Hypocoercivity without changing the scalar product

Gabriel STOLTZ

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

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Outline of the talk

- **Some hypocoercive dynamics**
  - Langevin dynamics and its overdamped limit
  - Random time HMC (linear Boltzmann)
  - Structural form of hypocoercive operators
  - Longtime convergence by a standard hypocoercive approach

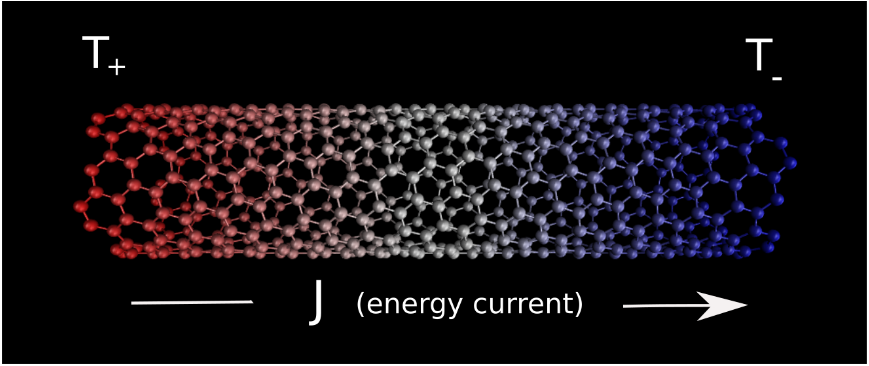
- **Hypocoercive approaches without changing the scalar product**
  - Space-time Poincare inequalities[1] and longtime convergence
  - Schur method and direct bound on the resolvent[2]

[1] Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)
[2] Bernard/Fathi/Levitt/Stoltz (2020)

Some hypocoercive dynamics

My motivation: computational statistical physics

- **Aims of computational statistical physics**
  - numerical microscope
  - computation of average properties, static or dynamic



"Given the structure and the laws of interaction of the particles, what are the macroscopic properties of the matter composed of these particles?"

Langevin dynamics (1)

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

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

Stochastic perturbation of the Hamiltonian dynamics

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

- Given (known) friction $\gamma > 0$ (could be a position-dependent matrix)

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 $\mathcal{L} = \mathcal{L}_{\mathrm{ham}} + \gamma\mathcal{L}_{\mathrm{FD}}$

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

- 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 $\mathcal{L}^*$

$$\mathcal{L}^* = -\mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}$$

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

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

Hamiltonian and overdamped limits

- As $\gamma \to 0$, recover Hamiltonian dynamics

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

Time $\sim \gamma^{-1}$ to change energy levels in this limit[3]

- Overdamped limit $\gamma \to +\infty$: 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 $\min\left(\gamma, \gamma^{-1}\right)$

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

Ergodicity results for Langevin dynamics (1)

- Almost-sure convergence[4] of ergodic averages $\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(q_s,p_s)\,ds$

- Asymptotic variance of ergodic averages

$$\sigma_\varphi^2 = \lim_{t\to+\infty} t\mathbb{E}\left[\widehat{\varphi}_t^2\right] = 2\int_{\mathcal{E}} \left(-\mathcal{L}^{-1}\mathscr{P}\varphi\right)\mathscr{P}\varphi\,d\mu$$

where $\mathscr{P}\varphi = \varphi - \mathbb{E}_\mu(\varphi)$

- A central limit theorem holds[5] when the equation has a solution in $L^2(\mu)$

Poisson equation in $L^2(\mu)$

$$-\mathcal{L}\Phi = \mathscr{P}\varphi$$

- Well-posedness of such equations?

[4] Kliemann, *Ann. Probab.* **15**(2), 690-707 (1987)
[5] Bhattacharya, *Z. Wahrsch. Verw. Gebiete* **60**, 185–201 (1982)

Ergodicity results for Langevin dynamics (2)

- Invertibility of $\mathcal{L}$ on subsets of $L_0^2(\mu) = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \, d\mu = 0 \right\}$?

$$-\mathcal{L}^{-1} = \int_0^{+\infty} \mathrm{e}^{t\mathcal{L}} \, dt$$

- Exponential convergence of $\mathrm{e}^{t\mathcal{L}}$ in various Banach spaces $E \cap L_0^2(\mu)$
  - Lyapunov techniques[6] $B_W^\infty(\mathcal{E}) = \left\{ \varphi \text{ measurable, } \sup \left| \frac{\varphi}{W} \right| < +\infty \right\}$
  - standard hypocoercive[7] setup $H^1(\mu)$
  - $E = L^2(\mu)$ after hypoelliptic regularization[8] from $H^1(\mu)$
  - Directly $E = L^2(\mu)$ (recently[9] Poincaré using $\partial_t - \mathcal{L}_{\mathrm{ham}}$)
  - coupling arguments[10]

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

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

[8] F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)

[9] Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)

[10] A. Eberle, A. Guillin and R. Zimmer, *Ann. Probab.* **47**(4), 1982-2010 (2019)

Random time HMC / linear Boltzmann

• PDMP: resampling of momenta at exponential times

$$\mathcal{L}_{\mathrm{FD}} = \Pi_0 - 1, \qquad (\Pi_0 \varphi)(q) = \int_{\mathbb{R}^d} \varphi(q,p)\, \kappa(dp)$$

• Other possibilities: resample momenta componentwise (Andersen dynamics), zigzag, BPS, ...

Generator of RTHMC $\mathcal{L} = \mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}$

$$\mathcal{L}_{\mathrm{ham}} = p^T M^{-1} \nabla_q - \nabla V^T \nabla_p, \qquad \mathcal{L}_{\mathrm{FD}} = \Pi_0 - 1$$

• **Proofs of convergence**: Lyapunov techniques[11], hypocoercivity[12], coupling techniques[13]

[11] Bou-Rabee/Sanz-Serna (2017), Bierkens/Roberts/Zitt (2019), ...

[12] Dolbeault/Mouhot/Schmeiser (2009), Andrieu/Durmus/Nüsken/Roussel (2018), Deligiannidis/Paulin/Bouchard-Côté/Doucet (2020)

[13] Bou-Rabee/Eberle/Zimmer (2020)

Common structure of the operators

- Hilbert space $\mathcal{H} = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \, \mu = 0 \right\}$
- Decomposition into symmetric and antisymmetric parts

$$\mathcal{L} = \mathcal{A} + \gamma \mathcal{S}$$

with $\mathcal{A} = \mathcal{L}_{\mathrm{ham}}$, and $\mathcal{S} = -\frac{1}{\beta} \nabla_p^* \nabla_p$ (Langevin) or $\mathcal{S} = \Pi_0 - 1$ (RTHMC)

- Note that $\Pi_0 \mathcal{A} \Pi_0 = 0$ and $\Pi_0 \mathcal{S} = \mathcal{S} \Pi_0 = 0$, so that

$$\mathcal{L} = \begin{pmatrix} 0 & \mathcal{A}_{0+} \\ \mathcal{A}_{+0} & \mathcal{L}_{++} \end{pmatrix}, \qquad \mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_+, \qquad \mathcal{H}_0 = \Pi_0 \mathcal{H}$$

Saddle-point like structure!

A standard hypocoercive approach

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

• The generator, considered on $L^2(\mu)$, is the sum of...

- a degenerate symmetric part $\mathcal{L}_{\mathrm{FD}} = -p^T M^{-1}\nabla_p + \frac{1}{\beta}\Delta_p$
- an antisymmetric part $\mathcal{L}_{\mathrm{ham}} = p^T M^{-1}\nabla_q - \nabla V^T \nabla_p$

• Standard strategy for coercive generators: consider φ with average 0 with respect to μ and compute

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

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

• Change of scalar product in order to use the antisymmetric part

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

- Assume that the potential V is smooth and[14]
  - the marginal measure ν satisfies a Poincaré inequality

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

  - 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 $\varphi \in L_0^2(\mu)$,

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

with convergence rate of order $\min(\gamma, \gamma^{-1})$: there exists $\overline{\lambda} > 0$ such that

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

[14] 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[15]

$$R = \left(1 + (\mathcal{L}_{\mathrm{ham}}\Pi_0)^*(\mathcal{L}_{\mathrm{ham}}\Pi_0)\right)^{-1}(\mathcal{L}_{\mathrm{ham}}\Pi_0)^* = \left(1 + \mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\mathcal{A}_{+0}^*$$

  - $R = \Pi_0 R(1-\Pi_0)$ 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 less quantitative (optimize scalar product)

- **Interest:** $\mathcal{A}_{+0}^*\mathcal{A}_{+0} = \beta^{-1}\nabla_q^*\nabla_q$ coercive in q, and

$$R\mathcal{L}_{\mathrm{ham}}\Pi_0 = \frac{\mathcal{A}_{+0}^*\mathcal{A}_{+0}}{1 + \mathcal{A}_{+0}^*\mathcal{A}_{+0}}$$

Note: could consider $R_\eta = \left(\eta + \mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\mathcal{A}_{+0}^*$ for any $\eta > 0$

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

Sketch of proof (2)

- Poincaré inequalities: $-\mathcal{S} \geqslant \beta^{-1} K_\kappa^2 \Pi_+$ and $\mathcal{A}_{+0}^* \mathcal{A}_{+0} \geqslant \beta^{-1} K_\nu^2 \Pi_0$

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

$$\begin{aligned}
\mathscr{D}[\varphi] &= \gamma \langle -\mathcal{S}\varphi, \varphi \rangle + \varepsilon \langle R \mathcal{L}_{\mathrm{ham}} \Pi_0 \varphi, \varphi \rangle + \mathrm{O}(\gamma\varepsilon) \\
&= \frac{\gamma}{\beta} \|\nabla_p \varphi\|_{L^2(\mu)}^2 + \varepsilon \left\langle \frac{\mathcal{A}_{+0}^* \mathcal{A}_{+0}}{1 + \mathcal{A}_{+0}^* \mathcal{A}_{+0}} \Pi_0 \varphi, \Pi_0 \varphi \right\rangle + \mathrm{O}(\gamma\varepsilon) \\
&\geqslant \frac{\gamma K_\kappa^2}{\beta} \|\Pi_+ \varphi\|_{L^2(\mu)}^2 + \frac{\varepsilon K_\nu^2}{\beta + K_\nu^2} \|\Pi_0 \varphi\|_{L^2(\mu)}^2 + \mathrm{O}(\gamma\varepsilon)
\end{aligned}$$

- Remainder involves elliptic estimates for $\Pi_+ \mathcal{L}_{\mathrm{ham}}^2 \Pi_0 \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0} \right)^{-1}$
- Gronwall inequality $\displaystyle \frac{d}{dt} \left(\mathcal{H}\left[\mathrm{e}^{t\mathcal{L}} \varphi \right] \right) = -\mathscr{D}\left[\mathrm{e}^{t\mathcal{L}} \varphi \right] \leqslant -\frac{2\lambda}{1+\varepsilon} \mathcal{H}\left[\mathrm{e}^{t\mathcal{L}} \varphi \right]$

Schur complements and direct bounds on the resolvent

Obtaining directly bounds on the resolvent (1)

- "Saddle-point like" structure for typical hypocoercive operators on $L_0^2(\mu)$

$$\mathcal{L} = \begin{pmatrix} 0 & \mathcal{A}_{0+} \\ \mathcal{A}_{+0} & \mathcal{L}_{++} \end{pmatrix}, \qquad \mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_+, \qquad \mathcal{H}_0 = \Pi_0 \mathcal{H}, \qquad \mathcal{A} = \mathcal{L}_{\mathrm{ham}}$$

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
  - $-\mathcal{S} \geqslant s\Pi_+ = s(1 - \Pi_0)$ (Poincaré on $\kappa(dp)$ for Langevin)
  - "macroscopic coercivity" $\|\mathcal{A}_{+0}\varphi\|_{L^2(\mu)} \geqslant a\|\Pi\varphi\|_{L^2(\mu)}$
    Amounts to $\mathcal{A}_{+0}^* \mathcal{A}_{+0} \geqslant a^2 \Pi_0$
    Guaranteed here by a Poincaré inequality for $\nu(dq)$, with $a^2 = K_\nu^2/\beta$

Obtaining directly bounds on the resolvent (2)

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

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

Abstract resolvent estimates in $\mathcal{B}(L_0^2(\mu))$

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

- Valid under the following additional technical assumptions
  - There exists an involution $\mathcal{R}$ on $\mathcal{H}$ such that

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

  - Operators $\mathcal{S}_{11}$ and $\mathcal{L}_{21}\mathcal{A}_{10}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}$ bounded: Schur again

$$\mathfrak{S}_0^{-1} = -\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\mathcal{A}_{10}^*\left(\mathcal{S}_{11} - \mathcal{L}_{12}\mathcal{L}_{22}^{-1}\mathcal{L}_{21}\right)\mathcal{A}_{10}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}$$

Scaling with the friction and the dimension

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

$$\left\|\mathcal{L}^{-1}\right\|_{\mathcal{B}(L_0^2(\mu))} \leqslant \frac{2\beta\gamma}{K_\nu^2} + \frac{4}{\gamma}\left(\frac{3}{4} + \left\|\Pi_+ \mathcal{L}_{\mathrm{ham}}^2 \Pi_0 \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0}\right)^{-1}\right\|_{\mathcal{B}(L_0^2(\mu))}^2\right)$$

- Estimate $2\left(C + C' K_\nu^{-2}\right)$ for 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 $\Delta V \leqslant c_1 d + \frac{c_2 \beta}{2}|\nabla V|^2$ (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 Poincaré inequalities

Poincaré inequality with antisymmetric part of generator

- "Macroscopic coercivity" $\|\mathcal{A}_{+0}\varphi\|_{L^2(\mu)} \geqslant a\|\Pi\varphi\|_{L^2(\mu)}$

Poincaré inequality with $\mathcal{A}$ (Theorem 1.2 in Armstrong/Mourrat)

Assume that the operators $\Pi_+\mathcal{A}^2\Pi_0\,(\mathcal{A}_{+0}^*\mathcal{A}_{+0})$ and $\mathcal{S}_{11}$ are bounded. Then,

$$\forall f \in C_c^\infty, \qquad \|f - \langle f, \mathbf{1}\rangle\| \leqslant C_1\|(1-\Pi_0)f\| + C_2\|(1-\mathcal{S})^{-1/2}\mathcal{A}f\|$$

- Note that $\left\|(1-\mathcal{S})^{-1/2}\cdot\right\|$ = norm on $L^2(\nu, H^{-1}(\kappa))$
- **Proof:** need only to control $\|\Pi_0 f\|$

$$\begin{aligned}
\|\Pi_0 f\|^2 &= \langle \mathcal{A}_{+0}f, \mathcal{A}_{+0}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\rangle = \langle \mathcal{A}\Pi_0 f, \mathcal{A}_{+0}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\rangle \\
&= \langle \mathcal{A}f, \mathcal{A}_{+0}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\rangle - \langle \mathcal{A}(1-\Pi_0)f, \mathcal{A}_{+0}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\rangle \\
&\leqslant \|(1-\mathcal{S})^{-1/2}\mathcal{A}f\|\left\|(1-\mathcal{S}_{11})^{1/2}\mathcal{A}_{10}\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\right\| \\
&\qquad + \|(1-\Pi_0)f\|\left\|\Pi_+\mathcal{A}^2\Pi_0\left(\mathcal{A}_{+0}^*\mathcal{A}_{+0}\right)^{-1}\Pi_0 f\right\|
\end{aligned}$$

- Bound works also with $\left\|(1-\mathcal{S})^{-1/2}(\mathrm{i}\omega + \mathcal{A})\left(f - \langle f, \mathbf{1}\rangle_{L^2(\mu)}\right)\right\|_{L^2(\mu)}$

Space-time Poincaré inequality

- Consider the Hilbert space (for a given time $T > 0$)

$$\mathcal{H}_T = \left\{ \varphi \in L^2(\widetilde{\mu}_T) \,\middle|\, \langle \varphi, \mathbf{1} \rangle_{L^2(\widetilde{\mu}_T)} = 0 \right\}, \qquad \widetilde{\mu}_T = \mu(dq\,dp) \otimes \frac{\mathbf{1}_{[0,T]}(t)\,dt}{T}$$

- Replace $\mathcal{L}$ by $-\partial_t + \mathcal{L}$: total antisymmetric part $-\partial_t + \mathcal{A}$

Poincaré inequality with $-\partial_t + \mathcal{A}$ (Armstrong/Mourrat, Prop. 7.2)

There exist $C_{1,T}, C_{2,T} \in \mathbb{R}_+$ such that, for any $f \in C_c^\infty([0,T] \times \mathcal{E})$,

$$\|f - \widetilde{\mu}_T(f)\|_{L^2(\widetilde{\mu}_T)} \leqslant C_{1,T} \|(1 - \Pi_0) f\|_{L^2(\widetilde{\mu}_T)} + C_{2,T} \left\| (1 - \mathcal{S})^{-1/2} (-\partial_t + \mathcal{A})\, f \right\|_{L^2(\widetilde{\mu}_T)}$$

- **Elements of proof:**
  - Formally amounts to replacing $\mathcal{A}$ by $-\partial_t \Pi_0 + \mathcal{A}_{+0}$
  - Issue with some integration by parts in the time variable[16]

[16] See Lemma 2.6 in Cao/Lu/Wang (2019)

Exponential decay from the space-time Poincaré inequality

- Show that $\varphi(t) = \mathrm{e}^{t\mathcal{L}}\varphi_0 \to 0$ for $\varphi_0 \in \mathcal{H}$ given

- Decay inequality from $-\gamma\mathcal{S}\varphi(t) = \Pi_+(-\partial_t + \mathcal{A})\varphi(t)$

$$\frac{d}{dt}\left(\frac{1}{2}\|\varphi(t)\|^2\right) = \gamma\,\langle\varphi(t), \mathcal{S}\varphi(t)\rangle = -\frac{1}{\gamma}\left\|(-\mathcal{S})^{-1/2}(-\partial_t + \mathcal{A})\varphi(t)\right\|^2$$
$$\leqslant -\frac{1}{\gamma}\left\|(1-\mathcal{S})^{-1/2}(-\partial_t + \mathcal{A})\varphi(t)\right\|^2$$

- Young inequality to keep some $\langle\varphi(t), \mathcal{S}\varphi(t)\rangle$ + integrate in time

$$\|\varphi(T)\|^2_{L^2(\mu)} - \|\varphi(0)\|^2_{L^2(\mu)}$$
$$\leqslant -\frac{\gamma s T}{\gamma^2 s C_{2,T}^2 + C_{1,T}^2}\left[C_{1,T}\,\|\Pi_+\varphi(t)\|_{L^2(\widetilde{\mu}_T)} + C_{2,T}\left\|(1-\mathcal{S})^{-1/2}(-\partial_t + \mathcal{A})\varphi(t)\right\|_{L^2(\widetilde{\mu}_T)}\right]^2$$
$$\leqslant -\frac{\gamma s T}{\gamma^2 s C_{2,T}^2 + C_{1,T}^2}\|\varphi\|^2_{L^2(\widetilde{\mu}_T)} \leqslant -\frac{\gamma s T}{\gamma^2 s C_{2,T}^2 + C_{1,T}^2}\|\varphi(T)\|^2_{L^2(\mu)},$$

- Exponential decay $\|\varphi(T)\| \leqslant \alpha_T\|\varphi(0)\|$ with $\log\alpha_T \sim \min\left(\gamma, \frac{1}{\gamma}\right)$

Generalizations/perspectives for direct resolvent estimates

- **Schur approach works for other hypocoercive dynamics**[17]
  - non-quadratic kinetic energies
  - Andersen dynamics
  - adaptive Langevin dynamics (additional Nosé–Hoover part)

- **Work needed to extend it approach to more degenerate dynamics**
  - PDMPs such as BPS and zigzag
  - generalized Langevin dynamics[18]
  - chains of oscillators[19]

- **Current work also on obtaining...**
  - resolvent estimates $(\mathrm{i}\omega - \mathcal{L})^{-1}$
  - space-time Poincaré inequalities with our algebraic framework

[17] E. Bernard, M. Fathi, A. Levitt, G. Stoltz, *arXiv preprint* **2003.00726**
[18] Ottobre/Pavliotis (2011), Pavliotis/Stoltz/Vaes (2021)
[19] Menegaki (2020)