat{B}_N & -\hat{C}_N \end{pmatrix}, \quad \begin{matrix} \{\hat{A}_i\}_{n\times n}, \\ \{\hat{B}_i\}_{n\times n}, \\ \{\hat{C}_i\}_{n\times n}, \end{matrix} \quad n = 2K+1\,.$$

Numerical results

$[\beta = 1,\ m = 1,\ U(q) = U_0(1 - \cos q)]$



[4] Kozlov, S. M., Math. Notes **45**, 360-368 (1989) and I., PhD Thesis, (2017).