Longtime convergence of some diffusion processes in molecular dynamics

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Outline of the talk

- **Computational statistical physics**
  - A general perspective
  - Langevin dynamics and its overdamped limit

- **Longtime convergence of overdamped Langevin dynamics**
  - Poincaré inequalities
  - Estimates on the asymptotic variance

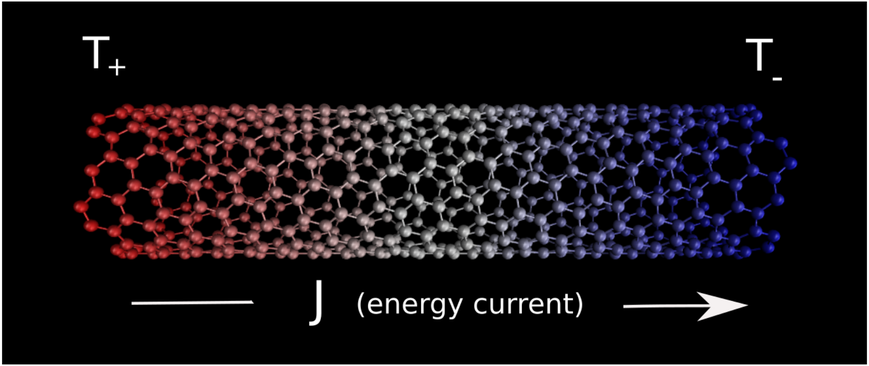
- **Longtime convergence of “hypocoercive” ODEs**

- **Longtime convergence of Langevin dynamics**
  - The need for a modified scalar product
  - One hypocoercive approach for Langevin dynamics
  - Direct estimates on the variance

Computational statistical physics

Computational statistical physics (1)

- **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?"

Computational statistical physics (2)

- Macrostate of the system described by a probability measure

Equilibrium thermodynamic properties (pressure,...)

$$\mathbb{E}_\mu(\varphi) = \int_{\mathcal{E}} \varphi(q,p)\,\mu(dq\,dp)$$

- Choice of thermodynamic ensemble
  - least biased measure compatible with the observed macroscopic data
  - Volume, energy, number of particles, ... fixed exactly or in average
  - Equivalence of ensembles (as $N \to +\infty$)

- Canonical ensemble = measure on (q,p), average energy fixed H

$$\mu_{\mathrm{NVT}}(dq\,dp) = Z_{\mathrm{NVT}}^{-1}\,\mathrm{e}^{-\beta H(q,p)}\,dq\,dp$$

with $\beta = \dfrac{1}{k_{\mathrm{B}}T}$ the Lagrange multiplier of the constraint $\displaystyle\int_{\mathcal{E}} H\,\rho\,dq\,dp = E_0$

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

$$\forall \varphi \in C_0^\infty(\mathcal{E}), \qquad \int_{\mathcal{E}} \mathcal{L}\varphi \, d\mu = 0$$

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

- Overdamped limit $\gamma \to +\infty$ (or masses going to 0)

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

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

- In both cases, slow convergence to equilibrium
  - it takes time to change energy levels in the Hamiltonian limit[1]
  - for fixed masses, time has to be rescaled by a factor γ

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

Ergodicity results for Langevin dynamics (1)

- Almost-sure convergence[2] of ergodic averages $\widehat{\varphi}_t = \dfrac{1}{t}\displaystyle\int_0^t \varphi(q_s,p_s)\,ds$

- 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[3] 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?

[2] Kliemann, *Ann. Probab.* **15**(2), 690-707 (1987)

[3] Bhattacharya, *Z. Wahrsch. Verw. Gebiete* **60**, 185–201 (1982)

Ergodicity results for Langevin dynamics (2)

- Invertibility of $\mathcal{L}$ on subsets of $L^2_0(\mu) = \left\{ \varphi \in L^2(\mu) \,\middle|\, \int_{\mathcal{E}} \varphi \, d\mu = 0 \right\}$?

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

- Prove exponential convergence of the semigroup $\mathrm{e}^{t\mathcal{L}}$
  - various Banach spaces $E \cap L^2_0(\mu)$
  - Lyapunov techniques[4] $B^\infty_W(\mathcal{E}) = \left\{ \varphi \,\text{measurable}, \sup \left| \frac{\varphi}{W} \right| < +\infty \right\}$
  - standard hypocoercive[5] setup $H^1(\mu)$
  - $E = L^2(\mu)$ after hypoelliptic regularization[6] from $H^1(\mu)$
  - Directly $E = L^2(\mu)$ (recently[7] Poincaré using $\partial_t - \mathcal{L}_{\mathrm{ham}}$)
  - coupling arguments[8]

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[4] Wu ('01); Mattingly/Stuart/Higham ('02); Rey-Bellet ('06); Hairer/Mattingly ('11)
[5] Villani (2009) and before Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004)
[6] F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)
[7] Armstrong/Mourrat (2019), Cao/Lu/Wang (2019)
[8] A. Eberle, A. Guillin and R. Zimmer, *Ann. Probab.* **47**(4), 1982-2010 (2019)

Convergence of overdamped Langevin dynamics

Overdamped Langevin dynamics and its generator

- Generator of Langevin dynamics (advection/diffusion)

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

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

$$\int_{\mathcal{D}} (\partial_{q_i}\varphi)\, \phi \, d\nu = -\int_{\mathcal{D}} \varphi\, (\partial_{q_i}\phi)\, d\nu - \int_{\mathcal{D}} \varphi\phi\, \partial_{q_i}\nu$$

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

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

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

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

Time evolution and decay estimates

- 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 $\varphi(t) \xrightarrow[t\to+\infty]{} \int_{\mathcal{D}} \varphi_0\,\nu$

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

- Decay estimate

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

Poincaré inequality and convergence of the semigroup

• Assume that a Poincaré inequality holds:

$$\forall \phi \in H^1(\nu) \cap L^2_0(\nu), \qquad \|\phi\|_{L^2(\nu)} \leqslant \frac{1}{K_\nu} \|\nabla_q \phi\|_{L^2(\nu)}$$

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

$$\left\| \mathrm{e}^{t\mathcal{L}} \right\|_{\mathcal{B}(L^2_0(\nu))} \leqslant \mathrm{e}^{-K_\nu^2 t/\beta}.$$

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

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 $\mathrm{div}(F\mathrm{e}^{-\beta V}) = 0$)

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

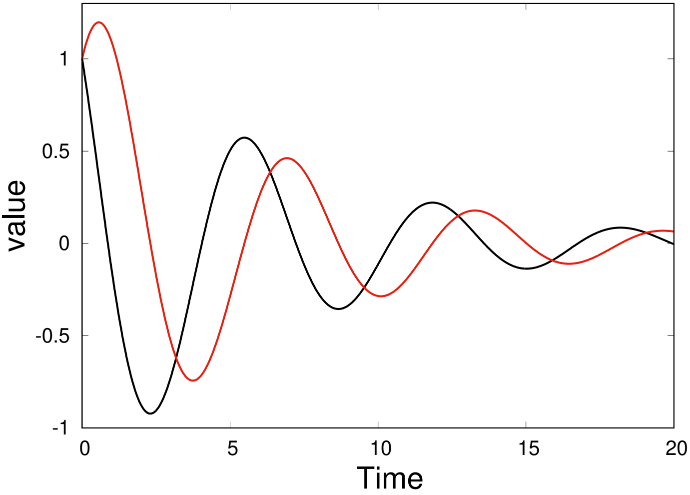
  determinant 1, trace γ, so eigenvalues $\lambda_\pm = \frac{\gamma}{2} \pm \left(\frac{\gamma^2}{4} - 1\right)^{1/2}$

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

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

• Change the scalar product with P positive definite:

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

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

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

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

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

• Optimal choice[9] 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 $-(PL + L^T P) \geqslant 2\lambda P$

• Therefore, $|X(t)|_P^2 \leqslant \mathrm{e}^{-2\lambda t}|X_0|_P^2$, 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 $+$ bound from degenerate dissipation

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

[9] 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 $\mathcal{L}_{\mathrm{FD}} = -p^T M^{-1}\nabla_p + \dfrac{1}{\beta}\Delta_p$
- 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

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

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

• 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[10,11]
  - 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

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

[10] Dolbeault, Mouhot and Schmeiser, *C. R. Math. Acad. Sci. Paris* (2009)

[11] 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 $\mathcal{H}[\varphi] = \dfrac{1}{2}\|\varphi\|^2_{L^2(\mu)} - \varepsilon \langle R\varphi, \varphi \rangle$ with[12]

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

  - $R = \Pi_0 R(1-\Pi_0)$ 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:** $(\mathcal{L}_{\mathrm{ham}}\Pi_0)^*(\mathcal{L}_{\mathrm{ham}}\Pi_0) = \beta^{-1}\nabla_q^*\nabla_q$ coercive in q, and

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

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

Sketch of proof (2)

- Recall Poincaré inequalities: $\nabla_p^*\nabla_p \geqslant K_\kappa^2(1-\Pi_0)$ and $\nabla_q^*\nabla_q \geqslant K_\nu^2\Pi_0$

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 (some elliptic estimates)

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

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

Obtaining directly bounds on the resolvent (1)

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

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

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
  - $-\dfrac{1}{2}(\mathcal{L} + \mathcal{L}^*) \geqslant s \Pi_+ = s(1 - \Pi_0)$ (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 $\Pi_1 = \mathcal{A}_{+0} \left(\mathcal{A}_{+0}^* \mathcal{A}_{+0}\right)^{-1} \mathcal{A}_{+0}^*$

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

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

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

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

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

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

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

Generalizations/perspectives for direct resolvent estimates

- **Approach works for other hypocoercive dynamics**[13]
  - non-quadratic kinetic energies
  - 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

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

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