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Langevin dynamics with space-time periodic nonequilibrium forcing

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Definition of the dynamics

- Periodic boundary conditions: position $q \in \mathcal{M} = (L\mathbb{T})^d$
- Nonequilibrium Langevin dynamics ($M \in \mathbb{R}^{d \times d}$ positive definite, $\gamma > 0$)

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

- Smooth potential V and force F, with F periodic in time with period T
- $F = 0$: inv. measure $\mu(dq\,dp) \propto \exp\left(-\beta \left[V(q) + \frac{1}{2} p^T M^{-1} p\right]\right) dq\,dp$

Questions

- what is the steady-state of the system?
- behavior under hyperbolic space-time scaling? (average velocity)
- fluctuations around the average velocity: longtime effective diffusion

P. Collet and S. Martínez, *J. Math. Biol.*, **56**(6) (2008) 765–792

G. Pavliotis, R. Joubaud and G. Stoltz, *J. Stat. Phys* **158**(1) (2015) 1–36

Convergence to the equilibrium state

Exponential convergence to a limiting cycle

- Lyapunov functions $\mathcal{K}_n(q,p) = 1 + |p|^{2n}$ (for $n \geqslant 1$) and corresponding L^∞ norms on functions $f(\theta, q, p)$

$$\|f\|_{L^\infty(L^\infty_{\mathcal{K}_n})} = \sup_{\theta \in T\mathbb{T}} \left\| \frac{f(\theta)}{\mathcal{K}_n} \right\|_{L^\infty}$$

Uniform convergence result for $\eta \in [-\eta_*, \eta_*]$

Unique probability measure $\psi_\eta(\theta, q, p)$ on $\mathcal{E} = T\mathbb{T} \times \mathcal{M} \times \mathbb{R}^d$ such that

$$\left| \mathbb{E}\Big(f([t], q_t^\eta, p_t^\eta) \Big) - \overline{f}_\eta([t]) \right| \leqslant C_n \, \mathrm{e}^{-\lambda_n t} \, \|f\|_{L^\infty(L^\infty_{\mathcal{K}_n})},$$

with time-dependent spatial average $\overline{f}_\eta(\theta) = \int_{\mathcal{M}\times\mathbb{R}^d} f(\theta, q, p) \psi_\eta(\theta, q, p) \, dq \, dp$

- In addition, convergence of the trajectorial average for any (q_0, p_0)

$$\frac{1}{t} \int_0^t f([s], q_s^\eta, p_s^\eta) \, ds \xrightarrow[t \to +\infty]{} \int_{\mathcal{E}} f \, \psi_\eta \qquad \text{a.s.}$$

Properties of the limiting cycle

- Time dependent generator $\mathcal{A}_0 + \eta \mathcal{A}_1$, adjoints on $L^2(\mathcal{E})$

$$\mathcal{A}_0 = M^{-1}p\cdot\nabla_q - \nabla V\cdot\nabla_p + \gamma\left(-M^{-1}p\cdot\nabla_p + \frac{1}{\beta}\Delta_p\right), \quad \mathcal{A}_1 = F(\theta,q)\cdot\nabla_p$$

Fokker-Planck equation for ψ_η

The invariant distribution is smooth, positive and satisfies

$$\left(-\partial_t + \mathcal{A}_0^\dagger + \eta\mathcal{A}_1^\dagger\right)\psi_\eta = 0, \qquad \int_{\mathcal{E}} \psi_\eta = 1.$$

- Finite moments of order $2n$ uniformly in the time variable

$$\forall\theta \in T\mathbb{T}, \qquad \int_{\mathcal{M}\times\mathbb{R}^d} \mathcal{K}_n(q,p)\,\psi_\eta(\theta,q,p)\,dq\,dp \leqslant R_n < +\infty$$

- Uniform marginals in time $\overline{\psi_\eta}(\theta) = \displaystyle\int_{\mathcal{E}} \psi_\eta(\theta,q,p)\,dq\,dp = \frac{1}{T}$

Elements of proof

- Exponential convergence of the sampled chain[1] $(Q_n^\eta, P_n^\eta) = (q_{nT}^\eta, p_{nT}^\eta)$

$$\left(U_{T,\eta} f\right)(q,p) = \mathbb{E}\left(f(Q_{n+1}^\eta, P_{n+1}^\eta) \,\middle|\, (Q_n^\eta, P_n^\eta) = (q,p) \right).$$

Uniform Lyapunov condition

For any $n \geqslant 1$ and $\eta_* > 0$, there exist $b > 0$ and $a \in [0,1)$ such that

$$\forall \eta \in [-\eta_*, \eta_*], \qquad U_{T,\eta} \mathcal{K}_n \leqslant a \mathcal{K}_n + b.$$

Uniform minorization condition

Fix any $p_{\max} > 0$. There exists a probability measure ν on $\mathcal{M} \times \mathbb{R}^d$ and a constant $\kappa > 0$ such that, for all $\eta \in [-\eta_*, \eta_*]$,

$$\forall B \in \mathscr{B}(\mathcal{M} \times \mathbb{R}^d), \qquad \mathbb{P}\left((Q_{k+1}^\eta, P_{k+1}^\eta) \in B \,\middle|\, \left|P_k^\eta\right| \leqslant p_{\max} \right) \geqslant \kappa\, \nu(B).$$

- Patch invariant measures for sampled chains $(q_{\theta+nT}^\eta, p_{\theta+nT}^\eta)_{n \geqslant 0}$

[1] M. Hairer and J. Mattingly, *Progr. Probab.*, **63** (2011) 109–117

Perturbative expansion for small forcings

- Write $\psi_\eta(t,q,p) = \rho_\eta(t,q,p)\mu(q,p)$: adjoints on $\mathcal{H} = L^2(\mathcal{E},\mu) \cap \{\mathbf{1}\}^\perp$

$$(-\partial_t + \mathcal{A}_0^* + \eta \mathcal{A}_1^*)\rho_\eta = 0, \qquad \psi_\eta = \rho_\eta \mu, \qquad \int_{\mathscr{E}} \rho_\eta \mu = 1$$

- Use the invertibility of $\partial_t + \mathcal{A}_0$ on $\mathcal{H}$ (Fourier series in time) and the relative boundedness of $\mathcal{A}_1$ with respect to $\partial_t + \mathcal{A}_0$

Series expansion of the invariant measure

There exists $C, r > 0$ such that, for $|\eta| < r$,

$$\rho_\eta = 1 + \eta \varrho_1 + \eta^2 \varrho_2 + \dots$$

with $\displaystyle\int_{\mathcal{E}} |\varrho_m(t,q,p)|^2 \mu(q,p)\, dq\, dp\, dt \leqslant \frac{C}{r^m}$ and $\displaystyle\int_{\mathscr{E}} \varrho_m \, \mu \, dq\, dp\, dt = 0$

- Functions ϱ_m not explicitely known: solutions of Poisson equations
- The leading order correction ϱ_1 governs the linear response

Linear response of the velocity

General result on the mobility

- Linear response of the time dependent spatially averaged velocity

$$\mathscr{V}(t) = \lim_{\eta \to 0} \frac{\overline{v}_\eta(t)}{\eta}, \qquad \overline{v}_\eta(t) = \int_{\mathcal{M}} \int_{\mathbb{R}^d} M^{-1} p \, \psi_\eta(t,q,p) \, dq \, dp$$

- Fourier series in time: $e_n(t) = \mathrm{e}^{\mathrm{i}n\omega t}$ $(\omega = 2\pi/T)$

$$F(t,q) = F_0(q) + 2 \sum_{n \geqslant 1} \mathrm{Re}\Big(F_n(q) e_n(t) \Big)$$

Space-time decomposition of the mobility

$$\mathscr{V}(t) = \beta \sum_{n \in \mathbb{Z}} e_n(t) \int_{\mathcal{M}} D_n(q) F_n(q) \, \widetilde{\mu}(q) \, dq, \qquad \widetilde{\mu}(q) = \widetilde{Z}^{-1} \mathrm{e}^{-\beta V(q)}$$

with the position-dependent diffusion matrix

$$D_n(q) = \int_0^{+\infty} \mathbb{E}\Big(\left(M^{-1} p_s\right) \otimes \left(M^{-1} p_0\right) \,\Big|\, q_0 = q \Big) \mathrm{e}^{\mathrm{i}n\omega s} \, ds$$

- In particular, the average (time-independent) velocity depends only on F_0

Numerical illustration (1)

- Timestep $\Delta t > 0$ such that $I \Delta t = T$
- Approximation (q^n, p^n) of $(q_{n\Delta t}, p_{n\Delta t})$ (omit η for simplicity)

$$\begin{cases} p^{n+1/2} = \alpha_{\Delta t} p^n + \dfrac{\Delta t}{2}\Big(-\nabla V(q^n) + \eta F(t^n, q^n) \Big) + \sqrt{\dfrac{1-\alpha_{\Delta t}^2}{\beta}}\, G^n, \\ q^{n+1} = q^n + \Delta t\, M^{-1} p^{n+1/2}, \\ p^{n+1} = \alpha_{\Delta t} p^{n+1/2} + \dfrac{\Delta t}{2}\Big(-\nabla V(q^{n+1}) + \eta F(t^{n+1}, q^{n+1}) \Big) + \sqrt{\dfrac{1-\alpha_{\Delta t}^2}{\beta}}\, G^{n+1/2}, \end{cases}$$

with $\alpha_{\Delta t} = \mathrm{e}^{-\gamma \Delta t\, M^{-1}/2}$ (Strang splitting)

- Empirical averages $\overline{v}_\eta(i\Delta t) \simeq \dfrac{I}{N} \displaystyle\sum_{j=1}^{N/I} M^{-1} p^{i+jI}$ and $\overline{\mathscr{V}} \simeq \dfrac{1}{I\eta} \displaystyle\sum_{i=1}^{I} \overline{v}_\eta(i\Delta t)$
- Numerical analysis[2] of the bias with respect to Δt

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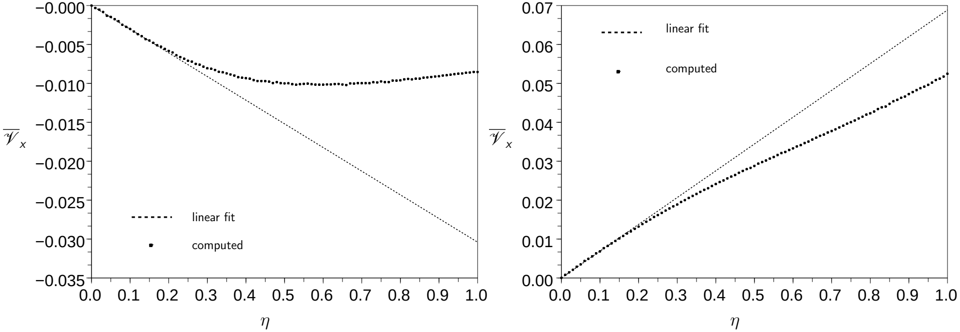
[2] B. Leimkuhler, Ch. Matthews, and G. Stoltz, *IMA J. Numer. Anal.* (2015)

Numerical illustration (2)

- 2-dimensional case $V(q) = 2\cos(2x) + \cos(y) + \cos(x - y)$
- Static, non-gradient forces $F_{0,n}(q) = \mathrm{e}^{\beta V(q)} \begin{pmatrix} \cos(nx) \\ 0 \end{pmatrix}$
- Parameters $\beta = \gamma = 1$, $M = \mathrm{Id}$, $\Delta t = 0.01$, 4.5×10^9 timesteps



$n = 1, \quad \overline{\mathscr{V}}_x = -3.04 \times 10^{-2}$ $\qquad$ $n = 2 \quad \overline{\mathscr{V}}_x = 6.88 \times 10^{-2}$

Negative mobility

- Decomposition of the real, $\mathcal{M}$-periodic and symmetric matrix

$$D_0(q) = \sum_{K \in \mathcal{L}^*} D_{0,K} \mathrm{e}^{-\mathrm{i}K\cdot q} = \sum_{K \in \mathcal{L}^*} a_{0,K} \cos(K\cdot q) + b_{0,K} \sin(K \cdot q),$$

- Related spatial decomposition of the external force

$$F_0(q) = \frac{1}{\widetilde{\mu}(q)|\mathcal{M}|} \left(\sum_{K \in \mathcal{L}^*} F_{0,K} \mathrm{e}^{-\mathrm{i}K\cdot q} \right), \qquad F_{0,K} = \overline{F_{0,-K}} \in \mathbb{C}^{d\times d}.$$

- Normalization such that $F_{0,0}$ = canonical equilibrium average of F_0

Spatial decomposition of the mobility

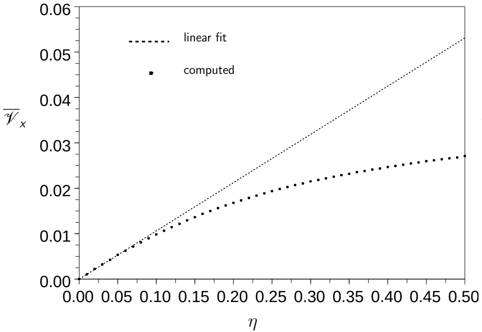
The space-time averaged linear response of the velocity reads

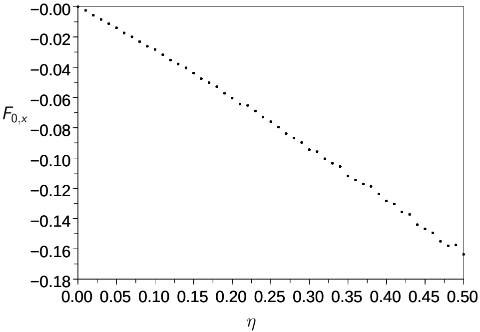
$$\overline{\mathscr{V}} = D_{0,0}F_{0,0} + \int_{\mathcal{M}} \Big(D_0(q) - D_{0,0}\Big)\Big(F_0(q)\widetilde{\mu}(q) - F_{0,0}\Big) dq$$

- Non-zero velocity produced either by constant forcing or as a result of some spatial resonance

Numerical illustration

- Time-independent force $F_0(q) = \mathrm{e}^{\beta V(q)} \begin{pmatrix} -1 + 3\cos(2x) \\ 0 \end{pmatrix}$





Left: Average observed velocity in the x direction.
Right: Average experienced force in the x direction.

Resonance of the frequency-dependent mobility

- Dependence on the period T of the forcing: fix $F_1(q)$ and consider

$$F(t,q) = 2\mathrm{Re}\left(F_1(q)\,\mathrm{e}^{\mathrm{i}\omega t}\right)$$

- Linear response result: $\mathscr{V}(t) = 2\beta\,\mathrm{Re}\left(\widehat{\mathscr{V}}(\omega)\,\mathrm{e}^{\mathrm{i}\omega t}\right)$ with

$$\widehat{\mathscr{V}}(\omega) = -2\beta \int_{\mathcal{M}} \int_{\mathbb{R}^d} \Big(\left[(\mathrm{i}\omega + \mathcal{A}_0)^{-1}\left(M^{-1}p\right)\right] \otimes \left(M^{-1}p\right) \Big) F_1\,\mu.$$

High-frequency decay of the linear response

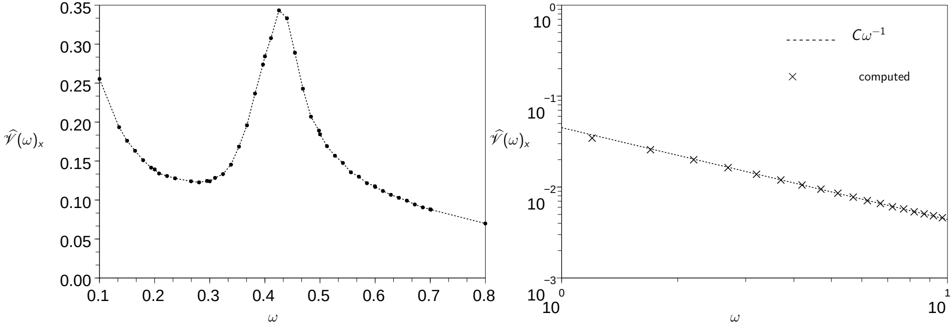
For any $n \geqslant 2$, there exists a constant $C_n > 0$ and $\nu_1, \dots, \nu_{n-1} \in \mathbb{C}^d$, such that, for all $\omega \geqslant 1$,

$$\left| \widehat{\mathscr{V}}(\omega) - \sum_{m=1}^{n-1} \frac{\nu_m}{\omega^m} \right| \leqslant \frac{C_n}{\omega^n}, \qquad \nu_1 = 2\mathrm{i}\beta M^{-1} \int_{\mathcal{M}} F_1(q)\,\widetilde{\mu}(q)\,dq$$

- Existence of a local/global maximum of $\left|\widehat{\mathscr{V}}(\omega)\right|$?

Numerical illustration

- Force $F(t,q) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cos(\omega t)$ and $\gamma = 0.1$



- Asymptotic behavior $\widehat{\mathscr{V}}(\omega)_x \sim \omega^{-1}$ since $\nu_1 \neq 0$

Longtime diffusive behavior

Convergence to an effective Brownian motion

- Diffusive rescaling on the dynamics not reprojected into $\mathcal{M}$
  - introduce $\mathscr{Q}_t^\eta = q_0^\eta + \int_0^t M^{-1} p_s^\eta \, ds$
  - remove average drift $\mathcal{V}_\eta = \int_{\mathcal{E}} M^{-1} p \, \psi_\eta(t,q,p) \, dt \, dq \, dp$
  - define $Q_t^\eta = \mathscr{Q}_t^\eta - t\mathcal{V}_\eta$ and rescale as $Q_t^{\eta,\varepsilon} = \varepsilon Q^\eta_{t/\varepsilon^2}$
- Stationary initial conditions $(q_0^\eta, p_0^\eta) \sim \psi_\eta(0,q,p) \, dq \, dp$

Weak convergence over finite time intervals

Limiting Brownian motion $d\overline{Q}_t = \sqrt{2}\, \mathscr{D}_\eta^{1/2} \, dB_t$ with $\overline{Q}_0 \sim \widetilde{\psi}_\eta(q) \, dq$ and symmetric, positive definite covariance matrix

$$\forall \xi \in \mathbb{R}^d, \qquad \xi^T \mathscr{D}_\eta \xi = \frac{\gamma}{\beta} \int_{\mathscr{E}} \left| \nabla_p \left(\xi^T \Phi_\eta \right) \right|^2 \psi_\eta.$$

- Covariance matrix determined by the solution of the Poisson equation

$$(\partial_t + \mathcal{A}_0 + \eta \mathcal{A}_1)\Phi_\eta(t,q,p) = M^{-1} p - \mathcal{V}_\eta, \qquad \int_{\mathscr{E}} \Phi_\eta \, \psi_\eta \, dt \, dq \, dp = 0.$$

Elements of proof

- Rewrite $\xi^T \left(Q_t^{\eta,\varepsilon} - Q_0^{\eta,\varepsilon} \right) = \varepsilon \int_0^{t/\varepsilon^2} \xi^T \left(M^{-1} p_s^\eta - \mathcal{V}_\eta \right) ds$ as

$$\varepsilon \xi^T \left(\Phi_\eta \left(\left[\frac{t}{\varepsilon^2} \right], \dots \right) - \Phi_\eta (0, \dots) \right) - \varepsilon \sqrt{\frac{2\gamma}{\beta}} \int_0^{t/\varepsilon^2} \nabla_p \left(\xi^T \Phi_\eta \right) ([\theta], q_\theta^\eta, p_\theta^\eta) \cdot dW_\theta$$

and use Martingale CLT (cv. finite dimensional laws) + thightness

Functional estimates (following Talay (2002) and Kopec (2013))

For a smooth function f with derivatives growing at most polynomially in p, the solution to the Poisson equation

$$(\partial_t + \mathcal{A}_0 + \eta \mathcal{A}_1) \Phi_\eta(t, q, p) = f(t, q, p) - \int_{\mathscr{E}} f \psi_\eta, \qquad \int_{\mathscr{E}} \Phi_\eta \, \psi_\eta = 0$$

is unique. For any $k \geqslant 1$ and $\eta_* > 0$, there exists a real constant $C > 0$ and integers $n, m, N \geqslant 1$ such that, for all $\eta \in [-\eta_*, \eta_*]$ and $|l| \leqslant k$,

$$\left| \partial^l \Phi_\eta(t, q, p) \right| \leqslant C \mathcal{K}_n(q, p) \sup_{|r| \leqslant N} \| \partial^r f \|_{L^\infty(L^\infty_{\mathcal{K}_m})}$$

Further properties of the covariance matrix

Perturbative expansion of the covariance matrix

$$\xi^T \mathscr{D}_\eta \xi = \xi^T \mathscr{D}_0 \xi + \eta \xi^T \mathcal{D}_1 \xi + \eta^2 \widetilde{\mathcal{D}}_{\eta,\xi}$$

with $\widetilde{\mathcal{D}}_{\eta,\xi}$ uniformly bounded for $|\xi| \leqslant 1$.

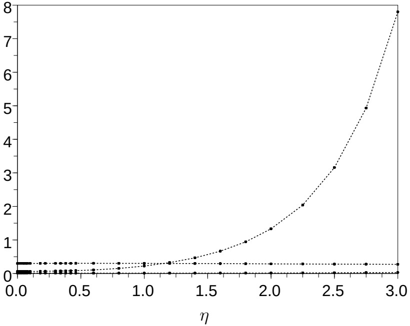
- Equilibrium covariance $\mathscr{D}_0 = \displaystyle\int_{\mathcal{M}} D_0(q)\, \widetilde{\mu}(q)\, dq$
- When the external force has time average 0 for all configurations

$$\forall q \in \mathcal{M}, \qquad \int_{T\mathbb{T}} F(t,q)\, dt = 0,$$

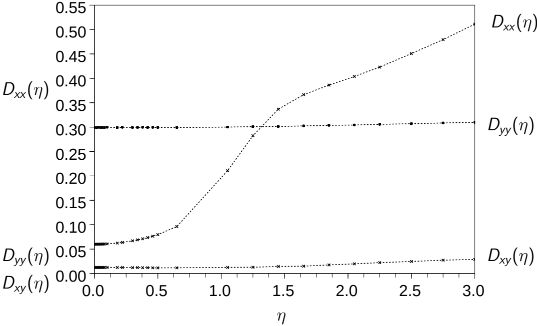
the first order correction vanishes: $\mathcal{D}_1 = 0$

Numerical illustration

- Simulations using $\mathscr{D}_\eta = \lim_{t\to\infty} \frac{\mathbb{E}\Big([\mathscr{Q}_t^\eta - \mathbb{E}(\mathscr{Q}_t^\eta)] \otimes [\mathscr{Q}_t^\eta - \mathbb{E}(\mathscr{Q}_t^\eta)] \Big)}{2t}$
- External forcing $F(t,q) = \mathrm{e}^{\beta V(q)} \begin{pmatrix} -1 + 3\cos(2x) \\ 0 \end{pmatrix} \cos(\omega t)$



$\omega = 0$



$\omega = 2\pi$

Conclusion and perspectives

Conclusion and perspectives

- Various resonance phenomena
  - "spatial" resonance leading to negative mobility
  - "frequency" resonance leading to enhanced synchronization
  - observed at the linear response level (already known in the nonlinear regime[3])

- Extension to thermal transport?

→ Some results for time-dependent drivings at the boundaries[4]

[3] Machura, Kostur, Talkner, Łuczka, Hänggi, *Phys. Rev. Lett.* (2007)

[4] A. Dhar, O. Narayan, A. Kundu, K. Saito, *Phys. Rev. E* (2011)