



Convergence en temps long de semigroupes d'évolution en dynamique moléculaire (et la naissance de l'hypocoercivité)

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Objectif

- Convergence en temps long de solutions d'équations d'évolution du type

$$\partial_t f(t, y) = (\mathcal{L}f)(t, y)$$

pour \mathcal{L} un opérateur **négalif** : pour un certain espace de Hilbert \mathcal{H} ,

$$\langle \mathcal{L}g, g \rangle_{\mathcal{H}} \leq 0$$

- Préservation de la masse $\int_{\mathcal{Y}} f(t, y) \mu(y) dy = \int_{\mathcal{Y}} f(0, y) \mu(y) dy$
→ regarder la **convergence vers 0** de

$$f(t, y) - \int_{\mathcal{Y}} f(t, z) \mu(z) dz$$

- **Intérêt pratique** (personnel) : brique de base pour comprendre les propriétés statistiques de méthodes de Monte Carlo

EDOs hypocoercives

et le changement de produit scalaire

A paradigmatic example of hypocoercive ODE

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

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

- **Structure of $-L$:**

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

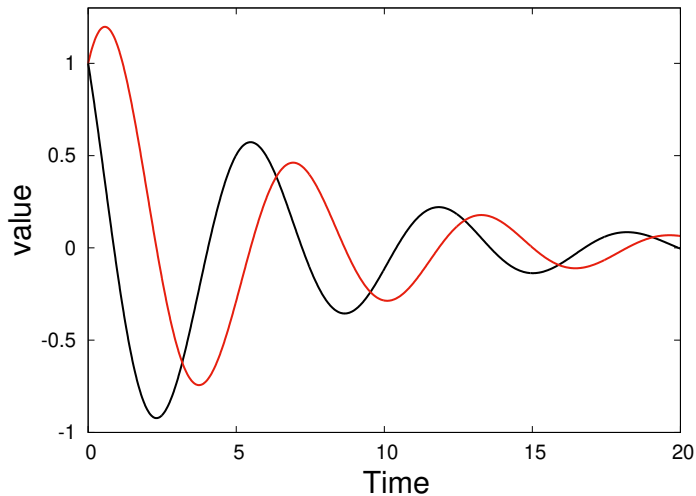
determinant 1, trace γ so eigenvalues $\lambda_{\pm} = \frac{\gamma}{2} \pm \left(\frac{\gamma^2}{4} - 1\right)^{1/2}$

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

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

$$X(t) = e^{tL} X(0), \quad |X(t)| \leq C e^{-\lambda t} |X(0)|$$

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”**: $\frac{d}{dt} \left(\frac{1}{2} |X(t)|^2 \right) = -\gamma X(t)^T S X(t) = -\gamma X_2(t)^2$

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

- Change the scalar product with P positive definite:

$$|X|_P^2 = X^T P X, \quad \frac{d}{dt} (|X(t)|_P^2) = X(t)^T (PL + L^T P) X(t)$$

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

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

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

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

Longtime convergence of this hypocoercive ODE (2)

- Optimal choice¹ for P ? Think of “ $L^T P \geq \lambda P$ ” and diagonalize L^T

$$P = a_- X_- \bar{X}_-^T + a_+ X_+ \bar{X}_+^T, \quad a_{\pm} > 0, \quad L^T X_{\pm} = \lambda_{\pm} X_{\pm}$$

Then $-(PL + L^T P) \geq 2\lambda P$

- Therefore, $|X(t)|_P^2 \leq e^{-2\lambda t} |X_0|_P^2$, and so, **by equivalence of scalar products**,

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

Decay rate given by spectral gap + bound from degenerate dissipation

- Prefactor $C \geq 1$ really needed!

Exponential convergence with $C = 1$ if and only if $-L$ is coercive (i.e. $-X^T L X \geq \alpha |X|^2$ with $\alpha > 0$)

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

Convergence dans le cas coercif

c'est Poincaré qui fait tout le boulot...

Overdamped Langevin dynamics and its generator

- Consider the operator (advection/diffusion)

$$\mathcal{L}_{\text{ovd}} = -\nabla V(x) \cdot \nabla_x + \frac{1}{\beta} \Delta_x = -\frac{1}{\beta} \sum_{i=1}^d \partial_{x_i}^* \partial_{x_i}$$

hence self-adjoint on $L^2(\nu)$ with $\nu(x) = Z_\nu^{-1} e^{-\beta V(x)}$. Indeed,

$$\int_{\mathbb{R}^d} (\partial_{x_i} \varphi) \phi \nu = - \int_{\mathbb{R}^d} \varphi (\partial_{x_i} \phi) \nu - \int_{\mathbb{R}^d} \varphi \phi \partial_{x_i} \nu$$

so that $\partial_{x_i}^* = -\partial_{x_i} + \beta \partial_{x_i} V$

- Generator unitarily equivalent to a Schrödinger operator on $L^2(\mathbb{R}^d)$

$$\tilde{\mathcal{L}}_{\text{ovd}} = \frac{1}{\beta} \Delta + \mathcal{V}, \quad \mathcal{V} = \frac{1}{2} \left(\Delta V - \frac{\beta}{2} |\nabla V|^2 \right)$$

by considering $\tilde{\mathcal{L}}_{\text{ovd}} g = \nu^{1/2} \mathcal{L}_{\text{ovd}} (\nu^{-1/2} g)$

Time evolution and decay estimates

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

$$\frac{d}{dt} \left(\int_{\mathbb{R}^d} \varphi(t) \nu \right) = \int_{\mathbb{R}^d} \mathcal{L}_{\text{ovd}}\varphi(t) \nu = \int_{\mathbb{R}^d} \varphi(t) (\mathcal{L}_{\text{ovd}}\mathbf{1}) \nu = 0$$

- Suggests the longtime limit $\varphi(t) \xrightarrow{t \rightarrow +\infty} \int_{\mathbb{R}^d} \varphi_0 \nu$

- Can assume w.l.o.g. that $\int_{\mathbb{R}^d} \varphi_0 \nu = 0$ (subspace $L_0^2(\nu)$ of $L^2(\nu)$)

- **Decay estimate**

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

Poincaré inequality and convergence of the semigroup

- Assume that a Poincaré inequality holds:

$$\forall \phi \in H^1(\nu) \cap L_0^2(\nu), \quad \|\phi\|_{L^2(\nu)}^2 \leq \frac{1}{K_\nu} \|\nabla \phi\|_{L^2(\nu)}^2$$

Various sufficient conditions (V uniformly convex, \mathcal{V} confining, etc)

Exponential decay of the semigroup

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

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

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

Several remarks:

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

EDP hypocoercives

deux opérateurs exemplaires

(Simple) Linear Boltzmann equation (1)

- Time evolution of density $f(t, x, v)$ (**Hamiltonian transport** + collision)

$$\partial_t f + \mathcal{L}_{\text{ham}} f = \gamma(\mathcal{P} - 1)f$$

where $f(0) = f_0 \geq 0$ and $\kappa(dv) = Z_\kappa^{-1} e^{-\beta|v|^2/2}$,

$$\mathcal{L}_{\text{ham}} = v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v, \quad (\mathcal{P}g)(x) = \left(\int_{\mathbb{R}^d} g(x, w) dw \right) \kappa(v)$$

- Note that $\int_{\mathbb{R}^d \times \mathbb{R}^d} f(t, x, v) dx dv = \int_{\mathbb{R}^d \times \mathbb{R}^d} f_0(x, v) dx dv = 1$

- **Steady-state?** Hamiltonian $H(x, v) = V(x) + \frac{|v|^2}{2}$

$$\mu(x, v) = Z^{-1} e^{-\beta H(x, v)} = \nu(x) \kappa(v), \quad \nu(x) = Z_\nu^{-1} e^{-\beta V(x)}$$

- Question: $\|f(t) - \mu\| \leq C e^{-\lambda t} \|f(0) - \mu\|$? (**which norm?**)

(Simple) Linear Boltzmann equation (2)

- Rewrite $f(t, x, v) = \varphi(t, x, v)\mu(x, v)$, **steady-state** $\varphi_\infty(x, v) = 1$

$$\partial_t \varphi + \mathcal{L}_{\text{ham}} \varphi = \gamma(\Pi_0 - 1)\varphi, \quad (\Pi_0 \phi)(x) = \int_{\mathbb{R}^d} \phi(x, w) \kappa(w) dw$$

- Consider $\|\varphi(t)\|_{L^2(\mu)}^2 = \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(t, x, v)^2 \mu(x, v) dx dv$

- Note that Π_0 is an **orthogonal projector** on $L^2(\mu)$

$$\|\phi\|_{L^2(\mu)}^2 = \|\Pi_0 \phi\|_{L^2(\mu)}^2 + \|(1 - \Pi_0)\phi\|_{L^2(\mu)}^2$$

In particular, $\Pi_0 - 1 \leq 0$ provides some dissipation

- Operator \mathcal{L}_{ham} **antisymmetric** on $L^2(\mu)$ (proof)

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} (\mathcal{L}_{\text{ham}} \varphi) \phi \mu = - \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi (\mathcal{L}_{\text{ham}} \phi) \mu$$

(Simple) Linear Boltzmann equation (3)

- **Issue:** prove that $\left\| \varphi(t) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi_0 \mu \right\|_{L^2(\mu)} \rightarrow 0$ as $t \rightarrow +\infty$
- Consider w.l.o.g. that $\int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(t) \mu = \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi_0 \mu = 0$
- Compute the decay of the $L^2(\mu)$ -norm

$$\begin{aligned} & \frac{d}{dt} \left(\frac{1}{2} \|\varphi(t)\|_{L^2(\mu)}^2 \right) \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} [\mathcal{L}_{\text{ham}} \varphi(t)] \varphi(t) \mu + \gamma \langle (\Pi_0 - 1) \varphi(t), \varphi(t) \rangle_{L^2(\mu)} \\ &= -\gamma \|(1 - \Pi_0) \varphi(t)\|_{L^2(\mu)}^2 \end{aligned}$$

- **Difficulty:** **missing dissipation** in $\|\Pi_0 \varphi(t)\|_{L^2(\mu)}$ in order to apply a Gronwall inequality...

Fokker-Planck operators

- Associated with Langevin dynamics in computational statistical physics
- Operator $\mathcal{L} = \mathcal{L}_{\text{ham}} + \gamma \mathcal{L}_{\text{FD}}$: (anti)symmetric parts on $L^2(\mu)$

$$\mathcal{L}_{\text{ham}} = v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v = \frac{1}{\beta} \sum_{i=1}^d \partial_{v_i}^* \partial_{x_i} - \partial_{v_i} \partial_{x_i}^*,$$

$$\mathcal{L}_{\text{FD}} = -v \cdot \nabla_v + \frac{1}{\beta} \Delta_v = -\frac{1}{\beta} \sum_{i=1}^d \partial_{v_i}^* \partial_{v_i}$$

since $\partial_{v_i}^* = -\partial_{v_i} + \beta v_i$ and $\partial_{x_i}^* = -\partial_{x_i} + \beta \partial_{x_i} V$

- **Degeneracy of the dissipation** provided by \mathcal{L}_{FD} : only in $v...$

- Question: $\left\| e^{t\mathcal{L}} \varphi - \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi \mu \right\|_{L^2(\mu)} \leq C e^{-\lambda t} \left\| \varphi - \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi \mu \right\|_{L^2(\mu)}$

Common structure of the operators

- Operator on $\mathcal{H} = \left\{ \varphi \in L^2(\mu) \mid \int_{\mathcal{E}} \varphi \mu = 0 \right\}$, (anti)symmetric parts
$$\mathcal{L} = \mathcal{A} + \gamma \mathcal{S}$$

We have seen $\mathcal{A} = \mathcal{L}_{\text{ham}}$ and $\mathcal{S} = -\beta^{-1} \nabla_v^* \nabla_v$ or $\Pi_0 - 1$ with

$$(\Pi_0 \varphi)(x) = \int_{\mathbb{R}^d} \varphi(x, w) \kappa(w) dw$$

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

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

- Since $-\langle \varphi, \mathcal{L} \varphi \rangle_{L^2(\mu)} = -\gamma \langle \varphi, \mathcal{S} \varphi \rangle_{L^2(\mu)} \geq \rho \gamma \|(1 - \Pi_0) \varphi\|_{L^2(\mu)}^2$ at best,

$$\frac{d}{dt} \left(\frac{1}{2} \|e^{t\mathcal{L}} \varphi\|_{L^2(\mu)}^2 \right) \leq -\rho \gamma \|(1 - \Pi_0) e^{t\mathcal{L}} \varphi\|_{L^2(\mu)}^2$$

Retrieve dissipation in x through **missing term** $\|\Pi_0 \varphi\|_{L^2(\mu)}^2 \dots$

Convergence dans le cas hypocoercif

un survol et une preuve (presque) complète

Exponential convergence: seminal ideas

- **Hypoellipticity**² gives **regularity** results for $\partial_t f = \mathcal{L}f$ when missing second order derivatives are recovered by commutators

Fokker–Planck operators with quadratic kinetic energies are hypoelliptic :

$$[\nabla_v, \mathcal{L}] = \nabla_x - \gamma \nabla_v$$

but **not the simple linear Boltzmann operator**...

- H^1 **setting for Langevin**³

$$\frac{d}{dt} \left(\frac{1}{2} \|(\nabla_x - a \nabla_v) e^{t\mathcal{L}} \varphi\|_{L^2(\mu)}^2 \right) = \dots - a \|\nabla_x e^{t\mathcal{L}} \varphi\|_{L^2(\mu)}^2$$

²Hörmander (1967)

³Talay (2002)

Exponential convergence: an incomplete survey

- Prove **exponential convergence** of the semigroup $e^{t\mathcal{L}}$ on subsets of $L_0^2(\mu)$
 - **Lyapunov** techniques⁴ $L_W^\infty(\mathcal{E}) = \left\{ \varphi \text{ measurable, } \left\| \frac{\varphi}{W} \right\|_{L^\infty} < +\infty \right\}$
 - standard **hypocoercive**⁵ setup $H^1(\mu)$
 - $E = L^2(\mu)$ after hypoelliptic regularization⁶ from $H^1(\mu)$
 - Directly⁷ $E = L^2(\mu)$ (recently⁸ Poincaré using $\partial_t - \mathcal{L}_{\text{ham}}$)
 - **coupling** arguments⁹ and other probabilistic proofs

⁴Wu ('01); Mattingly/Stuart/Higham ('02); Rey-Bellet ('06); Hairer/Mattingly ('11)

⁵Villani (2009), after Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004), ...

⁶F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)

⁷Hérau (2006), Dolbeault/Mouhot/Schmeiser (2009, 2015), ...

⁸Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)

⁹A. Eberle, A. Guillin and R. Zimmer, *Ann. Probab.* **47**(4), 1982-2010 (2019)

Direct $L^2(\mu)$ approach: lack of coercivity and a way around

- Decay estimates: $\varphi \in L^2_0(\mu)$, Fokker–Planck case,

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

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

- **Change of scalar product** to use the antisymmetric part \mathcal{L}_{ham} : modified square norm $\mathcal{H}[\varphi] = \frac{1}{2} \|\varphi\|_{L^2(\mu)}^2 - \varepsilon \langle R\varphi, \varphi \rangle$ for $\varepsilon \in (-1, 1)$ and¹⁰

$$R = \left(1 + (\mathcal{L}_{\text{ham}}\Pi_0)^*(\mathcal{L}_{\text{ham}}\Pi_0) \right)^{-1} (\mathcal{L}_{\text{ham}}\Pi_0)^*, \quad \Pi_0\varphi = \int_{v \in \mathbb{R}^d} \varphi d\kappa$$

- Approach less quantitative (**optimize scalar product**)

¹⁰Hérau (2006), Dolbeault/Mouhot/Schmeiser (2009, 2015), ...

Sketch of proof

- $R = \Pi_0 R(1 - \Pi_0)$ and $\mathcal{L}_{\text{ham}} R$ are bounded so that $\mathcal{H} \sim \|\cdot\|_{L^2(\mu)}^2$
- In fact, $(\mathcal{L}_{\text{ham}} \Pi_0)^*(\mathcal{L}_{\text{ham}} \Pi_0) = \beta^{-1} \nabla_x^* \nabla_x$ coercive in x

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

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

- Idea: Poincaré inequality for ∇_v and $\nabla_x^* \nabla_x \geq K_\nu^2 \Pi_0$

$$\begin{aligned} \mathcal{D}[\varphi] &= \gamma \langle -\mathcal{L}_{\text{FD}} \varphi, \varphi \rangle + \varepsilon \langle R \mathcal{L}_{\text{ham}} \Pi_0 \varphi, \varphi \rangle + \text{O}(\gamma \varepsilon) \\ &\geq \frac{\gamma}{\beta} \|\nabla_v \varphi\|_{L^2(\mu)}^2 + \varepsilon \left\langle \frac{\nabla_x^* \nabla_x}{\beta + \nabla_x^* \nabla_x} \Pi_0 \varphi, \Pi_0 \varphi \right\rangle + \text{O}(\gamma \varepsilon) \\ &\geq \frac{\gamma K_\kappa^2}{\beta} \|(1 - \Pi_0) \varphi\|_{L^2(\mu)}^2 + \frac{\varepsilon K_\nu^2}{\beta + K_\nu^2} \|\Pi_0 \varphi\|_{L^2(\mu)}^2 + \text{O}(\gamma \varepsilon) \end{aligned}$$

- Gronwall inequality $\frac{d}{dt} (\mathcal{H} [e^{t\mathcal{L}} \varphi]) = -\mathcal{D} [e^{t\mathcal{L}} \varphi] \leq -\frac{2\lambda}{1 + \varepsilon} \mathcal{H} [e^{t\mathcal{L}} \varphi]$

Un mot sur un travail récent

très “Matherials” pour arriver au résultat !

Obtaining directly bounds on the resolvent (1)

- Recall the following structure for typical hypocoercive operators

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

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

- $-\mathcal{S} \geq s\Pi_+ = 1 - \Pi_0$ (Poincaré on $\kappa(v)$ for Langevin)
- “macroscopic coercivity” $\|\mathcal{A}_{+0}\varphi\|_{L^2(\mu)} \geq a\|\Pi\varphi\|_{L^2(\mu)}$
Amounts to $\mathcal{A}_{+0}^* \mathcal{A}_{+0} \geq a^2 \Pi_0$

Guaranteed here by a Poincaré inequality for $\nu(x)$, with $a^2 = K_\nu^2/\beta$

Obtaining directly bounds on the resolvent (2)

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

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

- Additional technical assumptions:

- There exists an involution \mathcal{R} on \mathcal{H} such that

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

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

Abstract resolvent estimates

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

Scaling with the friction and the dimension

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

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

- 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 $\nabla_x^2 V \geq -K \text{Id}$ for some $K \geq 0$;
 - $C = 2$ and $C' = O(\sqrt{d})$ when $\Delta V \leq c_1 d + \frac{c_2 \beta}{2} |\nabla V|^2$ (with $c_2 \leq 1$) and $|\nabla^2 V|^2 \leq c_3^2 (d + |\nabla V|^2)$
- Better scaling $C' = O(\log d)$ when logarithmic Sobolev inequality and

$$\forall x \in \mathbb{R}^d, \quad \|\nabla^2 V(x)\|_{\mathcal{B}(\ell^2)} \leq c_3 (1 + |\nabla V(x)|_\infty)$$

Generalizations and perspectives

- **Approach works for other hypocoercive dynamics**¹¹
 - linear Boltzmann/randomized HMC
 - adaptive Langevin dynamics (additional Nosé–Hoover part)
- **Some work needed to extend it to more degenerate dynamics**
 - generalized Langevin dynamics
 - chains of oscillators
- **Current work also on obtaining...**
 - resolvent estimates $(i\omega - \mathcal{L})^{-1}$
 - space-time Poincaré inequalities with our algebraic framework

$$\left\| f - \langle f, \mathbf{1} \rangle_{L^2(\tilde{\mu}_T)} \right\|_{L^2(\tilde{\mu}_T)} \leq C_{1,T} \|(1-\Pi)f\|_{L^2(\tilde{\mu}_T)} + C_{2,T} \|(1-\mathcal{S})^{-1/2} (-\partial_t + \mathcal{A}) f\|_{L^2(\tilde{\mu}_T)}$$

¹¹E. Bernard, M. Fathi, A. Levitt, G. Stoltz, *arXiv preprint* **2003.00726**