The generalized Langevin equation: long-time behavior and diffusive transport in a periodic potential

CECAM workshop on GLEs – Sorbonne Université

Urbain Vaes
urbain.vaes@inria.fr
CERMICS – École des Ponts ParisTech & MATHERIALS – Inria Paris

October 12, 2021

Grigorios Pavliotis
Imperial College London
Department of Mathematics

Gabriel Stoltz
École des Ponts ParisTech
Inria
CERMICS & Inria

G. A. Pavliotis, G. Stoltz, and U. Vaes (2021). "Scaling limits for the generalized Langevin equation". In: J. Nonlinear Sci.

Table of contents:

Introduction

Long-time behavior

Effective diffusion coefficient

The generalized Langevin equation in its general form

The generalized Langevin equation is in general an integro-differential equation:

$$\ddot{q}_t = -V'(q) - \int_0^t \widehat{\gamma}(t-s)\,\dot{q}_s\,\mathrm{d}s + F(t).$$

- Simple setting: one particle, one dimension, unit mass.
- V is a periodic potential;
- $(q_t)_{t \geqslant 0}$ is the position process;
- $\widehat{\gamma}(\cdot)$ is a memory kernel;
- F is a stationary Gaussian noise process.

The kernel $\widehat{\gamma}(\cdot)$ and the noise F are related through the fluctuation/dissipation relation:

$$\mathbf{E}\big(F(s)F(t)\big) = \beta^{-1}\,\widehat{\gamma}(t-s).$$

Quasi-Markovian approximation for exponential memory kernels

When the memory kernel is of the form

$$\widehat{\gamma}(t) = \left\langle \mathrm{e}^{-\mathbf{A}|t|}\,\boldsymbol{\lambda}, \boldsymbol{\lambda} \right\rangle,$$

for $\mathbf{A} \in \mathbf{R}^{n\times n}$ with positive eigenvalues and $\boldsymbol{\lambda} \in \mathbf{R}^n$, the GLE is equivalent to

$$\begin{aligned}
\mathrm{d}q &= p\,\mathrm{d}t, \\
\mathrm{d}p &= -V'(q)\,\mathrm{d}t + \langle \boldsymbol{\lambda}, \mathbf{z} \rangle\,\mathrm{d}t, \\
\mathrm{d}\mathbf{z} &= -p\,\boldsymbol{\lambda}\,\mathrm{d}t - \mathbf{A}\,\mathbf{z}\,\mathrm{d}t + \boldsymbol{\Sigma}\,\mathrm{d}\mathbf{W}_t, \qquad \mathbf{z}(0) \sim \mathcal{N}(0, \beta^{-1}\mathbf{I}),
\end{aligned}$$

where $\Sigma \in \mathbf{R}^{n\times n}$ is related to $\mathbf{A}$ by the fluctuation/dissipation relation:

$$\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T = \beta^{-1}\,(\mathbf{A} + \mathbf{A}^T).$$

The simplest example: Ornstein–Uhlenbeck noise

Throughout this presentation, we focus on the simple case where

$$\widehat{\gamma}(t) = \gamma \exp\left(-\frac{t}{\nu^2}\right).$$

In this case GLE is equivalent to

$$\begin{cases} \mathrm{d}q_t = p_t \,\mathrm{d}t, \\ \mathrm{d}p_t = -V'(q_t)\,\mathrm{d}t + \frac{\sqrt{\gamma}}{\nu}\, z_t \,\mathrm{d}t, \\ \mathrm{d}z_t = -\frac{\sqrt{\gamma}}{\nu}\, p_t \,\mathrm{d}t - \frac{1}{\nu^2}\, z_t \,\mathrm{d}t + \sqrt{\frac{2\beta^{-1}}{\nu^2}}\,\mathrm{d}W_t. \end{cases}$$

Relation to other dynamics:

- When $\nu \to 0$: convergence in law to the solution of the Langevin equation[1]:
$$\ddot{q} = -V'(q) - \gamma \dot{q} + \sqrt{2\gamma\beta^{-1}}\,\dot{W}.$$
- When $\gamma \to \infty$: convergence in law to the overdamped Langevin equation[2]:
$$\dot{q} = -V'(q) + \sqrt{2\beta^{-1}}\,\dot{W}.$$

[1] M. Ottobre and G. A. Pavliotis (2011). “Asymptotic analysis for the generalized Langevin equation”. In: Nonlinearity.

[2] Z. Schuss (2010). Theory and applications of stochastic processes. Applied Mathematical Sciences. An analytical approach. Springer, New York.

Invariant measure and the associated Markov semigroup

Unique invariant measure over $\mathbf{T} \times \mathbf{R} \times \mathbf{R}$ (Boltzmann-Gibbs):

$$\mu(\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}z) \propto \exp\left(-\beta\left(V(q) + \frac{p^2}{2} + \frac{z^2}{2}\right)\right)\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}z.$$

We denote by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ the norm and inner product of $L^2(\mu)$, and

$$L_0^2(\mu) = \left\{\varphi \in L^2(\mu) : \langle\varphi, 1\rangle = \mathbf{E}_\mu\varphi = 0\right\}.$$

Associated Markov semigroup:

The semigroup associated with the dynamics is given by

$$\mathrm{e}^{t\mathcal{L}}\varphi(q,p,z) = \mathbf{E}_{(q,p,z)}\big(\varphi(q_t,p_t,z_t)\big),$$

with generator

$$\mathcal{L} = p\,\partial_q - V'(q)\,\partial_p + \sqrt{\gamma}\,\nu^{-1}(z\,\partial_p - p\,\partial_z) - \nu^{-2}(z\,\partial_z - \beta^{-1}\partial_z^2)$$

This operator is not elliptic, only hypoelliptic.

Aim 1: obtain long-time convergence estimates for the semigroup

Ergodic theorem[3]: for an observable $\varphi \in L^1(\mu)$,

$$\widehat{\varphi}_t = \frac{1}{t}\int_0^t \varphi(q_s, p_s, z_s)\,\mathrm{d}s \xrightarrow[t\to\infty]{a.s.} \mathbf{E}_\mu \varphi.$$

Central limit theorem[4]: If the following Poisson equation has a solution $\phi \in L^2(\mu)$,

$$-\mathcal{L}\phi = \varphi - \mathbf{E}_\mu \varphi,$$

then a central limit theorem holds:

$$\sqrt{t}\big(\widehat{\varphi}_t - \mathbf{E}_\mu \varphi\big) \xrightarrow[t\to\infty]{\text{Law}} \mathcal{N}(0, \sigma_\varphi^2), \qquad \sigma_\varphi^2 = \langle \phi, \varphi - \mathbf{E}_\mu \varphi \rangle .$$

Link between resolvent and semigroup: On $L_0^2(\mu)$, it holds that

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

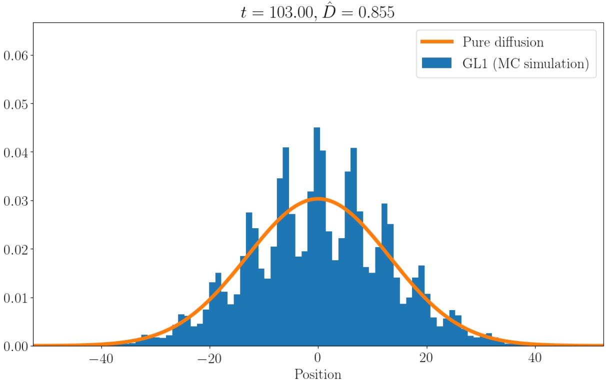
Aim 1: Understand the behaviour of $\mathrm{e}^{t\mathcal{L}}$ in different parameter regimes.

[3] W. Kliemann (1987). "Recurrence and invariant measures for degenerate diffusions". In: Ann. Probab.
[4] R. N. Bhattacharya (1982). "On the functional central limit theorem and the law of the iterated logarithm for Markov processes". In: Z. Wahrsch. Verw. Gebiete.

Aim 2: study the effective diffusion

In the particular case where $\varphi = p$, the CLT gives

$$\varepsilon\, x_{t/\varepsilon^2} \xrightarrow[\varepsilon \to 0]{} \mathcal{N}(0, 2D_{\gamma,\nu} t), \qquad x_t = \int_0^t p_s \,\mathrm{d}s.$$



Aim 2: Study the behaviour of $D_{\gamma,\nu}$ in asymptotic regimes of physical interest.

Indeed, applying Itô's formula to the solution ϕ of $-\mathcal{L}\phi = p$,

$$\mathrm{d}\phi(q_t, p_t, z_t) = -p_t \,\mathrm{d}t + \sqrt{2\beta^{-1}\nu^{-2}} \frac{\partial \phi}{\partial z}(q_t, p_t, z_t)\,\mathrm{d}W_t.$$

Therefore,

$$\varepsilon x_{t/\varepsilon^2} = \varepsilon \int_0^{t/\varepsilon^2} p_s \,\mathrm{d}s = -\underbrace{\varepsilon\left(\phi(q_{t/\varepsilon^2}, p_{t/\varepsilon^2}, z_{t/\varepsilon^2}) - \phi(q_0, p_0, z_0)\right)}_{\to 0 \text{ in } L^p(\Omega, C([0,T], \mathbf{R}))}$$
$$+ \underbrace{\sqrt{2\beta^{-1}\nu^{-2}}\varepsilon \int_0^{t/\varepsilon^2} \frac{\partial \phi}{\partial z}(q_s, p_s, z_s)\,\mathrm{d}W_s}_{\to \sqrt{2D_{\gamma,\nu}} W_t \text{ weakly in } C([0,\infty)) \text{ by MCLT}},$$

where

$$D_{\gamma,\nu} = \beta^{-1}\nu^{-2} \langle \partial_z \phi, \partial_z \phi \rangle = \beta^{-1}\nu^{-2} \langle \partial_z^* \partial_z \phi, \phi \rangle = -\langle \mathcal{L}\phi, \phi \rangle = \langle p, \phi \rangle.$$

Functional central limit theorem

$$\varepsilon x_{t/\varepsilon^2} \xrightarrow[\varepsilon \to 0]{} \sqrt{2D_{\gamma,\nu}}\, W_t \quad \text{weakly in } C([0,\infty)).$$

Outline

Introduction

Long-time behavior

Effective diffusion coefficient

The challenge: non-coercivity

The generator can be decomposed into symmetric and antisymmetric parts in $L^2(\mu)$:

$$\begin{aligned}\mathcal{L} &= \beta^{-1}\left(\partial_q\partial_p^* - \partial_q^*\partial_p\right) + \beta^{-1}\sqrt{\gamma}\nu^{-1}\left(\partial_p\partial_z^* - \partial_z^*\partial_p\right) - \beta^{-1}\nu^{-2}\partial_z^*\partial_z \\ &= B_1 + B_2 - A^*A.\end{aligned}$$

Therefore

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\|^2 = \left\langle \mathcal{L}\,\mathrm{e}^{t\mathcal{L}}\varphi, \mathrm{e}^{t\mathcal{L}}\varphi\right\rangle = -\left\|A\,\mathrm{e}^{t\mathcal{L}}\varphi\right\|^2$$

→ No instantaneous decay of the norm if $\varphi = \varphi(q,p)$;

⇒ There does not exist[5] $\lambda > 0$ such that

$$\left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\| \leqslant \mathrm{e}^{-\lambda t}\left\|\varphi\right\|.$$

Using a hypocoercivity approach, we will be able to show

$$\left\|\mathrm{e}^{t\mathcal{L}}\varphi\right\| \leqslant C\,\mathrm{e}^{-\lambda t}\left\|\varphi\right\|, \qquad C > 1.$$

[5] C. Villani (2009). "Hypocoercivity". In: Mem. Amer. Math. Soc.

Very brief review of some hypocoercivity techniques

- Lyapunov approaches give exponential convergence in weighted L^∞ spaces[6];
  - Difficult to be explicit in minorization condition.
- Standard $H^1(\mu)$ approach à la Villani[7];
  - Based on a modification of the inner product;
  - Can be combined with regularization to show $L^2(\mu)$ convergence.
- Direct $L^2(\mu)$ approach[8]:
  - More direct than "$H^1(\mu)$ + regularization" and usually quite flexible;
  - Seems difficult to apply in the case of the GLE.
- Entropic approach à la Villani gives convergence of the law in relative entropy;
  - Gives exponential convergence in a larger function space;
  - More restrictive assumptions than for $H^1(\mu)$ hypocoercivity.
- Schur complement approach[9]
  - Enables to prove resolvent estimates directly.

---

[6] J. C. Mattingly, A. M. Stuart, and D. J. Higham (2002). "Ergodicity for SDEs and approximations: locally Lipschitz vector fields and degenerate noise". In: Stochastic Process. Appl.

[7] C. Villani (2009). "Hypocoercivity". In: Mem. Amer. Math. Soc.

[8] J. Dolbeault, C. Mouhot, and C. Schmeiser (2009). "Hypocoercivity for kinetic equations with linear relaxation terms". In: C. R. Math. Acad. Sci. Paris.

[9] E. Bernard et al. (2020). "Hypocoercivity with Schur complements". In: arXiv preprint.

Hypocoercivity: a toy example

$$\dot{\mathbf{x}} = L\mathbf{x} := \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}\mathbf{x}, \qquad \mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix} \in \mathbf{R}^2.$$

Notice

$$\frac{\mathrm{d}}{\mathrm{d}t} |\mathbf{x}|^2 = -2y^2,$$

Defining $(\!(\mathbf{x},\mathbf{x})\!) = x^2 - 2\alpha xy + y^2$, with $0 < \alpha \ll 1$,

$$\frac{\mathrm{d}}{\mathrm{d}t} (\!(\mathbf{x},\mathbf{x})\!) = 2(\!(L\mathbf{x},\mathbf{x})\!) = -\mathbf{x}^T \begin{pmatrix} 2\alpha & -\alpha \\ -\alpha & 2-2\alpha \end{pmatrix}\mathbf{x} \leqslant -\xi |\mathbf{x}|^2 \leqslant -\widetilde{\xi}(\!(\mathbf{x},\mathbf{x})\!),$$

so $(\!(\mathbf{x}_t,\mathbf{x}_t)\!) \leqslant \mathrm{e}^{-\widetilde{\xi}t}(\!(\mathbf{x}_0,\mathbf{x}_0)\!)$.

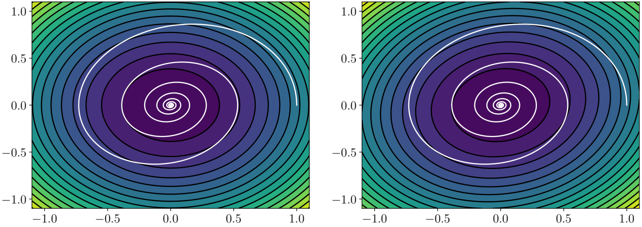


Figure: Level sets of $|\mathbf{x}|^2$ (left) and $(\!(\mathbf{x},\mathbf{x})\!)$ (right).

The $H^1(\mu)$ hypocoercivity approach for the GLE[10]

Define a modified inner product from the norm

$$(\!(h,h)\!) = \|h\|^2 + a_0\ \|\partial_z h\|^2 + a_1\ \|\partial_p h\|^2 + a_2\ \|\partial_q h\|^2 - 2b_0\langle \partial_z h, \partial_p h\rangle - 2b_1\langle \partial_p h, \partial_q h\rangle$$

- By the Cauchy–Schwarz inequality, we have

$$(\!(h,h)\!) \geqslant \|h\|^2 + \begin{pmatrix} \|\partial_z h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix}^T \underbrace{\begin{pmatrix} a_0 & -b_0 & 0 \\ -b_0 & a_1 & -b_1 \\ 0 & -b_1 & a_2 \end{pmatrix}}_{:=\mathbf{M}_1} \begin{pmatrix} \|\partial_z h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix},$$

- On the other hand, after some calculations,

$$-(\!(h,\mathcal{L}h)\!) \geqslant \begin{pmatrix} \|\partial_z \partial_z h\| \\ \|\partial_z \partial_p h\| \\ \|\partial_z \partial_q h\| \end{pmatrix}^T \left(\frac{\mathbf{M}_1}{\nu^2\beta}\right) \begin{pmatrix} \|\partial_z \partial_z h\| \\ \|\partial_z \partial_p h\| \\ \|\partial_z \partial_q h\| \end{pmatrix} + \begin{pmatrix} \|\partial_z h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix}^T \mathbf{M}_2 \begin{pmatrix} \|\partial_z h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix},$$

where $\mathbf{M}_2$ also depends on a_0, a_1, a_2, b_0, b_1.

$\rightarrow$ Simpler expression than in Villani's general hypocoercivity framework!

[10] M. Ottobre and G. A. Pavliotis (2011). "Asymptotic analysis for the generalized Langevin equation". In: Nonlinearity.

The $H^1(\mu)$ hypocoercivity approach for the GLE (continued)

Proposition

If $V'' \in L^\infty$, then there exists a choice of small parameters $a_0, a_1, a_2, b_0, b_1 \ll 1$ (dependent on ν and γ), and a constant $C > 0$ independent of γ and ν, such that

$$\forall \gamma, \nu > 0, \begin{cases} \mathbf{M}_2 \succcurlyeq C \min\left(\gamma, \dfrac{1}{\gamma}, \dfrac{\gamma}{\nu^4}\right) \mathbf{I}, \\ 0 \prec \mathbf{M}_1 \preccurlyeq \mathbf{I}. \end{cases}$$

Using this, we deduce the exponential convergence to equilibrium for $h \in H^1_0(\mu)$:

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}(\!(\mathrm{e}^{t\mathcal{L}} h, \mathrm{e}^{t\mathcal{L}} h)\!) \leqslant -C \min\left(\gamma, \frac{1}{\gamma}, \frac{\gamma}{\nu^4}\right) (\!(\mathrm{e}^{t\mathcal{L}} h, \mathrm{e}^{t\mathcal{L}} h)\!).$$

By Grönwall's lemma, this implies

$$(\!(\mathrm{e}^{\mathcal{L}t} h, \mathrm{e}^{\mathcal{L}t} h)\!) \leqslant \mathrm{e}^{-2\lambda(\nu,\gamma)t}(\!(h,h)\!), \qquad \lambda(\gamma,\nu) = C \min\left(\gamma, \frac{1}{\gamma}, \frac{\gamma}{\nu^4}\right).$$

Using the norm equivalence between $(\!(\cdot\,,\,\cdot)\!)$ and $\|\cdot\|_{H^1(\mu)}$, we have

$$\left\|\mathrm{e}^{\mathcal{L}t} h\right\|_{H^1(\mu)} \leqslant K(\gamma,\nu)\, \mathrm{e}^{-\lambda(\gamma,\nu)t} \|h\|_{H^1(\mu)}.$$

Obtaining a decay estimate in $L^2(\mu)$ by hypoelliptic regularization

Defining a Lyapunov functional[11]

$$N_h(t) = \|h\|^2 + a_0\, t\, \left\|\partial_z\, \mathrm{e}^{t\mathcal{L}}\, h\right\|^2 + a_1\, t^3\, \left\|\partial_p\, \mathrm{e}^{t\mathcal{L}}\, h\right\|^2 + a_2\, t^5\, \left\|\partial_q\, \mathrm{e}^{t\mathcal{L}}\, h\right\|^2 \\ - 2\, b_0\, t^2\, \left\langle \partial_z\, \mathrm{e}^{t\mathcal{L}}\, h, \partial_p\, \mathrm{e}^{t\mathcal{L}}\, h\right\rangle - 2\, b_1\, t^4\, \left\langle \partial_p\, \mathrm{e}^{t\mathcal{L}}\, h, \partial_q\, \mathrm{e}^{t\mathcal{L}}\, h\right\rangle,$$

where a_1, a_2, a_3, b_1, b_2 are the same parameters as before, we can show

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(N_h(t)\big) \leqslant 0 \qquad 0 \leqslant t \leqslant 1 \qquad \Rightarrow ((\mathrm{e}^{\mathcal{L}}\, h, \mathrm{e}^{\mathcal{L}}\, h)) \leqslant \|h\|^2.$$

From this we deduce, for $t \geqslant 1$,

$$\|\,\mathrm{e}^{\mathcal{L}t}\, h\| = \|\,\mathrm{e}^{\mathcal{L}(t-1)}\, \mathrm{e}^{\mathcal{L}}\, h\| \leqslant C\, \mathrm{e}^{-\bar{\lambda}\min\left(\gamma, \gamma^{-1}, \gamma\nu^{-4}\right)t}\, \|h\|.$$

Remark

$L^2(\mu)$ decay can also be obtained using a recent approach[12] based on introducing $Q_t = \mathrm{e}^{\mathcal{L}^* t}\, \mathrm{e}^{\mathcal{L}t}$ and using an inequality for self-adjoint operators[13].

---

[11] F. Hérau (2007). "Short and long time behavior of the Fokker-Planck equation in a confining potential and applications". In: J. Funct. Anal.

[12] G. Deligiannidis et al. (2018). "Randomized Hamiltonian Monte Carlo as Scaling Limit of the Bouncy Particle Sampler and Dimension-Free Convergence Rates". In: arXiv e-prints.

[13] M. Hairer, A. M. Stuart, and S. J. Vollmer (2014). "Spectral gaps for a Metropolis-Hastings algorithm in infinite dimensions". In: Ann. Appl. Probab.

The obtained decay rates are sharp

In the case where V is a quadratic potential, the quasi-Markovian GLE is a multidimensional Ornstein–Uhlenbeck process.

$\rightarrow$ the spectrum of the associated generator can be obtained explicitly in terms of the eigenvalues of the drift matrix $\mathbf{D}$[14]:

$$\sigma(\mathcal{L}) = \left\{ -\sum_{\mu \in \sigma(\mathbf{D})} \mu\, k_\mu, \quad k_\mu \in \mathbf{N} \right\}.$$

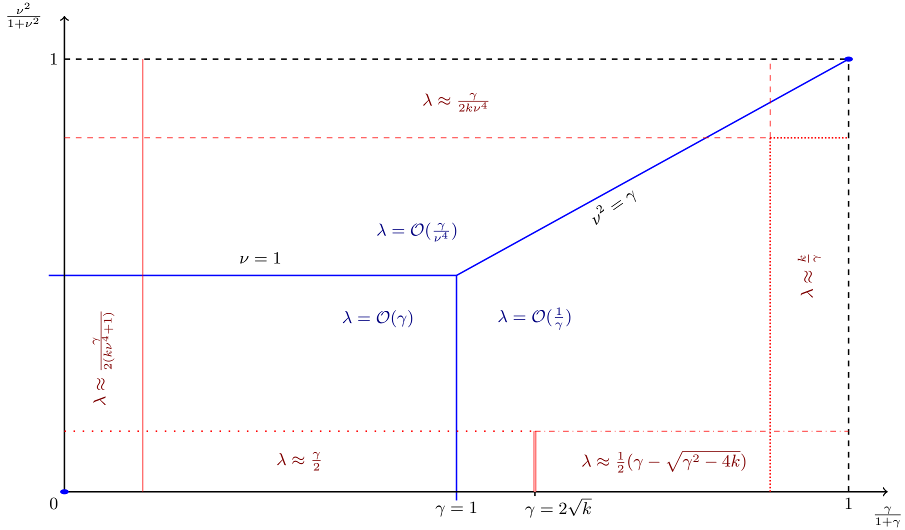
The characteristic polynomial of the drift matrix is

$$p(\lambda) = \lambda^3 + \frac{\lambda^2}{\nu^2} + \frac{\lambda\gamma}{\nu^2} + \lambda + \frac{1}{\nu^2}.$$

By asymptotic analysis, we can rigorously obtain the scaling w.r.t. γ and ν of the root with largest real part, and the obtained scalings match our general findings.

[14] G. Metafune, D. Pallara, and E. Priola (2002). "Spectrum of Ornstein-Uhlenbeck operators in L^p spaces with respect to invariant measures". In: J. Funct. Anal.

The rates in red correspond to $V(q) = k\frac{q^2}{2}$.



Outline

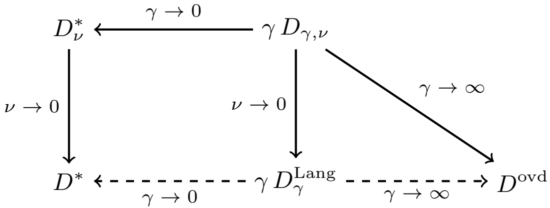
Introduction

Long-time behavior

Effective diffusion coefficient

- The underdamped limit: $\gamma \to 0$;
- The overdamped limit: $\gamma \to \infty$;
- The short memory limit: $\nu \to 0$.

Summary of our results:



The limits are found by formal asymptotics, and are then made rigorous by employing our explicit $L^2_0(\mu)$ resolvent estimate:

$$\left\| \mathcal{L}^{-1} \right\|_{L^2_0(\mu)} \leqslant \int_0^\infty \left\| \, \mathrm{e}^{t\mathcal{L}} \, \right\|_{L^2_0(\mu)} \mathrm{d}t \leqslant C \max\left(\gamma, \gamma^{-1}, \gamma^{-1}\nu^4\right).$$

Example: the short memory limit $\nu \to 0$

Recipe for finding and proving scalings of the effective diffusion coefficient:

- Decompose the generator according to the small parameter, here ν:

$$\mathcal{L} = \beta^{-1}\left(\partial_q \partial_p^* - \partial_q^* \partial_p\right) + \beta^{-1}\sqrt{\gamma}\nu^{-1}\left(\partial_p \partial_z^* - \partial_z^* \partial_p\right) - \beta^{-1}\nu^{-2}\partial_z^* \partial_z$$
$$=: \mathcal{L}_2 + \frac{1}{\nu}\mathcal{L}_1 + \frac{1}{\nu^2}\mathcal{L}_0.$$

- Expand the solution to the Poisson equation $-\mathcal{L}\phi_\nu = p$ as $\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \cdots$:

$$\begin{aligned}
\mathcal{O}(1/\nu^2) \qquad & \mathcal{L}_0\phi_0 = 0, \\
\mathcal{O}(1/\nu^1) \qquad & \mathcal{L}_0\phi_1 + \mathcal{L}_1\phi_0 = 0, \\
\mathcal{O}(1) \qquad & \mathcal{L}_0\phi_2 + \mathcal{L}_1\phi_1 + \mathcal{L}_2\phi_0 = -p, \\
\mathcal{O}(\nu) \qquad & \mathcal{L}_0\phi_{i+2} + \mathcal{L}_1\phi_{i+1} + \mathcal{L}_2\phi_i = 0, \qquad i = 1, 2, \ldots
\end{aligned}$$

- These equations can be solved successively, applying solvability solutions[15],

$$-\mathcal{L}^{\mathrm{Lang}}\phi_0 = p, \qquad \phi_1 = \ldots, \qquad \phi_2 = \ldots$$

[15] G. A. Pavliotis and A. M. Stuart (2008). Multiscale methods. Texts in Applied Mathematics. Averaging and homogenization. Springer, New York.

- By construction, it holds that

$$-\mathcal{L}\big(\phi_\nu - (\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \nu^3\phi_3)\big) = \nu^2 \text{rhs}$$

We now use a result from[16] to show that $\text{rhs} \in L^2_0(\mu)$: if $f(q,p) \in L^2_0(\mu)$ is a smooth function that grows, together with all its derivatives, at most polynomially as $|p| \to \infty$, then so is the solution in $L^2_0(\mu)$ of

$$-\mathcal{L}^{\text{Lang}}\phi_L = f(q,p).$$

- Apply the resolvent estimate found earlier (here uniform in ν) and take the limit $\nu \to 0$ to conclude that

$$\begin{aligned} \|\phi_\nu - (\phi_0 + \nu\phi_1 + \nu^2\phi_2 + \nu^3\phi_3)\| &= \mathcal{O}_{\nu\to 0}(\nu^2) \\ \Rightarrow \|\phi_\nu - \phi_0 - \nu\phi_1\| &= \mathcal{O}_{\nu\to 0}(\nu^2) \qquad \text{for fixed } \gamma. \end{aligned}$$

- Substitute in the expression $D^{\text{GLE}}_{\gamma,\nu} = \langle \phi_\nu, p\rangle$ of the effective diffusion to conclude

$$|D^{\text{GLE}}_{\gamma,\nu} - D^{\text{Lang}}_{\gamma}| = \mathcal{O}_{\nu\to 0}(\nu^2), \qquad \text{because } D^{\text{Lang}}_{\gamma} = \langle \phi_0 + \nu\phi_1, p\rangle.$$

[16] Marie Kopec (2015). "Weak backward error analysis for Langevin process". In: BIT Numer. Math.

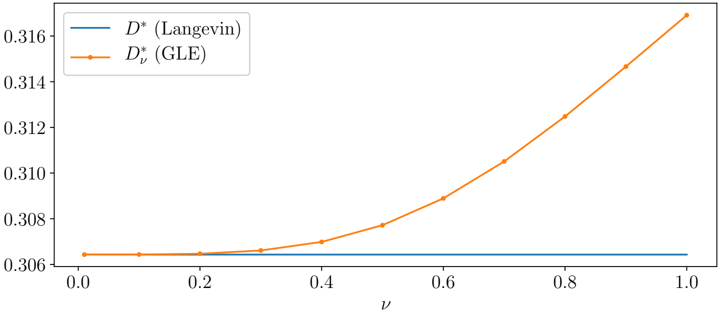
This approach not work for the underdamped limit...

...but a formal analysis enables to show that

$$\lim_{\gamma \to 0} \gamma D_{\nu,\gamma} \to D^*_\nu,$$

$$\lim_{\nu \to 0} D^*_\nu \to D^*,$$

In general $D^*_\nu \neq D^*$ for $\nu > 0$.



Numerical approaches for calculating of the effective diffusion coefficient

- Einstein's relation:

$$D_{\gamma,\nu} = \lim_{t\to\infty} \frac{1}{2t}\mathbf{E}\left|q(t) - q(0)\right|^2.$$

- Green–Kubo formula: Since $-\mathcal{L}^{-1} = \int_0^\infty \mathrm{e}^{t\mathcal{L}}\,\mathrm{d}t$,

$$D_{\gamma,\nu} = \int (-\mathcal{L}^{-1}p)\,p\,\mathrm{d}\mu = \int_0^\infty\int (\mathrm{e}^{t\mathcal{L}}\,p)p\,\mathrm{d}\mu\,\mathrm{d}t = \int_0^\infty \mathbf{E}_\mu(p_0 p_t)\,\mathrm{d}t.$$

- Linear response approach:

$$D_{\gamma,\nu} = \lim_{\eta\to 0}\frac{1}{\eta}\mathbf{E}_{\mu_\eta}\,p.$$

where μ_η is the invariant distribution of

$$\mathrm{d}q = p\,\mathrm{d}t,$$
$$\mathrm{d}p = \eta\,\mathrm{d}t - V'(q)\mathrm{d}t - \gamma p + \sqrt{2\gamma\beta^{-1}}\,\mathrm{d}W(t),$$

- Fourier/Hermite Galerkin method for the Poisson equation.

Fourier/Hermite Galerkin method

We employ a Fourier/Hermite spectral method for the Poisson equation, with the saddle-point formulation[17]:

$$\begin{aligned} &-\Pi_N \,\mathcal{L}\, \Pi_N \Phi_N + \alpha_N u_N = \Pi_N p, \\ &\langle \Phi_N, u_N \rangle = 0, \end{aligned} \tag{2}$$

where

- Π_N is the $L^2(\mu)$ projection operator on a finite-dimensional subspace V_N,
- $u_N = \Pi_N 1 / \|\Pi_N 1\|$. Eq. (2) ensures that the system is well-conditioned.

For V_N, we use the following basis functions:

$$e_{i,j,k} = \left(Z \, \mathrm{e}^{\beta\left(H(q,p) + |z|^2\right)} \right)^{\frac{1}{2}} G_i(q)\, H_j(p)\, H_k(z), \qquad 0 \leqslant i, j, k \leqslant N,$$

where $(G_i)_{i \geqslant 0}$ are trigonometric functions and $(H_j)_{i \geqslant 0}$ are Hermite polynomials.

[17] J. Roussel and G. Stoltz (2018). "Spectral methods for Langevin dynamics and associated error estimates". In: ESAIM: Math. Model. Numer. Anal.

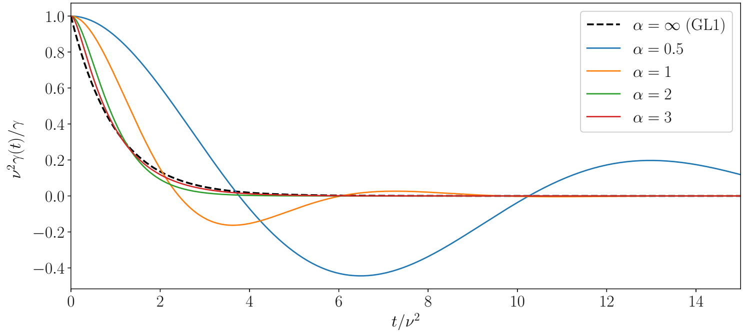
A slightly more general GLE

In numerical experiments, we consider the GLE with the following paramaters:

$$\boldsymbol{\lambda} = \frac{1}{\nu}\begin{pmatrix}\sqrt{\gamma}\\ 0\end{pmatrix}, \quad \mathbf{A} = \frac{1}{\nu^2}\begin{pmatrix}0 & -\alpha\\ \alpha & \alpha^2\end{pmatrix} \to \quad \boldsymbol{\Sigma} = \sqrt{\frac{2\,\beta^{-1}\,\alpha^2}{\nu^2}}\begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}.$$

In particular, we recover model GL1 as $\alpha \to \infty$ (the overdamped limit of the noise).

- ν^2 is horizontal scaling;
- γ is a vertical scaling;
- α encodes the shape;



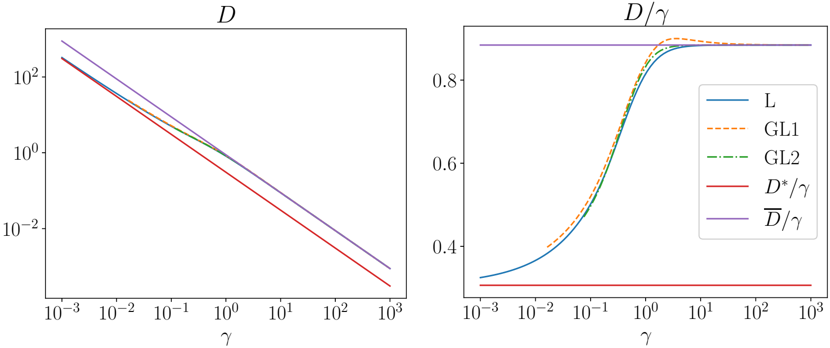


Figure: Diffusion coefficient as a function of γ, when $\nu = \alpha = 1$.

Dependence of D on ν and α

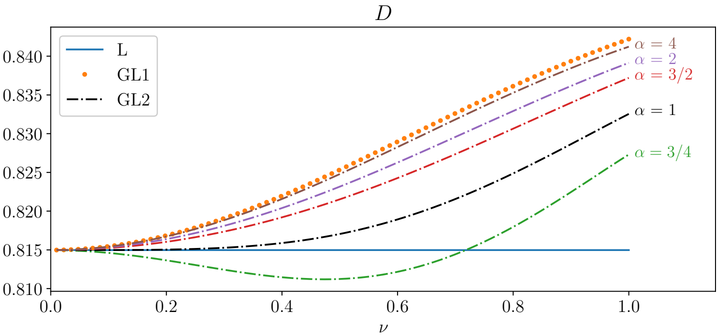


Figure: Effective diffusion coefficient against ν, for fixed values $\beta = \gamma = 1$.

Perspectives for future work

- Numerical study of the underdamped limit with variance reduction methods.
- Generalization to other systems? Higher-dimensional GLEs, atom chains, ...
- Direct $L^2(\mu)$ or Schur complement approach?
- Study of the spectral method, e.g. discrete hypocoercivity, convergence?

Thank you for your attention!