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

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

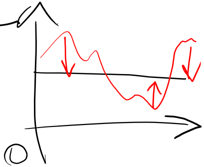
$\frac{d}{dt}\left(E(f)\right) \leq 0$ $\leq -\alpha E(f(t))$

pour $\mathcal{L}$ un opérateur négatif : pour un certain espace de Hilbert $\mathcal{H}$,

$i\partial_t \psi = \mathcal{L}\psi$ $\mathcal{L}$ auto. $\langle \mathcal{L}\psi, -i\mathcal{L}\psi\rangle = 0$

$\partial_t \psi = -i\mathcal{L}\psi$

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



- Préservation de la masse $\displaystyle\int_{\mathcal{Y}} f(t,y)\,\mu(y)\,dy = \int_{\mathcal{Y}} f(0,y)\,\boxed{\mu(y)}\,dy$

$\rightarrow$ regarder la convergence vers 0 de

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

- **Intérêt pratique** (personnel) : brique de base pour comprendre les propriétés statistiques de méthodes de Monte Carlo "$L^2(\mu)$"

EDOs hypocoercives

et le changement de produit scalaire

$\dot{x}_1 = -x_1 - \gamma x_1$

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

$\dot{x}_1 = -x_2 \,,\ \dot{x}_2 = +x_1 - \gamma x_1$

$$-L = A + \gamma S, \qquad \underbrace{A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\text{antisym.}}, \qquad \underbrace{S = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}}_{\text{sym.}}$$

A

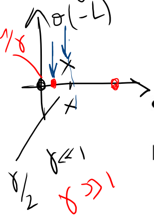
- **Structure of $-L$:**
  - Degenerate symmetric part $S \geqslant 0$
  - Antisymmetric part A coupling the kernel and the image of S
  - Smallest real part of eigenvalues (spectral gap) of order $\min(\gamma, \gamma^{-1})$

$$-L = \begin{pmatrix} 0 & 1 \\ -1 & \boxed{\gamma} \end{pmatrix}$$

negatif

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

$-L = U^{-1} D U$



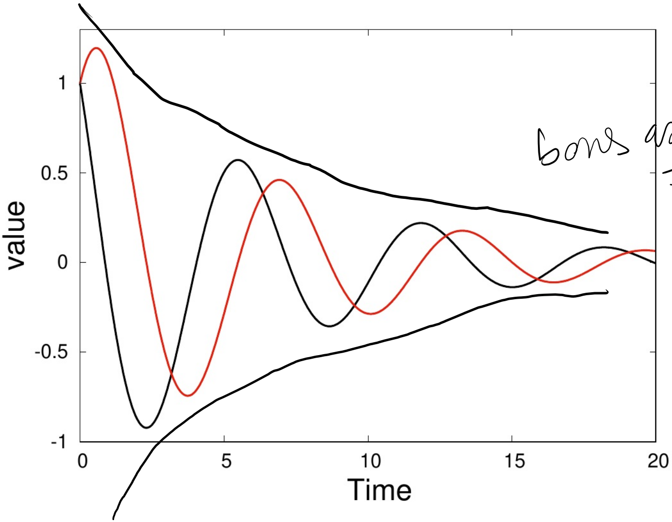
- **Longtime convergence of e^{tL}?** Use $\mathrm{e}^{tL} = U^{-1} \begin{pmatrix} \mathrm{e}^{-t\lambda_+} & 0 \\ 0 & \mathrm{e}^{-t\lambda_-} \end{pmatrix} U$

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

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

$C \geqslant 1$

Longtime convergence of hypocoercive ODE: illustration



bornes asymptotiques

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

- **“Elliptic PDE way”:** $\frac{d}{dt}\left(\frac{1}{2}|X(t)|^2\right) = -\gamma X(t)^T S X(t) = -\gamma X_2(t)^2 \leq 0$

$-X^T A X$

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

$|X(t)| \leq |X(0)|$

- Change the scalar product with P positive definite:

Change scalar product

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

$\leq -|X(t)|_P^2$

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

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

hypo. L^2

$\approx 2S$

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

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

Longtime convergence of this hypocoercive ODE (2)

- Optimal choice[1] for P? Think of "$L^T P \geqslant \lambda P$" and diagonalize L^T

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

Then $-(PL + L^T P) \geqslant 2\lambda P$ où $\lambda = \min \mathrm{Re}(\lambda_\pm)$ = trou spectral -

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

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

Decay rate given by spectral gap + bound from degenerate dissipation

- Prefactor $C \geqslant 1$ really needed!

$$-X(0)^T L X(0) \longleftarrow \frac{|X(t)|^2 - |X(0)|^2}{t} \leq \cdots \quad \lim_{t \to 0}$$

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

[1] F. 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

$\partial_t f = \mathcal{L}_{ovd} f$

sur $\mathbb{R}^d$ (ou $\mathbb{T}^d$)

- Consider the operator (advection/diffusion)

$\partial_{x_i}\nu = -\beta\,\partial_{x_i}V\cdot\nu$

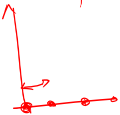
$$\mathcal{L}_{\rm ovd} = -\nabla V(x)\cdot\nabla_x + \frac{1}{\beta}\Delta_x = \boxed{-\frac{1}{\beta}\sum_{i=1}^d \partial_{x_i}^*\partial_{x_i}}$$

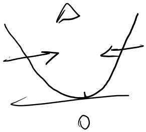
hence self-adjoint on $\boxed{L^2(\nu)}$ with $\boxed{\nu(x) = Z_\nu^{-1}\mathrm{e}^{-\beta V(x)}}$. Indeed,

$$\langle \partial_x \varphi, \phi\rangle_{L^2(\nu)} = \int_{\mathbb{R}^d} (\partial_{x_i}\varphi)\,\phi\,\nu = -\int_{\mathbb{R}^d} \varphi\,(\partial_{x_i}\phi)\,\nu - \int_{\mathbb{R}^d} \varphi\phi\,\boxed{\partial_{x_i}\nu}$$

so that $\partial_{x_i}^* = -\partial_{x_i} + \beta\,\partial_{x_i}V$ $\quad \frac{\partial_{x_i}\nu}{\nu}$ $\quad = -\langle \varphi, \partial_{x_i}\phi\rangle_{L^2(\nu)}$ $\quad \frac{\partial_{x_i}\nu}{\nu}\cdot\nu$

$\sigma(\mathcal{L}_{ovd})$





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

$-\frac{1}{\beta}\Delta + \mathcal{V}$ $\quad -$

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

$+\infty$ $\quad |\nabla V|^2 \gg \Delta V$

by considering $\widetilde{\mathcal{L}}_{\rm ovd} g = \nu^{1/2}\mathcal{L}_{\rm ovd}(\nu^{-1/2}g)$ $\quad |x| \to \infty$ $\quad |\nabla V|^2 \to +\infty$

Time evolution and decay estimates

$\mathcal{L}_{\rm ovd} = -\frac{1}{\beta} \nabla^* \nabla$

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

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

$= \langle \mathcal{L}_{\rm ovd}\varphi, 1 \rangle_{L^2(\nu)}$

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

$\varphi_0 \leftarrow \varphi_0 - \int \varphi_0 \nu$

- Can assume w.l.o.g. that $\int_{\mathbb{R}^d} \varphi_0\,\nu = 0$ (subspace $\boxed{L^2_0(\nu)}$ of $L^2(\nu)$)

- Decay estimate

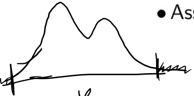
$= -\frac{1}{\beta}\langle \nabla^* \nabla \varphi, \varphi \rangle$

$$\frac{d}{dt}\left(\frac{1}{2}\|\varphi(t)\|^2_{L^2(\nu)}\right) = \langle \mathcal{L}_{\rm ovd}\varphi(t), \varphi(t)\rangle_{L^2(\nu)} = -\frac{1}{\beta}\|\nabla_x \varphi(t)\|^2_{L^2(\nu)} \leq 0$$

$= \int \mathcal{L}_{\rm ovd}\varphi(t) \cdot \varphi(t)\,\nu$

$\leq -\frac{K_\nu^2}{\beta}\|\varphi(t)\|^2_{L^2(\nu)}$

Poincaré inequality and convergence of the semigroup



K compact

- Assume that a Poincaré inequality holds:

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

$\nu(dx) = dx$ Poincaré-Wirtinger

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

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

$\|\varphi(t)\|_{L^2(\nu)} \le e^{-K_\nu t/\beta} \|\varphi_0\|$

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

$\mathcal{L}_{ovd} + \mathcal{A}$

Several remarks:

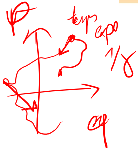
- The prefactor for the exponential convergence is 1
- The convergence rate is not degraded when one adds an antisymmetric part $\mathcal{A} = F \cdot \nabla$ to $\mathcal{L}$ (with $\operatorname{div}(F e^{-\beta V}) = 0$)

$-\langle \varphi, \mathcal{L}\varphi \rangle \geqslant \alpha \|\varphi\|^2$ in $L^2(\nu)$

EDP hypocoercives

deux opérateurs exemplaires

(Simple) Linear Boltzmann equation (1)



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

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

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

$|\kappa\rangle\langle 1| g$

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

$\dot q = p$

$\dot p = -\nabla V(q)$

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

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

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

$\mathcal{L}_{\mathrm{ham}}(F(H))$

$= F'(H) \underbrace{\mathcal{L}_{\mathrm{ham}} H}_{=0}$

$\beta = \dfrac{1}{k_B T}$

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

(Simple) Linear Boltzmann equation (2)

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

$L^2(\mu)$

$\Pi_0 1 = 1$

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

antisym. symm. diss.

$\mathcal{L}_{\mathrm{ham}}(\varphi\mu)$

$= \boxed{\mathcal{L}_{\mathrm{ham}}\varphi}\,\mu$

$+ \underbrace{\varphi\,\mathcal{L}_{\mathrm{ham}}\mu}_{=0}$

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

- Note that Π_0 is an orthogonal projector on $L^2(\mu)$ $\quad \Pi_0^2 = \Pi_0 = \Pi_0^*$

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

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

$\langle (\Pi_0 - 1)\varphi, \varphi\rangle$

$= -\langle (1-\Pi_0)\varphi, \varphi\rangle$

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

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

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

$\begin{pmatrix} 0 & 1 \\ -1 & \gamma \end{pmatrix}$

$P = I - \begin{pmatrix} 0 & \varepsilon \\ \varepsilon & 0 \end{pmatrix}$

$\langle x, Lx \rangle \geq \alpha |x|^2$

- **Issue:** prove that $\left\| \varphi(t) - \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi_0 \, \mu \right\|_{L^2(\mu)} \to 0$ as $t \to +\infty$

$\varphi_0 \leftarrow \varphi_0 - \int \varphi_0 \, \mu$

- Consider w.l.o.g. that $\displaystyle\int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(t) \, \mu = \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi_0 \, \mu = 0$
- Compute the decay of the $L^2(\mu)$-norm

$$\begin{aligned} \frac{d}{dt}\left(\frac{1}{2}\|\varphi(t)\|^2_{L^2(\mu)}\right) &= \int_{\mathbb{R}^d \times \mathbb{R}^d} [\mathcal{L}_{\mathrm{ham}}\varphi(t)]\, \varphi(t)\, \mu + \gamma \langle (\Pi_0 - 1)\varphi(t), \varphi(t) \rangle_{L^2(\mu)} \\ &= \underbrace{-\gamma \, \|(1 - \Pi_0)\varphi(t)\|^2_{L^2(\mu)}}_{\leq 0} \end{aligned}$$

manque $-\alpha \|\Pi_0 \varphi\|^2$

- 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 $\mathcal{L} = \mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}$: (anti)symmetric parts on $L^2(\mu)$

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

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

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 $\mathcal{L}_{\mathrm{FD}}$: only in v...

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

Common structure of the operators

- Operator on $\mathcal{H} = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \, \mu = 0 \right\}$, (anti)symmetric parts

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

$\partial_t f = \mathcal{L} f$

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

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

$(\mathcal{A}\Pi_0\varphi)(x,v)$
$= (v \cdot \nabla_x - \nabla V(x) \cdot \nabla_v)(\Pi_0\varphi)(x)$
$= v \cdot \nabla_x (\Pi_0 \varphi)(x)$

$(\Pi_0 - 1)\Pi_0 = 0$

$\nabla_v (\Pi_0 \varphi)(x) = 0$

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

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

$\Pi_0 \mathcal{A} \Pi_0 \varphi = 0$

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

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

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

Convergence dans le cas hypocoercif

un survol et une preuve (presque) complète

Exponential convergence: seminal ideas

$f(t,x) \in C^\infty$ si $t>0$

• **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...

$\mathcal{L}^{-1} \longrightarrow e^{t\mathcal{L}}$

• H^1 **setting for Langevin**[3]

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

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[2] Hörmander (1967)
[3] Talay (2002)

localisé vers $L^2(\mu)$

$H(x|v)$

$H(x v)$
$+ \alpha\, x \cdot v$

- Prove exponential convergence of the semigroup $\mathrm{e}^{t\mathcal{L}}$ on subsets of $L_0^2(\mu)$
  - Lyapunov techniques[4] $L_W^\infty(\mathcal{E}) = \left\{ \varphi \, \text{measurable}, \left\| \frac{\varphi}{W} \right\|_{L^\infty} < +\infty \right\}$
  - standard hypocoercive[5] setup $H^1(\mu)$
  - $E = L^2(\mu)$ after hypoelliptic regularization[6] from $H^1(\mu)$
  - Directly[7] $E = L^2(\mu)$ (recently[8] Poincaré using $\partial_t - \mathcal{L}_{\mathrm{ham}}$)
  - coupling arguments[9] and other probabilistic proofs

$L^2(\mu)$

$\neq$

$\boxed{-\nabla V}$

[4] Wu ('01); Mattingly/Stuart/Higham ('02); Rey-Bellet ('06); Hairer/Mattingly ('11)
[5] Villani (2009), after Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004), ...
[6] F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)
[7] Hérau (2006), Dolbeault/Mouhot/Schmeiser (2009, 2015), ...
[8] Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)
[9] A. 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

$\frac{\nabla^* \nabla}{1 + \nabla^* \nabla}$

- Decay estimates: $\varphi \in L_0^2(\mu)$, Fokker–Planck case,

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

$$= -\frac{\gamma}{\beta}\left\|\nabla_v \mathrm{e}^{t\mathcal{L}}\varphi\right\|_{L^2(\mu)}^2 \leqslant 0, \qquad \text{ou } -\gamma\|(1-\Pi_0)\varphi\|^2_{L^2(\mu)}$$

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

$\sqrt{\mathcal{L}_{\mathrm{ham}}\Pi}$

$\frac{\Pi \mathcal{L}_{\mathrm{ham}} \circ}{1 - \Pi \mathcal{L}_{\mathrm{ham}}^2 \Pi}$

$-\nabla_x^* \nabla_x$

- Change of scalar product to use the antisymmetric part $\mathcal{L}_{\mathrm{ham}}$: modified square norm $\mathcal{H}[\varphi] = \frac{1}{2}\|\varphi\|_{L^2(\mu)}^2 - \varepsilon\langle R\varphi, \varphi\rangle$ for $\varepsilon \in (-1, 1)$ and[10]

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

- Approach less quantitative (optimize scalar product)

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

Sketch of proof

$\begin{pmatrix} \gamma & O(1) \\ O(1) & 1/\gamma \end{pmatrix}$

- $R = \Pi_0 R(1-\Pi_0)$ and $\mathcal{L}_{\rm ham} R$ are bounded so that $\mathcal{H} \sim \|\cdot\|^2_{L^2(\mu)}$

$\frac{1}{2}\|\gamma K\|^2 - \varepsilon\langle R\varphi, \varphi\rangle$

$= \langle\langle \varphi, \varphi \rangle\rangle$

- In fact, $(\mathcal{L}_{\rm ham}\Pi_0)^*(\mathcal{L}_{\rm ham}\Pi_0) = \beta^{-1}\nabla_x^*\nabla_x$ coercive in x

$\min\left(\gamma, \frac{1}{\gamma}\right)$

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

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

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

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

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

$R\mathcal{L}$

$\downarrow$

$R\mathcal{L}_{\rm ham}$

$\downarrow$

$R\mathcal{L}_{\rm ham}\Pi$

$\gamma \ll 1 : \varepsilon = O(\gamma)$

$\gamma \gg 1 : \varepsilon = O\left(\frac{1}{\gamma}\right)$

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

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

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

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
  - $-\mathcal{S} \geqslant s\Pi_+ = 1 - \Pi_0$ (Poincaré on $\kappa(v)$ 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 $\nu(x)$, with $a^2 = K_\nu^2/\beta$

Obtaining directly bounds on the resolvent (2)

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

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

- Additional technical assumptions:
  - There exists an involution $\mathcal{R}$ on $\mathcal{H}$ such that

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

  - 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 $\max(\gamma, \gamma^{-1})$

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

- 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 $\nabla_x^2 V \geqslant -K\mathrm{Id}$ 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

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

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 $(\mathrm{i}\omega - \mathcal{L})^{-1}$
  - space-time Poincaré inequalities with our algebraic framework

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

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