(Non)equilibrium Langevin dynamics: convergence and numerical approximation

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Work also supported by ANR Funding ANR-14-CE23-0012 ("COSMOS")

Genève, Mars 2017

Outline

- **A quick introduction to computational statistical physics**
- **Equilibrium Langevin dynamics**
  - Various convergence results
  - A focus on the approach by Dolbeault, Mouhot and Schmeiser
- **Discretization by a spectral Galerkin method**
  - A priori error estimates for Poisson equations
  - Explicit convergence rates for a representative system
  - Numerical results
- **Nonequilibrium Langevin dynamics** (depending on time...)

A quick introduction to computational statistical physics

Computational statistical physics

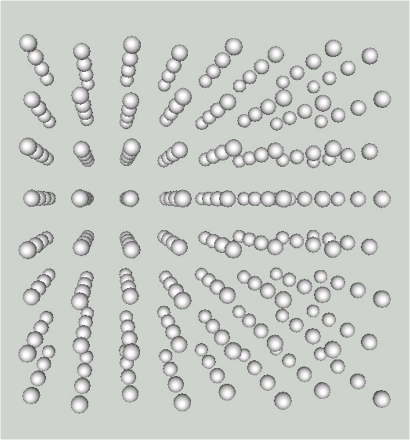
- *Predict macroscopic properties of matter from its microscopic description*

- **Microstate**
  - positions $q = (q_1, \ldots, q_N)$ and momenta $p = (p_1, \ldots, p_N)$
  - energy $V(q) + \sum_{i=1}^{N} \frac{p_i^2}{2m_i}$

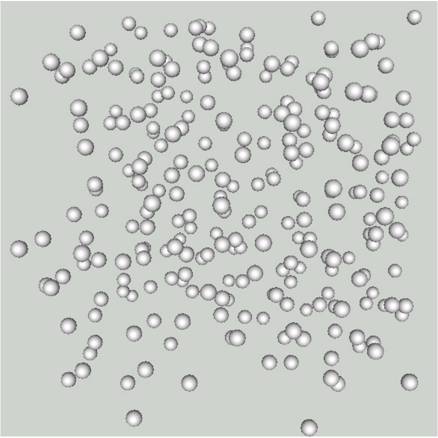
- **Macrostate**
  - described by a probability measure μ
  - constraints fixed exactly or in average (number of particles, volume, energy)

- **Properties :**
  - static $\langle A \rangle = \int_{\mathcal{E}} A(q,p)\, \mu(dq\, dp)$ (equation of state, heat capacity,...)
  - dynamic (transport coefficient, transition pathway, etc)

What is the melting temperature of Argon?



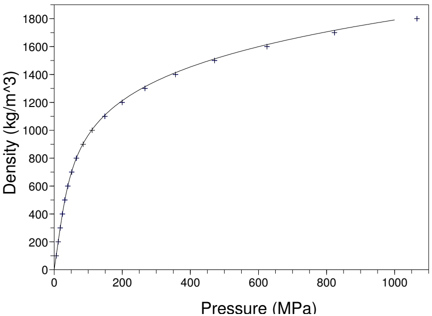
(a) Solid Argon (low temperature)

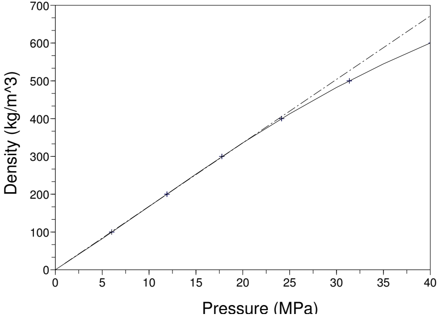


(b) Liquid Argon (high temperature)

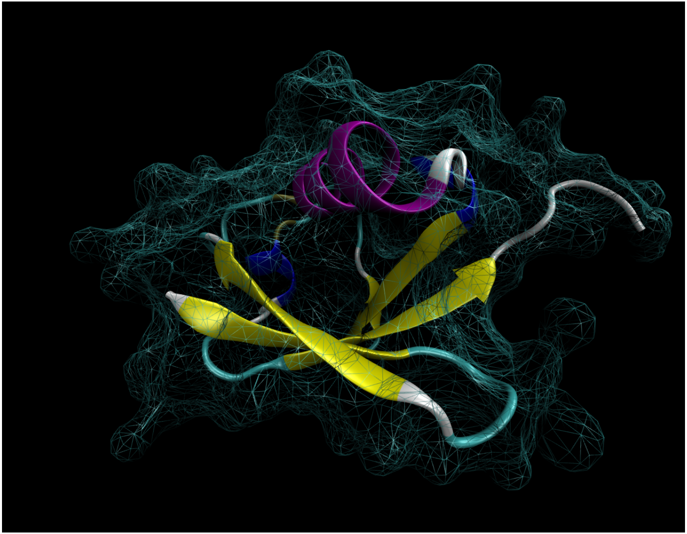
Examples of molecular systems (2)

Equation of state of Argon: density as a function of pressure at fixed temperature $T = 300$ K





Examples of molecular systems (3)



Ubiquitin: what is its structure? What are its conformational changes?

Some orders of magnitude...

- **Physical orders of magnitude**
  - distances ~ 1 $\mathring{A} = 10^{-10}$ m
  - energy per particle $\sim k_{\mathrm{B}} T \sim 4 \times 10^{-21}$ J at 300 K
  - atomic masses $\sim 10^{-26}$ kg
  - typical times $\sim 10^{-15}$ s
  - number of particles $\sim \mathcal{N}_A = 6.02 \times 10^{23}$

- **"Standards" simulations**
  - 10^6 particles ["heroic": from 10^9 particles on]
  - total time: (fraction of) ns ["heroic": (fraction of) μs]

- Computation of high dimensional integrals...

$\rightarrow$ Ergodic methods $\displaystyle \frac{1}{t}\int_0^t A(q_s, p_s)\, ds \xrightarrow[t\to+\infty]{} \langle A \rangle$

Equilibrium Langevin dynamics

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 $H(q,p) = V(q) + \frac{1}{2} p^T M^{-1} p$ (more general kinetic energies $U(p)$ can be considered[1])

Stochastic perturbation of the Hamiltonian dynamics

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

- Friction $\gamma > 0$ (could be a position-dependent matrix)

[1] Redon, Stoltz, Trstanova, *J. Stat. Phys.* (2016)

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 $m \to 0$

$$q_t - q_0 = -\frac{1}{\gamma}\int_0^t \nabla V(q_s)\,ds + \sqrt{\frac{2}{\gamma\beta}}W_t - \frac{1}{\gamma}(p_t - p_0)$$

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

- In both cases, slow convergence to equilibrium
  - it takes time to change energy levels in the Hamiltonian limit[2]
  - for m fixed, time has to be rescaled by a factor γ

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

Ergodicity results (1)

- Almost-sure convergence[3] of ergodic averages $\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(q_s, p_s)\, ds$
- Asymptotic variance of ergodic averages

$$\sigma_\varphi^2 = \lim_{t\to+\infty} t\mathbb{E}\left[\widehat{\varphi}_t^2\right] = 2\int_{\mathcal{E}} \left(-\mathcal{L}^{-1}\Pi_0\varphi\right)\Pi_0\varphi\, d\mu$$

where $\Pi_0\varphi = \varphi - \mathbb{E}_\mu(\varphi)$

- A central limit theorem holds[4] when the equation has a solution in $L^2(\mu)$

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

$$-\mathcal{L}\Phi = \Pi_0\varphi$$

- Well-posedness of such equations? Hypoelliptic operator

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

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

Ergodicity results (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[5,6] $L^\infty_W(\mathcal{E}) = \left\{ \varphi \, \text{measurable}, \, \left\| \frac{\varphi}{W} \right\|_{L^\infty} < +\infty \right\}$
  - standard hypocoercive[7] setup $H^1(\mu)$
  - $E = L^2(\mu)$ after hypoelliptic regularization[8] from $H^1(\mu)$

[5] L. Rey-Bellet, *Lecture Notes in Mathematics* (2006)
[6] Hairer and Mattingly, *Progr. Probab.* **63** (2011)
[7] Villani (2009) and before Talay (2002), Eckmann/Hairer (2003), Hérau/Nier (2004)
[8] F. Hérau, *J. Funct. Anal.* **244**(1), 95-118 (2007)

Direct $L^2(\mu)$ approach

- Assume that the potential V is smooth and[9,10]
  - the marginal measure ν satisfies a Poincaré inequality

$$\|\Pi_0\varphi\|^2_{L^2(\nu)} \leqslant \frac{1}{C_\nu}\|\nabla_q\varphi\|^2_{L^2(\nu)}.$$

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

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

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 exists $\overline{\lambda} > 0$ such that

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

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

[10] Dolbeault, Mouhot and Schmeiser, *Trans. AMS*, **367**, 3807–3828 (2015)

Sketch of proof

- Entropy functional $\mathcal{H}[\varphi] = \dfrac{1}{2}\|\varphi\|^2 - \varepsilon \langle A\varphi, \varphi\rangle$ for $\varepsilon \in (-1,1)$ and

$$A = \Big(1 + (\mathcal{L}_{\rm ham}\Pi_p)^*(\mathcal{L}_{\rm ham}\Pi_p)\Big)^{-1}(\mathcal{L}_{\rm ham}\Pi_p)^*, \qquad \Pi_p\varphi = \int_{\mathbb{R}^D} \varphi \, d\kappa$$

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

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

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

- Idea: control of $\|(1-\Pi_p)\varphi\|^2$ by $\langle -\mathcal{L}_{\rm FD}\varphi, \varphi\rangle$ (Poincaré); for $\|\Pi_p\varphi\|^2$,

$$\|\mathcal{L}_{\rm ham}\Pi_p\varphi\|^2 \geqslant \frac{DC_\nu}{\beta m}\|\Pi_p\varphi\|^2, \qquad \text{hence } A\mathcal{L}_{\rm ham}\Pi_p \geqslant \lambda_{\rm ham}\Pi_p$$

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

Discretization by a spectral Galerkin method

Motivation: control variate method

• The computation of transport coefficients by nonequilibrium steady-state techniques involves the computations of quantities of the form

$$\frac{\mathbb{E}_\tau(R)}{\tau}, \qquad |\tau| \ll 1$$

$\rightarrow$ **Magnification of the statistical error**

• Typical cases: $\mathcal{L}_\eta = \mathcal{L}_0 + \eta\widetilde{\mathcal{L}}$

- nonequilibrium perturbation (later on)
- coupling parameter between otherwise independent systems
- anharmonic part in an otherwise linear dynamics

• Control variate idea

- note that $\mathbb{E}_\tau(R - \mathcal{L}_\tau\Phi) = \mathbb{E}_\tau(R)$ for all Φ
- ...but it may happen that $\mathrm{Var}_\tau(R - \mathcal{L}_\tau\Phi) \ll \mathrm{Var}_\tau(R)$
- Optimal choice $\Phi = \mathcal{L}_\tau^{-1}(R - \mathbb{E}_\tau(R))$ unknown
- approximate it by $\mathcal{L}_0^{-1}(R - \mathbb{E}_0(R))$

Principle of Galerkin approximation

- Reference Poisson equation $-\mathcal{L}\Phi = \Pi_0 R$
- Galerkin space V_M: conformal ($V_M \subset L_0^2(\mu)$) or non-conformal

Variational formulation

$$\begin{cases} \text{Find } \Phi_M \in V_M \cap L_0^2(\mu) \text{ such that} \\ \forall \psi \in V_M, \ -\langle \psi, \mathcal{L}\Phi_M \rangle = \langle \psi, \Pi_0 R \rangle . \end{cases}$$

- In fact, $-\Pi_M \mathcal{L} \Pi_M \Phi_M = \Pi_M R$
- Error = (related to) consistency error + approximation error

$$\Phi_M - \Phi = (\Phi_M - \Pi_M \Phi) - (1 - \Pi_M)\Phi$$

- Well-posedness? Cannot apply Lax–Milgram[11]...
- Approximation error: for specific models

[11] Abdulle, Pavliotis, Vaes, *arXiv preprint* **1609.05097** (2016)

Well posedness of the Galerkin procedure (conformal case)

- Conformal space and $\|(A+A^*)(1-\Pi_M)\mathcal{L}\Pi_M\| \xrightarrow[M\to\infty]{} 0$

Invertibility of $-\Pi_M \mathcal{L} \Pi_M$

There exist $C \geqslant 1$ (independent of M, γ) and $M_0 \in \mathbb{N}$ such that, for any $M \geqslant M_0$, there is $\lambda_{\gamma,M} > 0$ for which

$$\forall \varphi \in V_M, \quad \forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t\Pi_M \mathcal{L} \Pi_M} \varphi \right\| \leqslant C \mathrm{e}^{-\lambda_{\gamma,M} t} \|\varphi\|.$$

Moreover, $\lambda_{\gamma,M} \xrightarrow[M\to\infty]{} \lambda_\gamma$ where $\lambda_\gamma > 0$.

- If $\mathcal{L}_{\mathrm{FD}}$ stabilizes V_M (i.e. $\Pi_M \mathcal{L}_{\mathrm{FD}} = \mathcal{L}_{\mathrm{FD}} \Pi_M$), uniform lower bound

$$\forall \gamma > 0, \qquad \lambda_{\gamma,M} \geqslant \overline{\lambda}_M \min(\gamma, \gamma^{-1}),$$

- Key inequality for the proof: $\mathscr{D}_M[\varphi] = -\langle\langle \varphi, \Pi_M \mathcal{L} \Pi_M \varphi \rangle\rangle$ such that

$$\mathscr{D}_M[\varphi] = \mathscr{D}[\varphi] + \varepsilon \langle A(1-\Pi_M)\mathcal{L}\varphi, \varphi \rangle + \varepsilon \langle \varphi, A^*(1-\Pi_M)\mathcal{L}\varphi \rangle$$

Well posedness in the non-conformal case

- Work on $V_{M,0} = V_M \cap L^2_0(\mu)$
- Projector $\Pi_M = \Pi_{M,0} + \Pi_{u_M}$ with $u_M = \dfrac{\Pi_M \mathbf{1}}{\|\Pi_M \mathbf{1}\|} \in V_M$
- Invertibility of $-\Pi_{M,0}\mathcal{L}\Pi_{M,0}$ under the additional condition

$$\|\mathcal{L}^* u_M\| \xrightarrow[M\to\infty]{} 0$$

Saddle-point formulation

For any $R \in L^2(\mu)$, there exist a unique $\Phi_M \in V_M$ and a unique $\alpha_M \in \mathbb{R}$ such that

$$\left\{ \begin{aligned} -\Pi_M \mathcal{L} \Pi_M \Phi_M + \alpha_M u_M &= \Pi_M R, \\ \langle \Phi_M, u_M \rangle &= 0. \end{aligned} \right.$$

Consistency error

- Poisson equation implies $-\Pi_{M,0}\mathcal{L}\Pi_{M,0}\Phi = \Pi_{M,0}R + \Pi_{M,0}\mathcal{L}(1-\Pi_{M,0})\Phi$

- Subtracting the equation for Φ_M,

$$\Pi_{M,0}\mathcal{L}\Pi_{M,0}(\Phi_M - \Pi_{M,0}\Phi) = \Pi_{M,0}\mathcal{L}(1-\Pi_{M,0})\Phi$$

Consistency error

$$\|\Phi_M - \Pi_{M,0}\Phi\|_{L^2(\mu)} \leqslant \frac{C}{\widehat{\lambda}_{\gamma,M}}\left(\|\Pi_M\mathcal{L}(1-\Pi_M)\Phi\|_{L^2(\mu)} + \|\mathcal{L}u_M\|\|\Phi\|\right)$$

- Explicit estimates/rates for specific models... Typically,

$$\|\Pi_M\mathcal{L}(1-\Pi_M)\Phi\|_{L^2(\mu)} \leqslant \|\Pi_M\mathcal{L}(1-\Pi_M)\|_{\mathcal{B}(L^2(\mu))}\|(1-\Pi_M)\Phi\|_{L^2(\mu)}$$

provided the second term is not too large and the last one is small

Spectral basis for Langevin operators

- Weighted Fourier modes in position

$$G_{2k}(q) = \sqrt{\frac{Z_{\beta,\nu}}{\pi}} \cos(kq) \, \mathrm{e}^{\beta V(q)/2}, \qquad G_{2k-1}(q) = \sqrt{\frac{Z_{\beta,\nu}}{\pi}} \sin(kq) \, \mathrm{e}^{\beta V(q)/2}$$

- Hermite functions H_ℓ for momenta (eigenfunctions of $\mathcal{L}_{\rm FD}$)

- Tensor basis of $2K-1$ Fourier and L Hermite modes: projector Π_{KL}

Approximation error

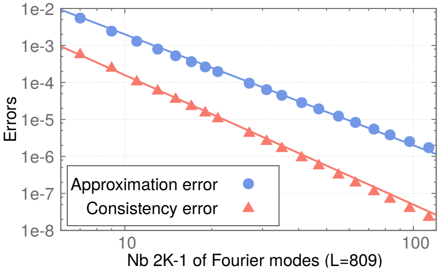
For any $s \in \mathbb{N}$, there exists $A_s \in \mathbb{R}_+$ such that, for all $\varphi \in H^s(\mu)$,

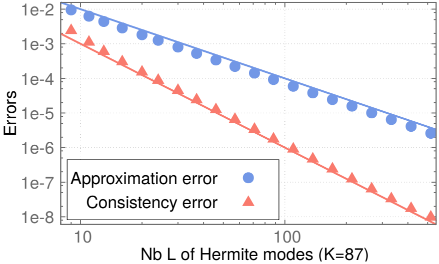
$$\forall K \geqslant 1, \; L \geqslant s, \qquad \|\varphi - \Pi_{KL}\varphi\|_{L^2(\mu)} \leqslant A_s \left(\frac{1}{K^s} + \frac{1}{L^{s/2}} \right) \|\varphi\|_{H^s(\mu)}$$

- Consistency error for $V(q) = 1 - \cos(q)$: bounds

$$\|\Pi_{KL}\mathcal{L}(1-\Pi_{KL})\|_{\mathcal{B}(L^2(\mu))} = \mathrm{O}(K\sqrt{L})$$

Observable $R = \sum_{k\in\mathbb{N},\ell\in\mathbb{N}} \max(1,k)^{-5/2}\max(1,\ell)^{-3/2} G_k H_\ell$ (almost $H^2(\mu)$)

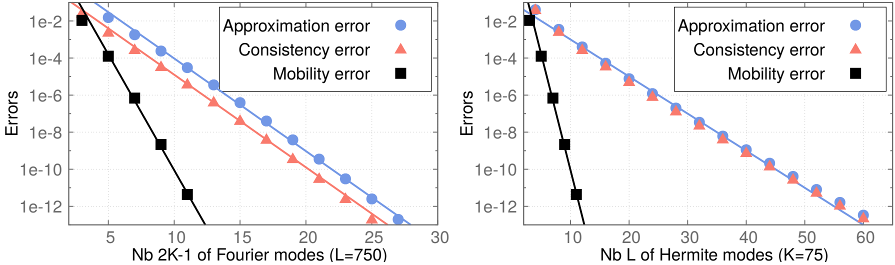




Left: approximation error $\sim K^{-3}$, consistency error $\sim K^{-7/2}$
Right: approximation error $\sim L^{-2}$, consistency error $\sim L^{-3}$
$\rightarrow$ "full" regularization by $\mathcal{L}^{-1}$!

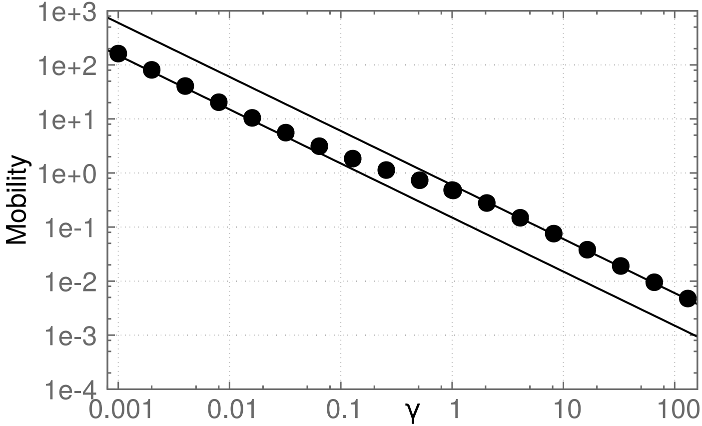
Estimation of the self-diffusion (1)

Definition $D(\gamma) = \int_0^{+\infty} \mathbb{E}\left(p_t p_0\right) dt = \left\langle -\mathcal{L}^{-1} p, p \right\rangle_{L^2(\mu)}$



Exponential rate of convergence

Estimation of the self-diffusion (2)

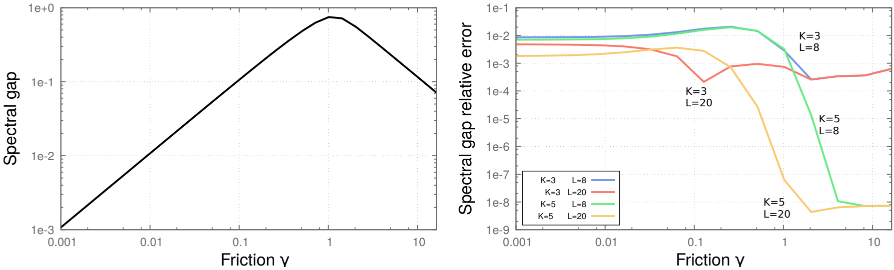


Scaling $D(\gamma) \sim \gamma^{-1}$ both for small and large frictions[12]

[12] M. Hairer and G. Pavliotis, *J. Stat. Phys.* (2008)

Errors on the spectral gap

Also exponential decay of the error on the spectral gap



Left: Spectral gap as a function of the friction γ
Right: Relative error on the spectral gap for several couples K, L. Note that it depends only on K in the overdamped regime

Nonequilibrium Langevin dynamics

Nonequilibrium perturbation of equilibrium dynamics

- Compact position space $\mathcal{D} = (2\pi\mathbb{T})^d$, constant force $|F| = 1$

Langevin dynamics perturbed by a constant force term

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

- Non-zero velocity in the direction F is expected in the steady-state
- F **does not derive from the gradient of a periodic function**
  - of course, $F = -\nabla W_F(q)$ with $W_F(q) = -F^T q$
  - ...but W_F is not periodic!

Existence and uniqueness of the steady state

- Generator $\mathcal{L}_{\gamma,\tau} = \mathcal{L}_{\rm ham} + \gamma \mathcal{L}_{\rm FD} + \tau \mathcal{L}_{\rm pert}$ with $\mathcal{L}_{\rm pert} = F \cdot \nabla_p$
- Lyapunov functions[13] $\mathcal{K}_n(q,p) = 1 + |p|^n$ for $n \geqslant 2$

Exponential convergence to equilibrium

Consider $\tau_* > 0$ and fix $\gamma > 0$. For any $\tau \in [-\tau_*, \tau_*]$, there is a unique invariant probability measure which admits a C^∞ density $\psi_\tau(q,p)$. Moreover, for any $n \geqslant 2$, there exist $C_n, \lambda_n > 0$ (depending on τ_*) such that, for any $\tau \in [-\tau_*, \tau_*]$ and for any $\varphi \in L^\infty_{\mathcal{K}_n}(\mathcal{E})$,

$$\forall t \geqslant 0, \qquad \left\| \mathrm{e}^{t\mathcal{L}_\tau}\varphi - \int_{\mathcal{E}} \varphi\, \psi_\tau \right\|_{L^\infty_{\mathcal{K}_n}} \leqslant C_n \mathrm{e}^{-\lambda_n t} \|\varphi\|_{L^\infty_{\mathcal{K}_n}}.$$

- Non-perturbative result (also non-quantitative unfortunately...)

[13] M. Hairer and J. Mattingly, *Progr. Probab.* (2011); Meyn and Tweedie (2009); Rey–Bellet (2006)

Perturbative expansion of the steady state

- Perturbative framework: operators considered on $L^2(\mu)$

$$\psi_\tau = h_\tau \mu, \qquad h_\tau \in L^2(\mu)$$

- Fokker–Planck equation $\mathcal{L}_{\gamma,\tau}^* h_\tau = 0$ with $\displaystyle\int_{\mathcal{E}} h_\tau \, d\mu = 1$

Power expansion of the invariant measure

For $|\tau| < r^{-1}$, it holds $h_\tau \in L^2(\mu)$ and

$$h_\tau = \left(1 + \tau \left(\mathcal{L}_{\mathrm{pert}} \mathcal{L}_{\gamma,0}^{-1}\right)^*\right)^{-1} \mathbf{1} = \left(1 + \sum_{n=1}^{+\infty} (-\tau)^n \left[\left(\mathcal{L}_{\mathrm{pert}} \mathcal{L}_{\gamma,0}^{-1}\right)^*\right]^n\right) \mathbf{1}.$$

- Spectral radius $r = \displaystyle\lim_{n \to +\infty} \left\| \left[\left(\mathcal{L}_{\mathrm{pert}} \mathcal{L}_{\gamma,0}^{-1}\right)^*\right]^n \right\|_{\mathcal{B}(L_0^2(\mu))}^{1/n}$. In fact,

$$\frac{1}{r} \geqslant \frac{\min(1,\gamma)}{\sqrt{\beta K}}$$

Provides magnitude of admissible perturbations for $L^2(\mu)$ convergence

Convergence rates

- Suboptimal results by the standard hypocoercive approach in $H^1(\mu)$
$\rightarrow$ nonequilibrium perturbation[14] of direct $L^2(\mu)$ strategy

Uniform rates for nonequilibrium perturbations

There exist $C, \delta_* > 0$ such that, for any $\delta \in [0, \delta^*]$, there is $\overline{\lambda}_\delta > 0$ for which, for all $\gamma \in (0, +\infty)$ and all $\tau \in [-\delta \min(\gamma, 1), \delta \min(\gamma, 1)]$,

$$\left\| \mathrm{e}^{t\mathcal{L}^*_{\gamma,\tau}} f - h_\tau \right\|_{L^2(\mu)} \leqslant C \mathrm{e}^{-\overline{\lambda}_\delta \min(\gamma,\gamma^{-1})t} \| f - h_\tau \|_{L^2(\mu)}.$$

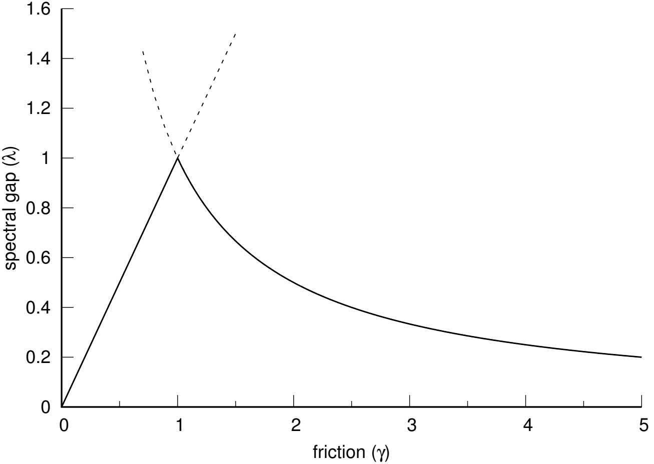
Moreover, $\overline{\lambda}_\delta = \overline{\lambda}_0 + \mathrm{O}(\delta)$.

- As a corollary: lower bounds on the spectral gap of order $\min(\gamma, \gamma^{-1})$

- Some elements on hypocoercive entropy estimates

[14] E. Bouin, F. Hoffmann, and C. Mouhot, *arXiv preprint* **1605.04121**

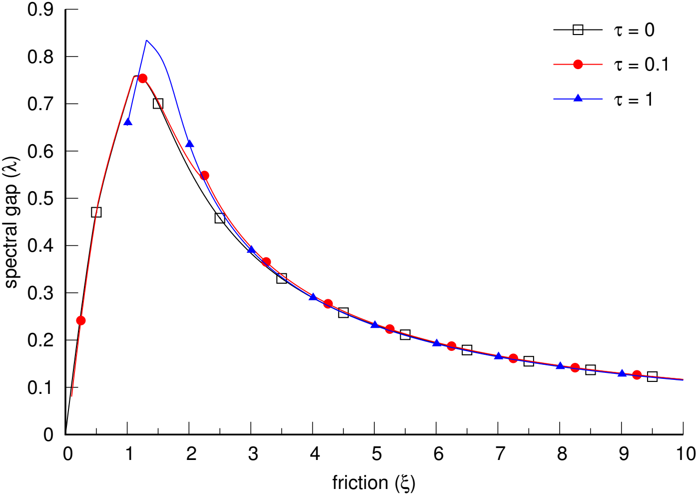
Numerical results (1)



Predicted spectral gap as a function of the friction γ when $V = 0$, $\beta = 1$ and $m = 1$ (solid line) vs. theoretical prediction[15]

[15] S. M. Kozlov, *Math. Notes* **45**, 360-368 (1989)

Numerical results (2)



Spectral gap as a function of γ for $\tau = 0, 0.1, 1$ when $V(q) = 1 - \cos(q)$

References

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