Hypocoercivity without changing the scalar product

Gabriel STOLTZ

(CERMICS, Ecole des Ponts & MATHERIALS team, Inria Paris)

Research funded by ANR SINEQ and ERC Synergy EMC2

Bernoulli, Lausanne, July 2025

Outline of the talk

- **Some hypocoercive dynamics**
  - Langevin dynamics and its overdamped limit
- **Longtime convergence of overdamped Langevin dynamics**
  - Poincaré inequalities
  - Estimates on the asymptotic variance
- **Longtime convergence of “hypocoercive” ODEs**
- **Longtime convergence of Langevin dynamics**
  - The need for a modified scalar product
  - One L^2-hypocoercive approach for Langevin dynamics
  - Direct estimates on the variance
  - Space-time approaches

Some hypocoercive dynamics

Langevin dynamics (1)

Computation of high-dimensional integrals... Ergodic averages

$$\int_{\mathcal{E}} \varphi \, d\mu = \lim_{t \to +\infty} \widehat{\varphi}_t, \qquad \widehat{\varphi}_t = \frac{1}{t} \int_0^t \varphi(q_s, p_s) \, ds$$

Almost-sure convergence (Kliemann, *Ann. Probab.* 1987)

- Positions $q \in \mathcal{D} = (L\mathbb{T})^d$ or $\mathbb{R}^d$, momenta $p \in \mathbb{R}^d$
$\rightarrow$ phase-space $\mathcal{E} = \mathcal{D} \times \mathbb{R}^d$

- Hamiltonian $H(q,p) = V(q) + \dfrac{1}{2} p^\top M^{-1} p$

Stochastic perturbation of the Hamiltonian dynamics (friction $\gamma > 0$)

$$\begin{cases} dq_t = M^{-1} p_t \, dt \\ dp_t = -\nabla V(q_t) \, dt - \gamma M^{-1} p_t \, dt + \sqrt{\dfrac{2\gamma}{\beta}} \, dW_t \end{cases}$$

Langevin dynamics (2)

- Evolution semigroup $\left(\mathrm{e}^{t\mathcal{L}}\varphi\right)(q,p) = \mathbb{E}\left[\varphi(q_t,p_t)\,\middle|\,(q_0,p_0)=(q,p)\right]$

- Generator of the dynamics $\mathcal{L}$

$$\frac{d}{dt}\left(\mathbb{E}\left[\varphi(q_t,p_t)\,\middle|\,(q_0,p_0)=(q,p)\right]\right) = \mathbb{E}\left[(\mathcal{L}\varphi)(q_t,p_t)\,\middle|\,(q_0,p_0)=(q,p)\right]$$

Generator of the Langevin dynamics $\mathcal{L} = \mathcal{L}_{\mathrm{ham}} + \gamma\mathcal{L}_{\mathrm{FD}}$

$$\mathcal{L}_{\mathrm{ham}} = p^\top M^{-1}\nabla_q - \nabla V^\top \nabla_p, \qquad \mathcal{L}_{\mathrm{FD}} = -p^\top M^{-1}\nabla_p + \frac{1}{\beta}\Delta_p$$

- Existence and uniqueness of the invariant measure characterized by

$$\forall \varphi \in C_{\mathrm{c}}^\infty(\mathcal{E}), \qquad \int_{\mathcal{E}} \mathcal{L}\varphi\, d\mu = 0$$

- Here, canonical measure

$$\mu(dq\,dp) = Z^{-1}\mathrm{e}^{-\beta H(q,p)}\,dq\,dp = \nu(dq)\,\kappa(dp)$$

Fokker–Planck equations

- Evolution of the law $\psi(t,q,p)$ of the process at time $t \geqslant 0$

$$\frac{d}{dt}\left(\int_{\mathcal{E}} \varphi\, \psi(t)\right) = \int_{\mathcal{E}} (\mathcal{L}\varphi)\, \psi(t)$$

- Fokker–Planck equation (with $\mathcal{L}^\dagger$ adjoint of $\mathcal{L}$ on $L^2(\mathcal{E})$)

$$\partial_t \psi = \mathcal{L}^\dagger \psi$$

- It is convenient to work in $L^2(\mu)$ with $f(t) = \psi(t)/\mu$
  - denote the adjoint of $\mathcal{L}$ on $L^2(\mu)$ by $\mathcal{L}^*$

$$\mathcal{L}^* = -\mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}, \quad \mathcal{L}_{\mathrm{FD}} = -\frac{1}{\beta}\sum_{i=1}^d \partial_{p_i}^* \partial_{p_i}, \quad \mathcal{L}_{\mathrm{ham}} = \frac{1}{\beta}\sum_{i=1}^d \partial_{p_i}^* \partial_{q_i} - \partial_{q_i}^* \partial_{p_i}$$

  - Fokker–Planck equation $\partial_t f = \mathcal{L}^* f$

Convergence results for $\mathrm{e}^{t\mathcal{L}}$ on $L^2(\mu)$ very similar to the ones for $\mathrm{e}^{t\mathcal{L}^*}$

Hamiltonian and overdamped limits

- As $\gamma \to 0$, the Hamiltonian dynamics is recovered

$$\frac{d}{dt}\mathbb{E}\left[H(q_t,p_t)\right] = -\gamma\left(\mathbb{E}\left[p_t^\top M^{-2} p_t\right] - \frac{1}{\beta}\mathrm{Tr}(M^{-1})\right) dt$$

Time $\sim \gamma^{-1}$ to change energy levels in this limit[1]

- Overdamped limit $\gamma \to +\infty$ with $M = \mathrm{Id}$: rescaling of time γt

$$\begin{aligned} q_{\gamma t} - q_0 &= -\frac{1}{\gamma}\int_0^{\gamma t} \nabla V(q_s)\, ds + \sqrt{\frac{2}{\gamma\beta}} W_{\gamma t} - \frac{1}{\gamma}\left(p_{\gamma t} - p_0\right) \\ &= -\int_0^t \nabla V(q_{\gamma s})\, ds + \sqrt{2\beta^{-1}} B_t - \frac{1}{\gamma}\left(p_{\gamma t} - p_0\right) \end{aligned}$$

which converges to the solution of $dQ_t = -\nabla V(Q_t)\, dt + \sqrt{2\beta^{-1}}\, dB_t$

- In both cases, slow convergence, with rate scaling as $\min\left(\gamma, \gamma^{-1}\right)$

[1] Hairer and Pavliotis, *J. Stat. Phys.*, **131**(1), 175-202 (2008)

Statistical error (1)

- **Asymptotic variance** $\sigma_\varphi^2 = \lim_{t\to+\infty} t \, \mathrm{Var}_\mu(\widehat{\varphi}_t)$: with $\Pi\varphi = \varphi - \int_{\mathcal{E}} \varphi \, d\mu$,

$$\sigma_\varphi^2 = \lim_{t\to+\infty} \int_0^t \left(1 - \frac{s}{t}\right) \mathbb{E}_\mu \left[\Pi\varphi(q_t,p_t)\Pi\varphi(q_0,p_0)\right] ds$$

$$= 2\int_0^{+\infty} \int_{\mathcal{E}} (\mathrm{e}^{s\mathcal{L}}\Pi\varphi)\Pi\varphi \, d\mu \, ds = 2\int_{\mathcal{E}} (-\mathcal{L}^{-1}\Pi\varphi)\Pi\varphi \, d\mu$$

Well-defined provided $-\mathcal{L}\Phi = \Pi\varphi$ has a solution in $L_0^2(\mu) = \Pi L^2(\mu)$

A Central Limit Theorem holds[2] in this case: $\boxed{\widehat{\varphi}_t - \mathbb{E}_\mu(\varphi) \simeq \frac{\sigma_\varphi}{\sqrt{t}} \mathcal{G}}$

- Sufficient condition: integrability of the semigroup, *e.g.*

$$\left\| \mathrm{e}^{t\mathcal{L}} \right\|_{\mathcal{B}(L_0^2(\mu))} \leqslant C \mathrm{e}^{-\lambda t}, \qquad -\mathcal{L}^{-1} = \int_0^{+\infty} \mathrm{e}^{s\mathcal{L}} \, ds$$

Question: dependence of σ_φ^2 on friction γ, potential V, ...

[2] R. N. Bhattacharya, *Z. Wahrsch. Verw. Gebiete* (1982)

Statistical error (2)

Prove exponential convergence of the semigroup $\mathrm{e}^{t\mathcal{L}}$ on $E \subset L_0^2(\mu)$

- Lyapunov techniques[3] $L^\infty_{\mathscr{K}}(\mathcal{E}) = \left\{ \varphi \text{ measurable}, \sup \left| \frac{\varphi}{\mathscr{K}} \right| < +\infty \right\}$
- "historic" hypocoercive[4] setup $H^1(\mu)$
- $L^2(\mu)$ after hypoelliptic regularization[5] from $H^1(\mu)$
- direct transfer from $H^1(\mu)$ to $L^2(\mu)$ by spectral argument[6]
- directly[7] $L^2(\mu)$ (recently[8] Poincaré using $\partial_t - \mathcal{L}_{\mathrm{ham}}$)
- coupling arguments[9]
- direct estimates on the resolvent using Schur complements[10]

Rate of convergence $\min\left(\gamma, \gamma^{-1}\right)$ so variance $\sim \max\left(\gamma, \gamma^{-1}\right)$

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[3] Wu ('01); Mattingly/Stuart/Higham ('02); Rey-Bellet ('06); Hairer/Mattingly ('11)

[4] Villani (2009) and before Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004),...

[5] Hérau, *J. Funct. Anal.* (2007)

[6] Deligiannidis/Paulin/Doucet, *Ann. Appl. Probab.* (2020)

[7] Hérau (2006), Dolbeaut/Mouhot/Schmeiser (2009, 2015)

[8] Albritton/Armstrong/Mourrat/Novack (2019), Cao/Lu/Wang (2019), Brigatti (2021), Dietert/Hérau/Hutridurga/Mouhot (2022), Brigati/Stoltz (2023)

[9] Eberle/Guillin/Zimmer, *Ann. Probab.* (2019)

[10] Bernard/Fathi/Levitt/Stoltz, *Annales Henri Lebesgue* (2022)

Convergence of overdamped Langevin dynamics

Overdamped Langevin dynamics and its generator

- Generator of overdamped Langevin dynamics (advection/diffusion)

$$\mathcal{L}_{\mathrm{ovd}} = -\nabla V(q) \cdot \nabla_q + \frac{1}{\beta}\Delta_q = -\frac{1}{\beta}\sum_{i=1}^{d} \partial_{q_i}^* \partial_{q_i}$$

hence self-adjoint on $L^2(\nu)$ with $\nu(dq) = Z_\nu^{-1} \mathrm{e}^{-\beta V(q)}\, dq$

- Solution $\varphi(t) = \mathrm{e}^{t\mathcal{L}_{\mathrm{ovd}}}\varphi_0$ to $\partial_t \varphi(t) = \mathcal{L}_{\mathrm{ovd}}\varphi(t)$: mass preservation

$$\frac{d}{dt}\left(\int_{\mathcal{D}} \varphi(t)\,\nu\right) = \int_{\mathcal{D}} \mathcal{L}_{\mathrm{ovd}}\varphi(t)\,\nu = \int_{\mathcal{D}} \varphi(t)\,(\mathcal{L}_{\mathrm{ovd}}\mathbf{1})\,\nu = 0$$

Suggests the longtime limit $\varphi(t) \xrightarrow[t\to+\infty]{} \int_{\mathcal{D}} \varphi_0 \, d\nu = 0$ for $\varphi_0 \in L_0^2(\nu)$

- Decay estimate

$$\frac{d}{dt}\left(\frac{1}{2}\|\varphi(t)\|_{L^2(\nu)}^2\right) = \langle \mathcal{L}_{\mathrm{ovd}}\varphi(t), \varphi(t)\rangle_{L^2(\nu)} = -\frac{1}{\beta}\|\nabla_q \varphi(t)\|_{L^2(\nu)}^2$$

Poincaré inequality and convergence of the semigroup

- Assume that a Poincaré inequality holds:

$$\forall \phi \in H^1(\nu) \cap L_0^2(\nu), \qquad \|\phi\|_{L^2(\nu)} \leqslant \frac{1}{K_\nu} \|\nabla_q \phi\|_{L^2(\nu)}$$

Various sufficient conditions (V uniformly convex, confining, etc)

Exponential decay of the semigroup

ν satisfies a Poincaré inequality with constant $K_\nu > 0$ if and only if

$$\left\| \mathrm{e}^{t\mathcal{L}} \right\|_{\mathcal{B}(L_0^2(\nu))} \leqslant \mathrm{e}^{-K_\nu^2 t/\beta}.$$

Proof: Gronwall inequality $\dfrac{d}{dt}\left(\dfrac{1}{2}\|\varphi(t)\|_{L^2(\nu)}^2\right) \leqslant -\dfrac{K_\nu^2}{\beta}\|\varphi(t)\|_{L^2(\nu)}^2$

Several remarks:

- The prefactor for the exponential convergence is 1
- The convergence rate is *not degraded* (but is it improved?) when one adds an antisymmetric part $\mathcal{A} = F \cdot \nabla$ to $\mathcal{L}$ (with $\mathrm{div}(F\mathrm{e}^{-\beta V}) = 0$)

Longtime convergence of hypocoercive ODEs

A paradigmatic example of hypocoercive ODE

- ODE $\dot{X} = LX \in \mathbb{R}^2$ with (for $\gamma > 0$)

$$-L = A + \gamma S, \qquad A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad S = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

- **Structure of $-L$:**
  - Degenerate symmetric part $S \geqslant 0$
  - Antisymmetric part A coupling the kernel and the image of S
  - Smallest real part of eigenvalues (spectral gap) of order $\min(\gamma, \gamma^{-1})$

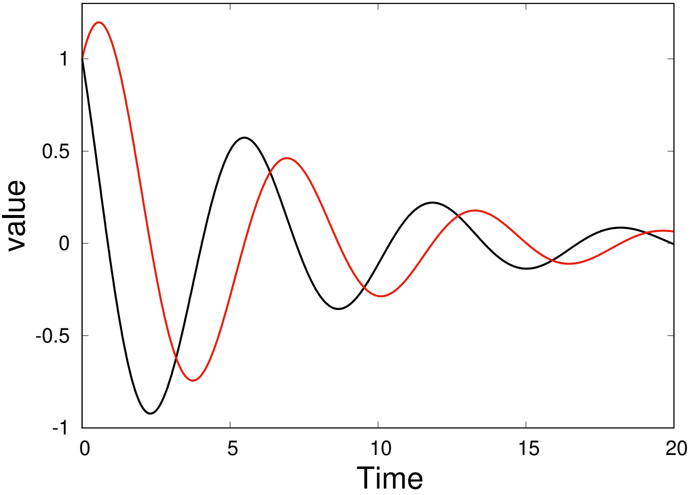
    determinant 1, trace γ, so eigenvalues $\lambda_\pm = \frac{\gamma}{2} \pm \left(\frac{\gamma^2}{4} - 1\right)^{1/2}$

- **Longtime convergence of e^{tL}?** Use $\mathrm{e}^{tL} = U^{-1} \begin{pmatrix} \mathrm{e}^{-t\lambda_+} & 0 \\ 0 & \mathrm{e}^{-t\lambda_-} \end{pmatrix} U$

Decay rate provided by the spectral gap $\lambda = \min\{\mathrm{Re}(\lambda_-), \mathrm{Re}(\lambda_+)\}$

$$X(t) = \mathrm{e}^{tL} X(0), \qquad |X(t)| \leqslant C\mathrm{e}^{-\lambda t} |X(0)|$$

Longtime convergence of hypocoercive ODE: illustration



Values $X_1(t), X_2(t)$ for $X(0) = (1,1)$ and $\gamma = 0.5$

Longtime convergence of this hypocoercive ODE (1)

- **"Elliptic PDE way":** $\dfrac{d}{dt}\left(\dfrac{1}{2}|X(t)|^2\right) = -\gamma X(t)^\top S X(t) = -\gamma X_2(t)^2$

No dissipation in X_1... cannot conclude that $|X(t)|$ converges to 0...

- Change the scalar product with P positive definite:

$$|X|_P^2 = X^\top P X, \qquad \frac{d}{dt}\left(|X(t)|_P^2\right) = X(t)^\top \left(PL + L^\top P\right) X(t)$$

- **Fundamental idea: couple X_1 and X_2.** Start perturbatively:

$$P = \mathrm{Id} - \varepsilon \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

so that $-(PL + L^\top P) = 2\gamma PS + 2\varepsilon \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \sim 2 \begin{pmatrix} \varepsilon & 0 \\ 0 & \gamma \end{pmatrix}$

This provides some (small...) dissipation in X_1!

Longtime convergence of this hypocoercive ODE (2)

• Optimal choice[11] for P? Think of "$L^\top P \geqslant \lambda P$" and diagonalize $L^\top$

$$P = a_- X_- \overline{X}_-^\top + a_+ X_+ \overline{X}_+^\top, \qquad a_\pm > 0, \qquad L^\top X_\pm = \lambda_\pm X_\pm$$

Then $-(PL + L^\top P) \geqslant 2\lambda P$

• Therefore, $|X(t)|_P^2 \leqslant \mathrm{e}^{-2\lambda t}|X_0|_P^2$ (no prefactor here), and so, by equivalence of scalar products,

$$|X(t)| \leqslant \min\left(1, C\mathrm{e}^{-\lambda t}\right)|X_0|$$

Decay rate given by spectral gap

• Prefactor $C \geqslant 1$ really needed!
Exponential convergence with $C = 1$ if and only if $-L$ is coercive (*i.e.* $-X^\top L X \geqslant \alpha |X|^2$ with $\alpha > 0$)

[11] F. Achleitner, A. Arnold, and D. Stürzer, *Riv. Math. Univ. Parma*, 6(1):1–68, 2015.

Convergence of Langevin dynamics

Direct $L^2(\mu)$ approach: lack of coercivity

- The generator, considered on $L^2(\mu)$, is the sum of...
  - a degenerate symmetric part $\mathcal{L}_{\mathrm{FD}} = -p^\top M^{-1}\nabla_p + \dfrac{1}{\beta}\Delta_p$
  - an antisymmetric part $\mathcal{L}_{\mathrm{ham}} = p^\top M^{-1}\nabla_q - \nabla V^\top \nabla_p$

- Standard strategy for coercive generators:

$$\begin{aligned}\frac{d}{dt}\left(\left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\|^2_{L^2(\mu)}\right) &= \left\langle \mathrm{e}^{t\mathcal{L}}\varphi, \mathcal{L}\mathrm{e}^{t\mathcal{L}}\right\rangle_{L^2(\mu)} = \left\langle \mathrm{e}^{t\mathcal{L}}\varphi, \mathcal{L}_{\mathrm{FD}}\mathrm{e}^{t\mathcal{L}}\right\rangle_{L^2(\mu)} \\ &= -\frac{1}{\beta}\left\|\nabla_p \mathrm{e}^{t\mathcal{L}}\varphi\right\|^2_{L^2(\mu)} \leqslant 0,\end{aligned}$$

but no control of $\|\phi\|_{L^2(\mu)}$ by $\|\nabla_p\phi\|_{L^2(\mu)}$ for a Gronwall estimate...

Two options:

- change of scalar product (use antisymmetric part)
- average in time (dissipation vanishes only exceptionally)

Almost direct $L^2(\mu)$ approach: convergence result

- Assume that the potential V is smooth and[12,13]
  - the marginal measure ν satisfies a Poincaré inequality

$$\|\varphi - \nu(\varphi)\|_{L^2(\nu)} \leqslant \frac{1}{K_\nu}\|\nabla_q \varphi\|_{L^2(\nu)}$$

  - there exist $c_1 > 0$, $c_2 \in [0,1)$ and $c_3 > 0$ such that V satisfies

$$\Delta V \leqslant c_1 + \frac{c_2}{2}|\nabla V|^2, \qquad \left|\nabla^2 V\right| \leqslant c_3\left(1 + |\nabla V|\right)$$

There exist $C > 0$ and $\lambda_\gamma > 0$ such that, for any $\varphi \in L^2_0(\mu)$,

$$\forall t \geqslant 0, \qquad \left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\|_{L^2(\mu)} \leqslant C\mathrm{e}^{-\lambda_\gamma t}\|\varphi\|_{L^2(\mu)}$$

with convergence rate of order $\min(\gamma, \gamma^{-1})$: there is $\overline{\lambda} > 0$ for which

$$\lambda_\gamma \geqslant \overline{\lambda}\min(\gamma, \gamma^{-1})$$

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

Sketch of proof (1)

- Change of scalar product to use the antisymmetric part $\mathcal{L}_{\mathrm{ham}}$:
  - bilinear form $\mathcal{H}[\varphi] = \frac{1}{2}\|\varphi\|^2_{L^2(\mu)} - \varepsilon \langle R\varphi, \varphi\rangle$ with[14]

$$R = \Big(1 + (\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p)\Big)^{-1}(\mathcal{L}_{\mathrm{ham}}\Pi_p)^*, \quad \Pi_p\varphi = \int_{p\in\mathbb{R}^d} \varphi \, d\kappa$$

  - $R = \Pi_p R(1-\Pi_p)$ and $\mathcal{L}_{\mathrm{ham}}R$ are bounded
  - modified square norm $\mathcal{H} \sim \|\cdot\|^2_{L^2(\mu)}$ for $\varepsilon \in (-1,1)$
  - Approach not fully quantitative (optimize scalar product, here ε)

- **Interest:** $(\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p) = \beta^{-1}\nabla_q^*\nabla_q$ coercive in q, and

$$R\mathcal{L}_{\mathrm{ham}}\Pi_p = \frac{(\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p)}{1 + (\mathcal{L}_{\mathrm{ham}}\Pi_p)^*(\mathcal{L}_{\mathrm{ham}}\Pi_p)}$$

[14] Hérau (2006), Dolbeault/Mouhot/Schmeiser (2009, 2015), ...

Sketch of proof (2)

- Recall Poincaré inequalities: $\nabla_p^*\nabla_p \geqslant K_\kappa^2(1-\Pi_p)$ and $\nabla_q^*\nabla_q \geqslant K_\nu^2\Pi_p$

Coercivity in the scalar product $\langle\langle\cdot,\cdot\rangle\rangle$ induced by $\mathcal{H}$

$$\mathscr{D}[\varphi] := \langle\langle -\mathcal{L}\varphi,\varphi\rangle\rangle \geqslant \lambda\|\varphi\|^2$$

- Upon controlling the remainder terms (some elliptic estimates)

$$\begin{aligned}
\mathscr{D}[\varphi] &= \gamma\left\langle -\mathcal{L}_{\mathrm{FD}}\varphi,\varphi\right\rangle + \varepsilon\left\langle R\mathcal{L}_{\mathrm{ham}}\Pi_p\varphi,\varphi\right\rangle + \mathrm{O}(\gamma\varepsilon) \\
&= \frac{\gamma}{\beta}\|\nabla_p\varphi\|^2_{L^2(\mu)} + \varepsilon\left\langle \frac{\nabla_q^*\nabla_q}{\beta+\nabla_q^*\nabla_q}\Pi_p\varphi,\Pi_p\varphi\right\rangle + \mathrm{O}(\gamma\varepsilon) \\
&\geqslant \frac{\gamma K_\kappa^2}{\beta}\|(1-\Pi_p)\varphi\|^2_{L^2(\mu)} + \frac{\varepsilon K_\nu^2}{\beta+K_\nu^2}\|\Pi_p\varphi\|^2_{L^2(\mu)} + \mathrm{O}(\gamma\varepsilon)
\end{aligned}$$

- Gronwall inequality $\dfrac{d}{dt}\left(\mathcal{H}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right]\right) = -\mathscr{D}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right] \leqslant -\dfrac{2\lambda}{1+\varepsilon}\mathcal{H}\left[\mathrm{e}^{t\mathcal{L}}\varphi\right]$

Obtaining directly bounds on the resolvent (1)

"Saddle-point like" structure[15] for typical hypocoercive operators on $L^2_0(\mu)$

$$\mathcal{L} = \begin{pmatrix} 0 & \mathcal{A}_{0+} \\ \mathcal{A}_{+0} & \mathcal{L}_{++} \end{pmatrix}, \qquad \mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_+, \qquad \mathcal{H}_0 = \Pi_p \mathcal{H}, \qquad \mathcal{A} = \mathcal{L}_{\mathrm{ham}}$$

Formal inverse with Schur complement $\mathfrak{S}_0 = \mathcal{A}_{+0}^* \mathcal{L}_{++}^{-1} \mathcal{A}_{+0}$

$$\mathcal{L}^{-1} = \begin{pmatrix} \mathfrak{S}_0^{-1} & -\mathfrak{S}_0^{-1} \mathcal{A}_{0+} \mathcal{L}_{++}^{-1} \\ -\mathcal{L}_{++}^{-1} \mathcal{A}_{+0} \mathfrak{S}_0^{-1} & \mathcal{L}_{++}^{-1} + \mathcal{L}_{++}^{-1} \mathcal{A}_{+0} \mathfrak{S}_0^{-1} \mathcal{A}_{0+} \mathcal{L}_{++}^{-1} \end{pmatrix}$$

Invertibility of $\mathfrak{S}_0$ is the crucial element: two ingredients

- $-\dfrac{1}{2}(\mathcal{L} + \mathcal{L}^*) \geqslant s\Pi_+ = s(1 - \Pi_p)$ (Poincaré on $\kappa(dp)$ for Langevin)
- "macroscopic coercivity" $\|\mathcal{A}_{+0}\varphi\|_{L^2(\mu)} \geqslant a\|\Pi_p \varphi\|_{L^2(\mu)}$
  Amounts to $\mathcal{A}_{+0}^* \mathcal{A}_{+0} \geqslant a^2 \Pi_p$
  Guaranteed here by a Poincaré inequality for $\nu(dq)$, with $a^2 = K_\nu^2/\beta$

[15] E. Bernard, M. Fathi, A. Levitt and G. Stoltz, *Annales Henri Lebesgue* (2022)

Obtaining directly bounds on the resolvent (2)

- Further decompose $\mathcal{L}$ using $\Pi_1 = \mathcal{A}_{+0} \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0}\right)^{-1} \mathcal{A}_{+0}^*$

$$\mathcal{L} = \begin{pmatrix} 0 & \mathcal{A}_{01} & 0 \\ \mathcal{A}_{10} & \mathcal{L}_{11} & \mathcal{L}_{12} \\ 0 & \mathcal{L}_{21} & \mathcal{L}_{22} \end{pmatrix}, \qquad \mathcal{A}_{01} = -\mathcal{A}_{10}^*.$$

- Additional technical assumptions ($\mathcal{S} = \gamma \mathcal{L}_{\mathrm{FD}}$ symmetric part):
  - There exists an involution $\mathcal{R}$ (e.g. momentum flip) on $\mathcal{H}$ such that

$$\mathcal{R}\Pi_0 = \Pi_0 \mathcal{R} = \Pi_0, \qquad \mathcal{R}\mathcal{S}\mathcal{R} = \mathcal{S}, \qquad \mathcal{R}\mathcal{A}\mathcal{R} = -\mathcal{A}$$

  - The operators $\mathcal{S}_{11}$ and $\mathcal{L}_{21}\mathcal{A}_{10} \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0}\right)^{-1}$ are bounded

Abstract resolvent estimates

$$\|\mathcal{L}^{-1}\| \leqslant 2 \left(\frac{\|\mathcal{S}_{11}\|}{a^2} + \frac{\|\mathcal{R}_{22}\| \|\mathcal{L}_{21}\mathcal{A}_{10}(\mathcal{A}_{+0}^*\mathcal{A}_{+0})^{-1}\|^2}{s} \right) + \frac{3}{s}$$

Scaling with the friction and the dimension

- Final estimate for Fokker–Planck operators: scaling $\max(\gamma, \gamma^{-1})$

$$\left\|\mathcal{L}^{-1}\right\|_{\mathcal{B}(L_0^2(\mu))} \leqslant \frac{2\beta\gamma}{K_\nu^2} + \frac{4}{\gamma}\left(\frac{3}{4} + \left\|\Pi_+ \mathcal{L}_{\mathrm{ham}}^2 \Pi_p \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0}\right)^{-1}\right\|^2\right)$$

- Estimate $2\left(C + C' K_\nu^{-2}\right)$ for squared operator norm on r.h.s.
  - $C = 1$ and $C' = 0$ when V is convex;
  - $C = 1$ and $C' = K$ when $\nabla_q^2 V \geqslant -K\mathrm{Id}$ for some $K \geqslant 0$;
  - $C = 2$ and $C' = \mathrm{O}(\sqrt{d})$ when $\Delta V \leqslant c_1 d + \dfrac{c_2 \beta}{2}|\nabla V|^2$ (with $c_2 \leqslant 1$) and $\left|\nabla^2 V\right|^2 \leqslant c_3^2\left(d + |\nabla V|^2\right)$

- Better scaling $C' = \mathrm{O}(\log d)$ when logarithmic Sobolev inequality and

$$\forall x \in \mathbb{R}^d, \qquad \left\|\nabla^2 V(q)\right\|_{\mathcal{B}(\ell^2)} \leqslant c_3\left(1 + |\nabla V(q)|_\infty\right)$$

Space-time approaches

Average decay[16] over $[t,t+\tau]$ for $\tau>0$: with $\mathrm{U}_\tau(dt)=\mathbf{1}_{[0,\tau]}(s)\dfrac{dt}{\tau}$,

$$\frac{d}{dt}\left(\int_0^\tau \|f(t+s,\cdot,\cdot)\|^2_{L^2(\mu)}\,\mathrm{U}_\tau(ds)\right)\leqslant -2\gamma\int_0^\tau \|\nabla_p f(t+s,\cdot,\cdot)\|^2_{L^2(\mu)}\,\mathrm{U}_\tau(ds)$$

- For $h(t)=\mathrm{e}^{t\mathcal{L}}h_0$, control dissipation with full space-time antisymmetric part

$$\|(\partial_t-\mathcal{L}_{\mathrm{ham}})h\|_{L^2(\mathrm{U}_\tau\otimes\nu;H^{-1}(\kappa))}\leqslant\gamma\|\nabla_p h\|_{L^2(\mathrm{U}_\tau\otimes\mu)}$$

- Space-time-velocity Poincaré inequality ($\mu(h)=0$)

$$\begin{aligned}\bar{\lambda}\|h\|^2_{L^2(\mathrm{U}_\tau\otimes\mu)}&\leqslant\|(\partial_t-\mathcal{L}_{\mathrm{ham}})h\|^2_{L^2(\mathrm{U}_\tau\otimes\nu;H^{-1}(\kappa))}+\|(\mathrm{Id}-\Pi_p)h\|^2_{L^2(\mathrm{U}_\tau\otimes\mu)}\\&\leqslant\|(\partial_t-\mathcal{L}_{\mathrm{ham}})h\|^2_{L^2(\mathrm{U}_\tau\otimes\nu;H^{-1}(\kappa))}+\frac{1}{K_\kappa}\|\nabla_p h\|^2_{L^2(\mathrm{U}_\tau\otimes\mu)}\end{aligned}$$

Combination leads to exponential convergence through Gronwall estimate (**explicit constants:** scaling in γ, τ, dimension, Poincaré constants, etc.)

[16] G. Brigati and G. Stoltz, *SIAM J. Math. Anal.* (2025)

Space-time-velocity Poincaré inequality

Aim: sufficient to control $\Pi_p h \to$ space-time functions (no velocity)

Two key ingredients: a Poincaré–Lions inequality

$$\left\| g - \iint_{[0,\tau]\times\mathcal{D}} g(t,q)\, \mathrm{U}_\tau(dt)\, \nu(dq) \right\|^2_{L^2(\mathrm{U}_\tau\otimes\nu)} \leqslant C_\tau^{\mathrm{Lions}} \|\nabla_{t,q} g\|^2_{H^{-1}(\mathrm{U}_\tau\otimes\nu)}$$

and an averaging result

$$\|\nabla_{t,q}\Pi_p h\|^2_{H^{-1}} \leqslant K_{\mathrm{avg}}\Big(\|(\mathrm{Id}-\Pi_p)h\|^2_{L^2} + \|(\partial_t - \mathcal{L}_{\mathrm{ham}})h\|^2_{L^2(\mathrm{U}_\tau\otimes\nu, H^{-1}(\kappa))}\Big)$$

Directly leads to $\bar{\lambda} = \dfrac{1}{1 + C_\tau^{\mathrm{Lions}} K_{\mathrm{avg}}}$

Same conditions on V as DMS approach

Averaging lemma

Based on identities such as ($z = z(t,q)$)

$$\begin{aligned}\int_0^\tau \int_{\mathcal{D}} (\partial_t \Pi_p h)\, z \, d\mathrm{U}_\tau \, d\mu &= \int_0^\tau \int_{\mathcal{D}} \int_{\mathbb{R}^3} [(\partial_t {\color{red}-\mathcal{L}_{\mathrm{ham}}}) \Pi_p h]\, z \, d\mathrm{U}_\tau \, d\nu \, d\kappa \\ &= \int_0^\tau \int_{\mathcal{D}} \int_{\mathbb{R}^3} [(\partial_t - \mathcal{L}_{\mathrm{ham}}) h]\, z \, d\mathrm{U}_\tau \, d\mu \\ &\quad + \int_0^\tau \int_{\mathcal{D}} \int_{\mathbb{R}^3} [(\mathrm{Id} - \Pi_p) h]\, (\partial_t - \mathcal{L}_{\mathrm{ham}}) z \, d\mathrm{U}_\tau \, d\mu \\ &\leqslant \|(\partial_t - \mathcal{L}_{\mathrm{ham}}) h\|_{L^2(\mathrm{U}_\tau \otimes \nu, H^{-1}(\kappa))} \|z\|_{L^2(\mathrm{U}_\tau \otimes \nu)} \|1\|_{H^1(\kappa)} \\ &\quad + \|(\mathrm{Id} - \Pi_p) h\|_{L^2(\mathrm{U}_\tau \otimes \mu)} \|(\partial_t - \mathcal{L}_{\mathrm{ham}}) z\|_{L^2(\mathrm{U}_\tau \otimes \mu)}\end{aligned}$$

for $z \in \mathrm{H}^1_{\mathrm{DC}}(\mathrm{U}_\tau \otimes \nu)$ with $\|z\|^2_{H^1(\mathrm{U}_\tau \otimes \nu)} \leqslant 1$

(Dirichlet boundary conditions $z(0) = z(\tau) = 0$ used for integration by parts in time)

Explicit expression for K_{avg} in terms of kinetic energy $E_{\mathrm{kin}}(p)$

Poincaré–Lions inequality (1/2)

Reduction to divergence equation: for $f \in L^2_0(\mathrm{U}_\tau \otimes \nu)$, find a solution $Z = (Z_0, Z_1, \dots, Z_d) \in H^1_{\mathrm{DC}}(\mathrm{U}_\tau \otimes \nu)^{d+1}$ satisfying

$$-\partial_t Z_0 + \sum_{i=1}^d \partial_{q_i}^\star Z_i = f$$

with estimates $\|Z\|_{H^1(\mathrm{U}_\tau\otimes\nu)} \leqslant C_\tau^{\mathrm{div}} \|f\|_{L^2(\mathrm{U}_\tau\otimes\nu)}$

Beware the boundary conditions in time for Z!

Proceed by duality (f with average 0 w.r.t. $\mathrm{U}_\tau \otimes \nu$)

$$\begin{aligned}\|f\|^2_{\mathrm{L}^2(\mathrm{U}_\tau\otimes\nu)} &= \int_0^\tau \int_{\mathcal{D}} \left(-\partial_t Z_0 + \sum_{i=1}^d \partial_{q_i}^\star Z_i\right) f \, d\mathrm{U}_\tau \, d\nu \\ &= \langle \nabla_{t,q} f, Z \rangle_{H^{-1}(\mathrm{U}_\tau\otimes\nu), H^1_{\mathrm{DC}}(\mathrm{U}_\tau\otimes\nu)} \\ &\leqslant C_\tau^{\mathrm{div}} \|f\|_{L^2(\mathrm{U}_\tau\otimes\nu)} \|\nabla_{t,q} f\|_{H^{-1}(\mathrm{U}_\tau\otimes\nu)}\end{aligned}$$

Poincaré–Lions inequality (2/2)

Decompose f in $\mathcal{N}$ and its orthogonal, with $L = \left(\nabla_q^\star \nabla_q\right)^{1/2}$ and

$$\mathcal{N} = \left\{ \mathrm{e}^{-tL} g_+ + \mathrm{e}^{-(\tau - t)L} g_-, \quad g_+, g_- \in L^2_0(\nu) \right\}$$

By construction, $(-\partial_t^2 + \nabla_q^\star \nabla_q) g = 0$ for $g \in \mathcal{N}$

Explicit solution to divergence equation (non unique)

$$Z = \nabla_{t,q} \mathscr{W}^{-1} \mathscr{P}_{\mathcal{N}^\perp} f + \begin{pmatrix} F_0(t,L) \\ \partial_{q_1} F_1(t,L) \\ \vdots \\ \partial_{q_d} F_1(t,L) \end{pmatrix} \mathscr{P}_{\mathcal{N},+} f + \begin{pmatrix} F_0(\tau - t,L) \\ \partial_{q_1} F_1(\tau - t,L) \\ \vdots \\ \partial_{q_d} F_1(\tau - t,L) \end{pmatrix} \mathscr{P}_{\mathcal{N},-} f$$

where $\mathcal{W} = -\partial_t^2 + \nabla_q^\star \nabla_q$ with Neumann BC in time, and

$$-\partial_t \Big[\underbrace{F_0(t,L)\mathrm{e}^{-tL}}_{P_0(\mathrm{e}^{-tL})} \Big] + L^2 \underbrace{F_1(t,L)\mathrm{e}^{-tL}}_{P_1(\mathrm{e}^{-tL})} = \mathrm{e}^{-tL}$$

Generalizations/perspectives

These approaches work for other hypocoercive dynamics

- non-quadratic kinetic energies (but still Poincaré inequality)[17]
- weak confinements and/or heavy tail distributions of velocities[18]
- adaptive Langevin dynamics (additional Nosé–Hoover part)[19]
- linear Boltzmann (HMC)/piecewise deterministic Markov processes

Possibly stretched exponential or algebraic convergence rates

Some work needed to extend the approaches to...

- more degeneracy: generalized Langevin,[20] chains of oscillators[21]
- non-gradient forcings (steady-state nonequilibrium dynamics)[22]

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[20] Ottobre/Pavliotis (2011), Pavliotis/Stoltz/Vaes (2021), Brigati/Lörler/Wang (2024)

[21] A. Menegaki (2020)

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