Séminaire de Mathématiques Appliquées du CERMICS

École des Ponts
ParisTech

The generalized Langevin equation in a periodic potential

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20 juin 2019

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June 21, 2019

Outline

Why use molecular simulation?

Statistical physics provides a bridge between the macroscopic and microscopic properties of matter.

Using molecular simulation, we can calculate macroscopic quantities of interest:

- Static, thermodynamic properties, such as heat capacities;
- Dynamical properties, such as transport coefficients and Arrhenius constants for chemical kinetics.

In this talk, we are interested in the diffusion coefficient, also know as the mobility, associated with the microscopic description of matter provided by the Generalized Langevin equation.

Models

We consider the following hierarchy of models:

$$\dot{q} = - V'(q) + \sqrt{2\,\beta^{-1}}\,\dot{W}, \tag{OL}$$

$$\ddot{q} = - V'(q) - \gamma\,\dot{q} + \sqrt{2\,\gamma\,\beta^{-1}}\,\dot{W}, \tag{L}$$

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

where

- V is the periodic potential $\frac{1}{2}(1-\cos(q))$;
- γ is the friction coefficient;
- $\gamma(\cdot)$ is the memory kernel;
- F is a non-Markovian noise process.

The kernel $\gamma(\cdot)$ and the noise F are related by the fluctuation/dissipation relation:

$$\langle F(t)F(s)\rangle = \beta^{-1}\,\gamma(t-s).$$

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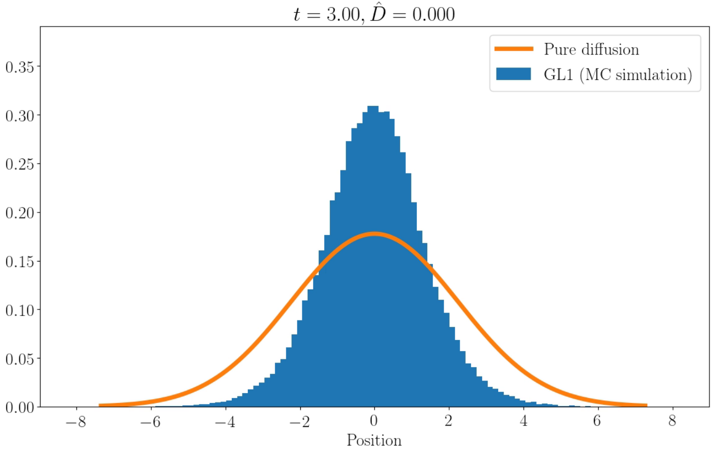
Effective diffusion

For all these models, it is possible to show that a functional central limit theorem holds:

$$x(t/\varepsilon^2) := \varepsilon\, q(t/\varepsilon^2) \to \sqrt{2\,D}\, W(t),$$

in the sense of weak convergence of probability measures.



Some background material on the Langevin equation

The (one-particle) Langevin equation can be rewritten as:

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

The position and momentum $\{p_t, q_t\}$ define a Markov process with generator

$$\mathcal{L}_L = \left(p \frac{\partial}{\partial q} - V'(q) \frac{\partial}{\partial p} \right) + \gamma \left(-p \frac{\partial}{\partial p} + \beta^{-1} \frac{\partial^2}{\partial p^2} \right) =: \mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}.$$

The formal L^2 adjoint of $\mathcal{L}_L$ is the Fokker–Planck operator

$$\mathcal{L}_L^{\dagger} = \left(-p \frac{\partial}{\partial q} + V'(q) \frac{\partial}{\partial p} \right) + \gamma \left(\frac{\partial}{\partial p}(p\,\cdot) + \beta^{-1} \frac{\partial^2}{\partial p^2} \right) =: -\mathcal{L}_{\mathrm{ham}} + \gamma \mathcal{L}_{\mathrm{FD}}^{\dagger}.$$

- $\mathcal{L}_{\mathrm{ham}}$ is the Liouville operator corresponding to the Hamiltonian dynamics

$$\begin{cases} \mathrm{d}q_t = \dfrac{\partial H}{\partial p}(q_t, p_t)\,\mathrm{d}t, \\ \mathrm{d}p_t = -\dfrac{\partial H}{\partial q}(q_t, p_t)\,\mathrm{d}t. \end{cases} \qquad H(q,p) = V(q) + \frac{p^2}{2}.$$

  Its null space consists of function of the type $f = f(H(q,p))$:

$$\mathcal{L}_{\mathrm{ham}} f(H(q,p)) = \frac{\partial H}{\partial p}\frac{\partial H}{\partial q} f' - \frac{\partial H}{\partial q}\frac{\partial H}{\partial p} f' = 0.$$

- The null space of $\mathcal{L}_{\mathrm{FD}}^{\dagger}$ consists of functions of the type $f = f(q)\,\mathrm{e}^{-\beta\,\frac{p^2}{2}}$.

It follows that $\ker(\mathcal{L}_L^{\dagger})$ is spanned by the canonical measure

$$\mu(q,p) = \frac{1}{\mathcal{Z}}\,\mathrm{e}^{-\beta H(q,p)} = \frac{1}{\mathcal{Z}}\,\mathrm{e}^{-\beta\left(V(q) + \frac{p^2}{2}\right)}, \quad \text{on } \mathbf{T} \times \mathbf{R}.$$

The Langevin equation: long-time behavior

In $L^2(\mu)$,

- The fluctuation/dissipation part is symmetric:

$$\langle \mathcal{L}_{\mathrm{FD}} u, v \rangle_{L^2(\mu)} = \langle u, \mathcal{L}_{\mathrm{FD}} v \rangle_{L^2(\mu)} = -\beta^{-1} \langle u', v' \rangle_{L^2(\mu)}.$$

  and in fact $\mathcal{L}_{\mathrm{FD}} = -\frac{1}{\beta} \partial_p^* \partial_p$.

- The Hamiltonian part is antisymmetric:

$$\langle \mathcal{L}_{\mathrm{ham}} u, v \rangle_{L^2(\mu)} = -\langle u, \mathcal{L}_{\mathrm{ham}} v \rangle_{L^2(\mu)}.$$

  and in fact $\mathcal{L}_{\mathrm{ham}} = \frac{1}{\beta} \left(\partial_p^* \partial_q - \partial_q^* \partial_p \right)$.

Therefore, if $u(t) = \mathrm{e}^{\mathcal{L}_L t} u_0$ for $u_0 \in L^2(\mu)$, then

$$\frac{1}{2} \frac{\partial}{\partial t} \|u\|_{L^2(\mu)}^2 = \langle \mathcal{L}_L u, u \rangle = -\gamma \, \beta^{-1} \, \|\partial_p u\|_{L^2(\mu)}^2.$$

Since the right-hand side is zero when $u = u(q)$, $\mathcal{L}_L$ is not coercive.

The Langevin equation: long-time behavior

Let us define:

$$L_0^2(\mu) = \left\{ u \in L^2(\mu) : \int u \, \mathrm{d}\mu = 0 \right\}, \qquad H_0^1(\mu) = H^1(\mu) \cap L_0^2.$$

It is possible to construct inner products $(\!(\cdot, \cdot)\!)_{L^2(\mu)}$ and $(\!(\cdot, \cdot)\!)_{H^1(\mu)}$ such that:

- $(\!(\cdot, \cdot)\!)_{L^2(\mu)}$ induces a norm equivalent to $\| \cdot \|_{L^2(\mu)}$ and

$$(\!(\mathcal{L}_L u, u)\!)_{L^2(\mu)} \leq -\lambda \, (\!(u, u)\!)_{L^2(\mu)} \qquad \forall u \in L_0^2(\mu).$$

- $(\!(\cdot, \cdot)\!)_{H^1(\mu)}$ induces a norm equivalent to $\| \cdot \|_{H^1(\mu)}$ and

$$(\!(\mathcal{L}_L u, u)\!)_{H^1(\mu)} \leq -\lambda \, (\!(u, u)\!)_{H^1(\mu)} \qquad \forall u \in H_0^1(\mu).$$

For all $u_0 \in X_0$, $u = \mathrm{e}^{\mathcal{L}_L t} u_0$ satisfies

$$\begin{aligned}
&\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} (\!(u, u)\!)_X = (\!(\mathcal{L}_L u, u)\!)_X \leq -\lambda (\!(u, u)\!)_X, \\
&\Rightarrow (\!(u(\cdot, t), u(\cdot, t))\!) \leq \mathrm{e}^{-2\lambda t} (\!(u(\cdot, 0), u(\cdot, 0))\!) \\
&\Rightarrow \|u(\cdot, t)\|_X \leq C \, \mathrm{e}^{-\lambda t} \, \|u(\cdot, 0)\|_X
\end{aligned}$$

$-\mathcal{L}_L$ is said to be hypocoercive on $L_0^2(\mu)$ and $H_0^1(\mu)$.

The Langevin equation: effective diffusion

After

- introducing the non-periodized position x;
- applying the diffusive rescaling $x \mapsto x/\varepsilon$, $t \mapsto t/\varepsilon^2$;

the Langevin equation can be recast as a fast/slow system of SDEs:

$$\begin{aligned} \mathrm{d}x_t^\varepsilon &= \frac{1}{\varepsilon}\, p_t^\varepsilon \,\mathrm{d}t, \quad x_t^\varepsilon \in \mathbf{R}, \\ \mathrm{d}q_t^\varepsilon &= \frac{1}{\varepsilon^2}\, p_t^\varepsilon \,\mathrm{d}t, \quad q_t^\varepsilon \in \mathbf{T}, \\ \mathrm{d}p_t^\varepsilon &= \frac{1}{\varepsilon^2}\left(-V'(q_t^\varepsilon)\,\mathrm{d}t - \gamma p_t^\varepsilon \,\mathrm{d}t\right) + \frac{1}{\varepsilon}\sqrt{2\gamma\beta^{-1}}\,\mathrm{d}W_t. \end{aligned}$$

To relate D to $\mathcal{L}_L$, we consider the backward Kolmogorov equation associated with the rescaled dynamics:

$$\frac{\partial u}{\partial t} = \mathcal{L}_L^\varepsilon u, \qquad u(x,q,p,t=0) = U_0,$$

where

$$\mathcal{L}_L^\varepsilon = \frac{1}{\varepsilon^2}\mathcal{L}_L + \frac{1}{\varepsilon}\left(p\frac{\partial}{\partial x}\right)$$

The Langevin equation: effective diffusion

Expanding the solution in powers of ε,

$$u = u_0 + \varepsilon\, u_1 + \varepsilon^2\, u_2 + \cdots\,,$$

and grouping the terms multiplying equal powers of ε,

$$\begin{aligned}
\mathcal{O}(\varepsilon^{-2}) &\quad \mathcal{L}_L u_0 = 0,\\
\mathcal{O}(\varepsilon^{-1}) &\quad \mathcal{L}_L u_1 + (p\,\partial_x u_0) = 0,\\
\mathcal{O}(\varepsilon^{0}) &\quad \mathcal{L}_L u_2 + (p\,\partial_x u_1) - \partial_t u_0 = 0,\\
&\quad \vdots
\end{aligned}$$

The equation $-\mathcal{L}_L u = f$ admits a solution if and only if f is orthogonal to $\ker(\mathcal{L}_L^\dagger)$:

$$\int f\,\mathrm{d}\mu = 0. \qquad \text{(Centering condition)}$$

The first and second equations give $u_0 = u_0(x)$ and

$$u_1(x,q,p) = (-\mathcal{L}_L^{-1} p)\, u_0'(x)$$

The Langevin equation: effective diffusion

The centering condition, applied to the third equation, gives:

$$
\begin{aligned}
0 &= \int (p\,\partial_x u_1 - \partial_t u_0)\,\mu(\mathrm{d}q\,\mathrm{d}p) \\
&= \int \big(p\,(-\mathcal{L}_L^{-1} p)\,u_0''(x) - \partial_t u_0(x)\big)\,\mu(\mathrm{d}q\,\mathrm{d}p) \\
&= \left(\int (-\mathcal{L}_L^{-1} p)\,p\,\mu(\mathrm{d}q\,\mathrm{d}p)\right) u_0''(x) - \partial_t u_0(x).
\end{aligned}
$$

This suggests that $x^\varepsilon(t)$ converges to a Brownian motion multiplied by $\sqrt{2D}$, where

$$
\begin{aligned}
D &= \int (-\mathcal{L}_L^{-1} p)\,p\,\mu(\mathrm{d}q\,\mathrm{d}p), \\
&= \int -\phi\,\mathcal{L}_L \phi\,\mu(\mathrm{d}q\,\mathrm{d}p) \qquad \text{where } \phi := -\mathcal{L}_L^{-1} p, \\
&= \gamma\beta^{-1} \int |\partial_p \phi|^2\;\mu(\mathrm{d}q\,\mathrm{d}p).
\end{aligned}
$$

The Langevin equation: effective diffusion

To show this rigorously, apply Itô's formula to $\phi := -\mathcal{L}_L^{-1} p$:

$$\begin{aligned}
\mathrm{d}\phi(q_t^\varepsilon, p_t^\varepsilon) &= \frac{1}{\varepsilon^2} \mathcal{L}_L \phi(q_t^\varepsilon, p_t^\varepsilon) + \cancel{\frac{1}{\varepsilon} p \frac{\partial \phi}{\partial x}} + \frac{1}{\varepsilon} \sqrt{2\gamma\beta^{-1}} \frac{\partial \phi}{\partial p}(q_t^\varepsilon, p_t^\varepsilon)\, \mathrm{d}W_t, \\
&= \frac{1}{\varepsilon^2} p_t^\varepsilon + \frac{1}{\varepsilon} \sqrt{2\gamma\beta^{-1}} \frac{\partial \phi}{\partial p}(q_t^\varepsilon, p_t^\varepsilon)\, \mathrm{d}W_t.
\end{aligned}$$

Therefore,

$$x_t^\varepsilon = \frac{1}{\varepsilon} \int_0^t p_s^\varepsilon \, \mathrm{d}s = \underbrace{\varepsilon(\phi(q_t^\varepsilon, p_t^\varepsilon) - \phi_(q_0, p_0))}_{\to 0 \text{ in } L^p(\Omega, C([0,T], \mathbf{R}))} + \sqrt{2\gamma\beta^{-1}} \int_0^t \frac{\partial \phi}{\partial p}(q_s^\varepsilon, p_s^\varepsilon)\, \mathrm{d}W_s.$$

The martingale term has quadratic variation

$$\begin{aligned}
\langle M \rangle_t &= 2\,\gamma\,\beta^{-1} \int_0^t \left|\partial_p \phi(q_s^\varepsilon, p_s^\varepsilon)\right|^2 \, \mathrm{d}s \\
&= 2\,\varepsilon^2\,\gamma\,\beta^{-1} \int_0^{t/\varepsilon^2} \left|\partial_p \phi(q_s, p_s)\right|^2 \, \mathrm{d}s \quad \underset{\varepsilon \to 0}{\to} \quad 2\gamma\beta^{-1}\, t \int \left|\partial_p \phi(q,p)\right|^2 \, \mu(\mathrm{d}q\,\mathrm{d}p),
\end{aligned}$$

after which the central limit theorem for martingales gives the conclusion.

The Langevin equation: underdamped limit

Parameters: $\gamma = 0.01$, $\beta = 1$.

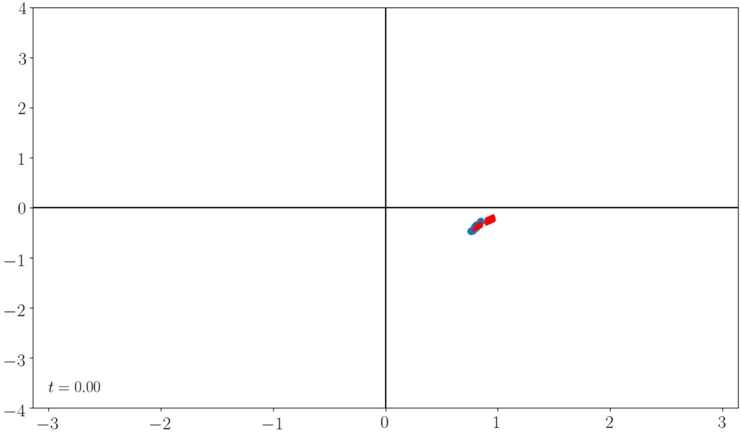


Figure: GL1 dynamics in the $q - p$ plane.

The Langevin equation: overdamped limit

Parameters: $\gamma = 100$, $\varepsilon = 1$, $\beta = 1$.

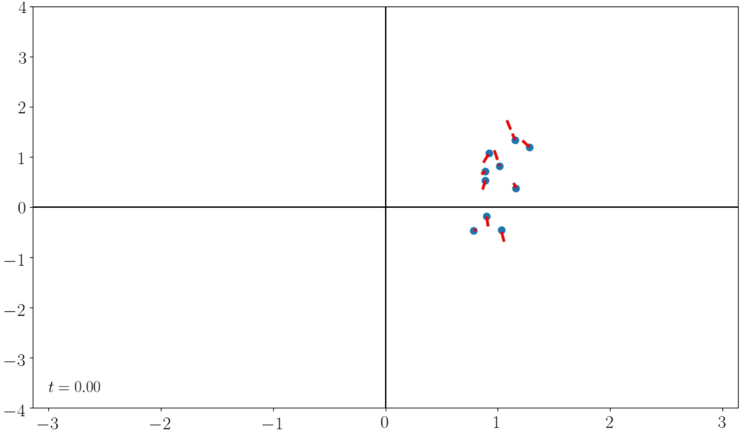


Figure: GL1 dynamics in the $q - p$ plane.

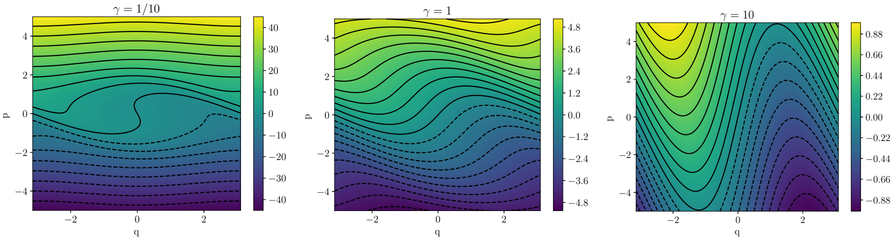
The $\gamma \to \infty$ (overdamped) and $\gamma \to 0$ (underdamped) limits are well understood for the Langevin equation.

$$\lim_{\gamma \to 0} \gamma D_\gamma =: D^*,$$

$$\lim_{\gamma \to \infty} \gamma D_\gamma =: \overline{D},$$

$$D^* \leq \gamma\, D_\gamma \leq \overline{D} \quad \forall \gamma \in (0, \infty).$$

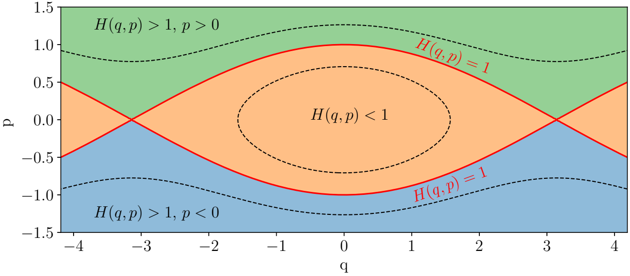
In addition $\overline{D}$ coincides with the effective diffusion coefficient associated with the overdamped Langevin dynamics.

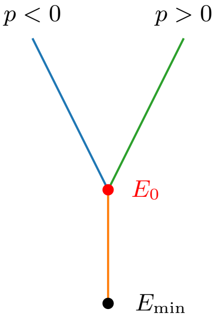


As $\gamma \to 0$, the Hamiltonian of the rescaled process

$$\begin{cases} q_\gamma(t) = q(t/\gamma), \\ p_\gamma(t) = p(t/\gamma), \end{cases}$$

converges weakly to a diffusion process on a graph.





The Langevin equation: effective diffusion in the overdamped limit

As $\gamma \to \infty$, the rescaled position $q(\gamma t)$ converges weakly to the solution of the overdamped Langevin equation:

$$\dot{q} = -V'(q) + \sqrt{2\,\beta^{-1}}\,\dot{W}.$$

To study the effective diffusion in the overdamped regime, we use the expansion

$$\phi_\gamma = \phi_0 + \frac{1}{\gamma}\phi_1 + \frac{1}{\gamma^2}\phi_2 + \cdots$$

in the Poisson equation $-\mathcal{L}_L \phi = p$. Grouping terms:

$$\begin{aligned}
\mathcal{O}(\gamma) \quad & -\mathcal{L}_{\mathrm{FD}}\phi_0 = 0, \\
\mathcal{O}(1) \quad & -\mathcal{L}_{\mathrm{FD}}\phi_1 - \mathcal{L}_{\mathrm{ham}}\phi_0 = p, \\
\mathcal{O}(1/\gamma) \quad & -\mathcal{L}_{\mathrm{FD}}\phi_2 - \mathcal{L}_{\mathrm{ham}}\phi_1 = 0 \ldots
\end{aligned}$$

Solving these equations as previously, we obtain

$$\begin{aligned}
\phi_0(q) &= \left(-V'(q)\partial_q + \beta^{-1}\partial_q^2\right)^{-1} V'(q), \\
\phi_1(q,p) &= p\,(1 + \partial_q\phi_0) + \xcancel{\psi_1(q)}, \\
\phi_2(q,p) &= (p^2/2)\,\partial_q^2\phi_0 + \xcancel{p\,\partial_q\psi_1} + \psi_2(q).
\end{aligned}$$

The Langevin equation: effective diffusion in the overdamped limit

Truncating the series at the third term, we have

$$-\mathcal{L}_L \left(\phi_0 + \frac{1}{\gamma}\phi_1 + \frac{1}{\gamma^2}\phi_2 - \phi_\gamma \right) = -\frac{1}{\gamma^2}\,\mathcal{L}_{\text{ham}}\phi_2.$$

If one can show that

- The right-hand side $\mathcal{L}_{\text{ham}}\phi_2 \in X$,
- The operator norm $\|\mathcal{L}_L^{-1}\|_X/\gamma^2 \to 0$ as $\gamma \to \infty$.

Then, taking $\gamma \to \infty$, we obtain

$$\|\phi_0 - \phi_\gamma\|_X \to 0 \quad \text{as} \quad \gamma \to \infty.$$

The second condition is guaranteed by hypocoercivity:

Hypocoercivity implies the boundedness of the inverse

If

$$\|\,\mathrm{e}^{\mathcal{L}t}\, h\|_X \leq C\,\mathrm{e}^{-\lambda t}\,\|h\|_X, \qquad \forall h \in X$$

then

$$\|\mathcal{L}^{-1}\|_{\mathcal{B}(X)} \leq \frac{C}{\lambda}.$$

Back to the GLE: a simple quasi-Markovian model

Assume that the memory kernel is of the form $\gamma(t) = \lambda^2 \, \mathrm{e}^{-a|t|}$. The corresponding GLE is equivalent to

$$
\begin{aligned}
\mathrm{d}q_t &= p_t \, \mathrm{d}t, \\
\mathrm{d}p_t &= -V'(q_t) \, \mathrm{d}t + \lambda \, z_t \, \mathrm{d}t, \\
\mathrm{d}z_t &= -\lambda \, p_t \, \mathrm{d}t - a \, z_t \, \mathrm{d}t + \sqrt{2a\beta^{-1}} \, \mathrm{d}W_t, \qquad z(0) \sim \mathcal{N}(0, \beta^{-1})
\end{aligned}
$$

Indeed, integrating the third equation:

$$
z_t = \mathrm{e}^{-at} \, z_0 - \lambda \int_0^t \mathrm{e}^{-a(t-s)} \, p_s \, \mathrm{d}s + \sqrt{2a\beta^{-1}} \int_0^t \mathrm{e}^{-a(t-s)} \, \mathrm{d}W_s.
$$

Substituting in the equation for p:

$$
\mathrm{d}p_t = -V'(q_t) \, \mathrm{d}t - \int_0^t \gamma(t-s) \, p_s \, \mathrm{d}s + \underbrace{\left(\lambda \, \mathrm{e}^{-at} \, z_0 + \lambda \sqrt{2a\beta^{-1}} \int_0^t \mathrm{e}^{-a(t-s)} \, \mathrm{d}W_s \right)}_{=:F(t)},
$$

$F(t)$ is a stationary mean-zero Gaussian process with variance $\beta^{-1}\lambda^2$, so

$$
\mathbf{E}\left(F(s)F(t)\right) = \int_{\mathbf{R}} (\mathrm{e}^{L_{\mathrm{OU}} t} \, x) \, x \, \mathcal{N}(0, \lambda^2 \beta^{-1}) \, \mathrm{d}x = \beta^{-1} \, \lambda^2 \, \mathrm{e}^{-at},
$$

where $\mathcal{L}_{\mathrm{OU}} = -a \, x \, \partial_x + a \, \beta^{-1} \, \lambda^2 \, \partial_x^2$.

General quasi-Markovian approximation

When the memory kernel is of the form

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

for (possibly nonsymmetric) $\mathbf{A} \in \mathbf{R}^{n\times n}$ with nonnegative eigenvalues and $\boldsymbol{\lambda} \in \mathbf{R}^n$, eq. (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:

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

Invariant density:

$$\mu(\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}\mathbf{z}) = \frac{1}{\mathcal{Z}} \exp\left(-\beta\left(H(q,p) + \frac{|\mathbf{z}|^2}{2}\right)\right).$$

where $H(q,p) = V(q) + \frac{p^2}{2}$.

Relationship with the Langevin dynamics

Let us consider the scaling $\mathbf{A} \mapsto \mathbf{A}/\nu^2$, $\boldsymbol{\lambda} \mapsto \boldsymbol{\lambda}/\nu$, then

Theorem (Ottobre 2011[1])

Let $\{q(t), p(t), \mathbf{z}(t)\}$ be the solution of the quasi-Markovian GLE, with $V \in C^1(\mathbf{T})$ and initial conditions having finite moments of any order. Then the process $\{q, p\}$ on $[0, T]$ converges weakly to the solution of the Langevin equation:

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

with

$$\gamma = \int_0^\infty \gamma(t)\,\mathrm{d}t.$$

[1] M. Ottobre and G. A. Pavliotis. Asymptotic analysis for the generalized Langevin equation. *Nonlinearity*, 24(5):1629–1653, 2011. ISSN: 0951-7715.

Example: sum of exponentials

If $\gamma(t) = \sum_{i=1}^{n} \lambda_i^2 \, \mathrm{e}^{-a_i |t|}$, then

$$\boldsymbol{\lambda} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_n \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{pmatrix}$$

This leads to the following system:

$$\begin{aligned} \mathrm{d}q &= p \, \mathrm{d}t, \\ \mathrm{d}p &= -V'(q) \, \mathrm{d}t + \left(\sum_{i=1}^{n} \lambda_i z_t^i \right) \mathrm{d}t, \\ \mathrm{d}z_t^i &= -\lambda_i \, p_t \, \mathrm{d}t - a_i \, z_t^i \, \mathrm{d}t + \sqrt{2 a_i \beta^{-1}} \, \mathrm{d}W_t, \qquad i = 1, 2, \dots, n. \end{aligned}$$

Example: continued fraction

If the Laplace transform $\tilde{\gamma}$ is of the form

$$\tilde{\gamma}(s) = \cfrac{\lambda^2}{\theta_1 + s + \cfrac{\varepsilon_1^2}{\theta_2 + s + \cfrac{\varepsilon_2^2}{\theta_3 + s + \cfrac{\varepsilon_3^2}{\ddots}}}},$$

then quasi-Markovian approximations can be constructed via

$$\mathbf{A} = \begin{pmatrix} \theta_1 & \varepsilon_1 & & & & \\ -\varepsilon_1 & \theta_2 & \varepsilon_2 & & & \\ & -\varepsilon_1 & \theta_3 & \varepsilon_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -\varepsilon_{n-2} & \theta_{n-1} & \varepsilon_{n-1} \\ & & & & -\varepsilon_{n-1} & \theta_n, \end{pmatrix} \quad \text{and} \quad \boldsymbol{\lambda} = \begin{pmatrix} \lambda \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

Models: quasi-Markovian approximations of interest

We are interested in two particular Markovian approximations:

GL1: Scalar OU noise,

$$\mathrm{d}z = (-\sqrt{\gamma}\, p/\nu - z/\nu^2)\,\mathrm{d}t + \sqrt{2\,\beta^{-1}/\nu^2}\,\mathrm{d}W_t, \quad z(0) \sim \mathcal{N}(0, \beta^{-1}).$$

The associated memory kernel is $\gamma(t) = \frac{\gamma}{\nu^2}\, \mathrm{e}^{-\frac{|t|}{\nu^2}}$.

GL2: Harmonic noise,

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

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

Models: quasi-Markovian approximations of interest

Influence of the paramaters on the autocorrelation function of the noise:

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

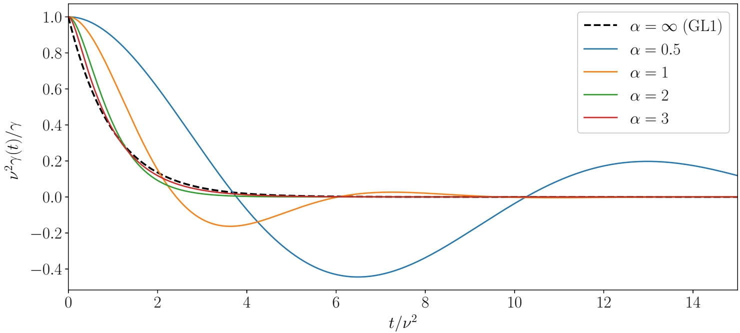


Figure: Autocorrelation function of the noise for model GL2.

Calculation of the effective diffusion

After

- introducing the non-periodized position x;
- applying the diffusive rescaling $x \mapsto x/\varepsilon$, $t \mapsto t/\varepsilon^2$;

the (quasi-Markovian) GLE can be recast as a fast/slow system of SDEs:

$$\begin{aligned}
\mathrm{d}x &= \frac{1}{\varepsilon}\, p \,\mathrm{d}t, \\
\mathrm{d}q &= \frac{1}{\varepsilon^2}\, p \,\mathrm{d}t, \\
\mathrm{d}p &= \frac{1}{\varepsilon^2}\, \big(-V'(q) + \langle \boldsymbol{\lambda}, \mathbf{z} \rangle\big)\, \mathrm{d}t, \\
\mathrm{d}\mathbf{z} &= -\frac{1}{\varepsilon^2}\, (p\,\boldsymbol{\lambda} + \mathbf{A}\,\mathbf{z})\, \mathrm{d}t + \frac{1}{\varepsilon}\, \boldsymbol{\Sigma}\, \mathrm{d}\mathbf{W}_t, \quad \mathbf{z}(0) \sim \mathcal{N}(0, \beta^{-1}\mathbf{I}).
\end{aligned}$$

The effective diffusion coefficient can be obtained by solving a Poisson equation:

$$\begin{aligned}
-\mathcal{L}\,\phi &= p, \\
D &= \int_{\mathbf{T}\times\mathbf{R}\times\mathbf{R}^n} \phi\, p\, \mu(\mathrm{d}q\,\mathrm{d}p\,\mathrm{d}\mathbf{z}).
\end{aligned}$$

Decomposing the generator as

$$\mathcal{L} = \left(p \, \frac{\partial}{\partial q} - \frac{\partial V}{\partial q} \, \frac{\partial}{\partial p} + \langle \boldsymbol{\lambda}, \mathbf{z} \rangle \, \frac{\partial}{\partial p} - p \, \boldsymbol{\lambda} \cdot \nabla_{\mathbf{z}} - \mathbf{A}_a \, \mathbf{z} \cdot \nabla_{\mathbf{z}} \right) + \big(-\mathbf{A}_s \, \mathbf{z} \cdot \nabla_{\mathbf{z}} + \beta^{-1} \, \mathbf{A} : (\nabla_{\mathbf{z}} \nabla_{\mathbf{z}}) \big) \, ,$$

the effective diffusion coefficient can be written as

$$D = \beta^{-1} \int_{\mathbf{T} \times \mathbf{R} \times \mathbf{R}^n} \mathbf{A}_s : (\nabla_{\mathbf{z}} \phi \otimes \nabla_{\mathbf{z}} \phi) \, \mu(\mathrm{d}q \, \mathrm{d}p \, \mathrm{d}\mathbf{z}).$$

Asymptotic analysis: limits of interest

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

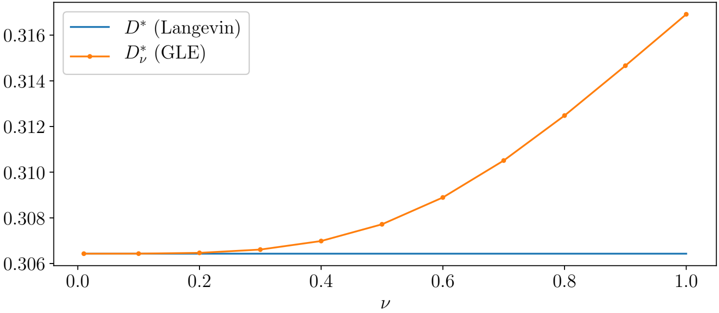
Results

Underdamped limit for the GLE

It holds that:

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

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



Idea of the (formal) proof

Decomposing the generator as

$$\mathcal{L}_0 + \sqrt{\gamma}\mathcal{L}_1 := \left(p\,\frac{\partial}{\partial q} - \frac{\partial V}{\partial q}\,\frac{\partial}{\partial p} + \frac{1}{\nu^2}\left(-z\frac{\partial}{\partial z} + \frac{\partial^2}{\partial z^2}\right)\right) + \frac{\sqrt{\gamma}}{\nu}\,\left(z\,\frac{\partial}{\partial p} - p\,\frac{\partial}{\partial z}\right),$$

and considering the asymptotic expansion $\phi = \frac{1}{\gamma}\,\phi_0 + \frac{1}{\sqrt{\gamma}}\,\phi_1 + \cdots$

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

Then use that $-\mathcal{L}_0\phi = f$ admits a solution only if $f = f(q,p)$ and

$$\int_{\mathbf{T}\times\mathbf{R}} f(q,p)\,F\left(V(q) + \frac{p^2}{2}\right)\,\mathrm{d}p\,\mathrm{d}q = 0,$$

for all smooth, rapidly decaying F. The solvability condition of the third equation gives an equation for $\phi_0 = \phi_0\left(V(q) + \frac{p^2}{2}\right)$:

$$\left(\beta^{-1}\,S_\nu'(E) - S_\nu(E)\right)\,\phi_0'(E) + \beta^{-1}\,S_\nu(E)\,\phi_0''(E) = \begin{cases} -2\pi, & \text{for } p > 0, E > E_0,\\ 2\pi, & \text{for } p < 0, E > E_0,\\ 0, & \text{for } E_{\min} < E < E_0.\end{cases}$$

Results

Overdamped limit for the GLE

It holds that:

$$\lim_{\gamma \to \infty} \gamma \, D_{\nu,\gamma} = \overline{D}, \qquad \forall \nu > 0.$$

Short memory limit

In the limit $\nu \to 0$,

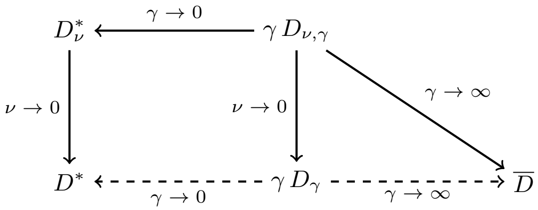
$$D_{\nu,\gamma} = D_\gamma + \mathcal{O}(\nu^4), \qquad \text{when } \alpha = 1,$$
$$D_{\nu,\gamma} = D_\gamma + \mathcal{O}(\nu^2), \qquad \text{otherwise.}$$

In addition, the $\mathcal{O}(\nu^2)$ and $\mathcal{O}(\nu^4)$ corrections can be calculated by solving Poisson equations of the type

$$-\mathcal{L}_L \phi = f,$$

where $\mathcal{L}_L$ is the generator of the Langevin dynamics.

Asymptotic analysis: summary



Hypocoercivity: a toy example

$$\dot{\mathbf{x}} = \begin{pmatrix} 0 & -1 \\ 1 & -\gamma \end{pmatrix} \mathbf{x}, \quad \gamma > 0, \ \mathbf{x} \in \mathbf{R}^2.$$

Writing $\mathbf{x} = (x, y)^T$,

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

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

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

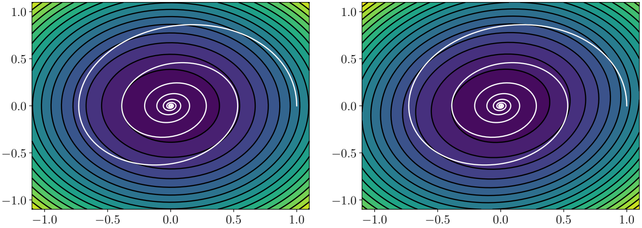


Figure: Level sets of $|\mathbf{x}|^2$ (left) and $(\!(\mathbf{x}, \mathbf{x})\!)$ (right).

By decomposing the generator as

$$\begin{aligned} -\mathcal{L} =& \beta^{-1}\,\nu^{-2}\,\alpha^2\,\partial_{z_2}^*\,\partial_{z_2} \\ &+\nu^{-2}\,\alpha(z_1\,\partial_{z_2} - z_2\,\partial_{z_1}) + \sqrt{\gamma}\,\nu^{-1}(p\,\partial_{z_1} - z_1\,\partial_p) + (\partial_q V\,\partial_p - p\,\partial_q) \\ =&: A^* A + B, \end{aligned}$$

we observe that

$$\langle -\mathcal{L}u, u\rangle_{L^2(\mu)} = \beta^{-1}\,\nu^{-2}\,\alpha^2\,\|\partial_{z_2} u\|^2.$$

we can apply Villani's framework for hypocoercivity.

$$\begin{aligned} ((h,h)) = &\|h\|^2 + a_0\,\|\partial_{z_2} h\|^2 + a_1\,\|\partial_{z_1} h\|^2 + a_2\,\|\partial_p h\|^2 + a_3\,\|\partial_q h\|^2 \\ &- b_0\,\langle \partial_{z_2} h, \partial_{z_1} h\rangle - b_1\,\langle \partial_{z_1} h, \partial_p h\rangle - b_2\,\langle \partial_p h, \partial_q h\rangle\,. \end{aligned}$$

Convergence to equilibrium

By Cauchy–Schwarz,

$$((h,h)) - \|h\|^2 \geq \begin{pmatrix} \|\partial_{z_2} h\| \\ \|\partial_{z_1} h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix}^T \underbrace{\begin{pmatrix} a_0 & -b_0 & 0 & 0 \\ 0 & a_1 & -b_1 & 0 \\ 0 & 0 & a_2 & -b_2 \\ 0 & 0 & 0 & a_3 \end{pmatrix}}_{:=M_1} \begin{pmatrix} \|\partial_{z_2} h\| \\ \|\partial_{z_1} h\| \\ \|\partial_p h\| \\ \|\partial_q h\| \end{pmatrix}. \tag{3}$$

On the other hand, after some calculations,

$$-((h, \mathcal{L}h)) \geq \begin{pmatrix} \|\partial_{z_2}\, \partial_{z_2}\, h\| \\ \|\partial_{z_2}\, \partial_{z_1}\, h\| \\ \|\partial_{z_2}\, \partial_p\, h\| \\ \|\partial_{z_2}\, \partial_q\, h\| \end{pmatrix}^T (\alpha^2 \nu^{-2} M_1) \begin{pmatrix} \|\partial_{z_2}\, \partial_{z_2}\, h\| \\ \|\partial_{z_2}\, \partial_{z_1}\, h\| \\ \|\partial_{z_2}\, \partial_p\, h\| \\ \|\partial_{z_2}\, \partial_q\, h\| \end{pmatrix} + \begin{pmatrix} \|\partial_{z_2}\, h\| \\ \|\partial_{z_1}\, h\| \\ \|\partial_p\, h\| \\ \|\partial_q\, h\| \end{pmatrix}^T M_2 \begin{pmatrix} \|\partial_{z_2}\, h\| \\ \|\partial_{z_1}\, h\| \\ \|\partial_p\, h\| \\ \|\partial_q\, h\| \end{pmatrix}.$$

where M_2 also depends on $a_0, a_1, a_2, a_3, b_0, b_1, b_2$.

Combining the two inequalities, and using the coercivity of

$$\partial_{z_2}^* \partial_{z_2} + \partial_{z_1}^* \partial_{z_1} + \partial_p^* \partial_p + \partial_q^* \partial_q$$

we conclude to the exponential convergence to equilibrium:

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} (\!(h, h)\!) \leq -\frac{c_2}{C_1 + \kappa^{-1}} (\!(h, h)\!),$$

where C_1 is the largest eigenvalue of the symmetric part of M_1 and c_2 is the smallest eigenvalue of the symmetric part of M_2.

To obtain the best possible rate of convergence, we solve

$$\max_{\substack{a_0, a_1, a_2, a_3 \\ b_0, b_1, b_2 \\ c_2, C_1}} \quad \frac{c_2}{C_1 + \kappa^{-1}} \quad \text{subject to} \quad \begin{cases} \frac{1}{2}(M_2 + M_2^T) - c_2 I \succeq 0, \\ C_1 I - \frac{1}{2}(M_1 + M_1^T) \succeq 0, \end{cases} \tag{4}$$

Convergence to equilibrium: results

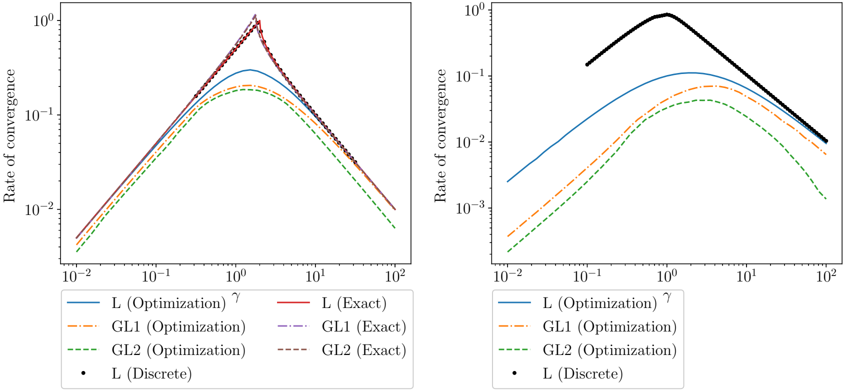


Figure: Convergence rate of the dynamics for the three models when $\mathcal{X} = \mathbf{R}, V(q) = q^2/2$ (left) and $\mathcal{X} = \mathbf{T}, V(q) = (1/2)\,(1 - \cos(q))$ (right). In both cases, $\nu = \alpha^{-1} = 1/3$.

Numerical approaches for the calculation of the effective diffusion coefficient

Ensemble average of second moment

$$D = \lim_{t \to \infty} \frac{1}{2t} \mathbf{E}(q(t) - q(0))^2$$

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

$$D = \int (-\mathcal{L}^{-1} p)\, p \,\mathrm{d}\mu = \int_0^\infty \int (\mathrm{e}^{\mathcal{L}t}\, p) p \,\mathrm{d}\mu \,\mathrm{d}t = \int_0^\infty C_p(t) \,\mathrm{d}t.$$

Non-equilibrium technique Considering a small forcing,

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

the effective diffusion can also be obtained as

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

Fourier/Hermite Galerkin method for the Poisson equation

Numerical experiments

Goals:

- Verify asymptotic results;
- Corroborate and complement early results.

We employ a Fourier/Hermite spectral method for the Poisson equation, with the saddle-point formulation[2].

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

where

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

The constraint $\langle \Phi_N, u_N \rangle = 0$ ensures that the system is well-conditioned.

[2] J. Roussel and G. Stoltz. Spectral methods for Langevin dynamics and associated error estimates. *ESAIM: Math. Model. Numer. Anal.*, 52(3):1051–1083, 2018.

In the case of harmonic noise, we use the following basis functions:

$$e_{i,j,k,l} = \left(\mathcal{Z} \, \mathrm{e}^{\beta \left(H(q,p) + |\mathbf{z}|^2 \right)} \right)^{\frac{1}{2}} G_i(q) \, H_j(p) \, H_k(z_1) \, H_l(z_2), \qquad 0 \leq i, j, k, l \leq N.$$

where G_i are trigonometric functions,

$$G_i(q) = \begin{cases} 1/\sqrt{2\pi}, & \text{if } i = 0, \\ \sin\left(\frac{i+1}{2} q\right) / \sqrt{\pi}, & \text{if } i \text{ is odd}, \\ \cos\left(\frac{i}{2} q\right) / \sqrt{\pi}, & \text{if } i \text{ is even, } i > 0. \end{cases}$$

and H_j are rescaled normalized Hermite functions,

$$H_j(p) = \frac{1}{\sqrt{\sigma}} \, \psi_j\left(\frac{p}{\sigma}\right), \qquad \psi_j(p) := (2\pi)^{-\frac{1}{4}} \frac{(-1)^j}{\sqrt{j!}} \, \mathrm{e}^{\frac{p^2}{4}} \, \frac{\mathrm{d}^j}{\mathrm{d}p^j} \left(\mathrm{e}^{-\frac{p^2}{2}} \right).$$

Unitary transformation

Let $\rho_\infty = \frac{1}{\mathcal{Z}}\, \mathrm{e}^{-\beta\left(H(q,p)+|\mathbf{z}|^2\right)}$ be the density of μ.

Since it is more convenient to work in the flat $L^2\left(\mathbf{R}^n\right)$, we rewrite the problem using the following unitary transformation:

$$\sqrt{\rho_\infty} : L^2\left(\mu\right) \to L^2\left(\mathrm{d}q\, \mathrm{d}p\, \mathrm{d}\mathbf{z}\right).$$

The Poisson equation for the calculation of the effective diffusion coefficient becomes:

$$-\underbrace{(\rho_\infty^{1/2} \mathcal{L}\, \rho_\infty^{-1/2})}_{=:\mathcal{H}}\underbrace{(\rho_\infty^{1/2}\boldsymbol{\phi})}_{=:\boldsymbol{\psi}} = (\rho_\infty^{1/2} p).$$

In the case of the overdamped Langevin equation, the operator $\mathcal{H}$ obtained by the transformation is a Schrödinger operator:

$$\mathcal{H} = \Delta - \left(\frac{1}{4}|\boldsymbol{\nabla} V|^2 - \frac{1}{2}\Delta V\right).$$

With this formulation, the effective coefficient is simply $\langle \psi, p \rangle_{L^2}$.

Choice of the scaling factor

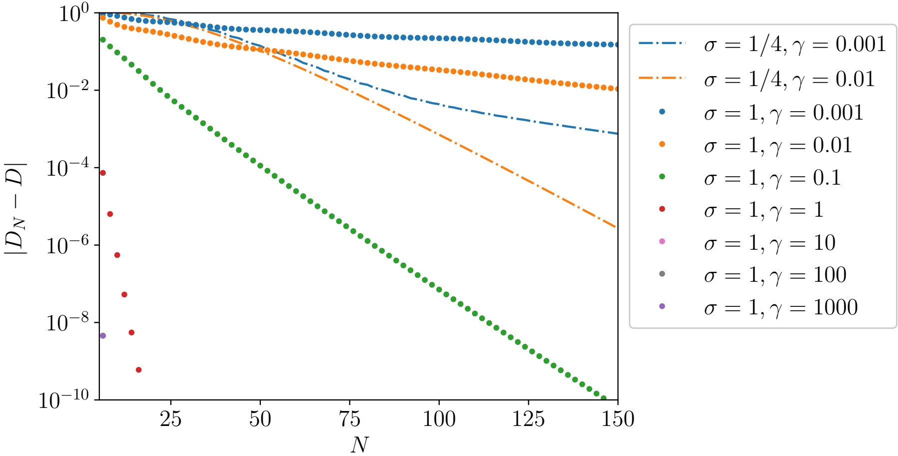
We recall that

- The Hermite functions are the eigenfunctions of the Fourier transform;
- A contraction in real space leads to a dilation in Fourier space;
- The final inflection point of ψ_j occurs at $x \propto \sqrt{4j+2}$;
- Using Plancherel identity: $\langle u, H_j^\sigma \rangle = \left\langle \tilde{u}, H_j^{1/\sigma} \right\rangle$.

To favor exploration in Fourier space, e.g. because $u(x)$ is expected to decay rapidly as $|x| \to \infty$, it is useful to choose $\sigma = \sigma(N)$.

In particular, with $\sigma(N) \propto \sqrt{N}$, the window of resolution in real space does not grow as N increases.

Improving the convergence by rescaling the Hermite functions



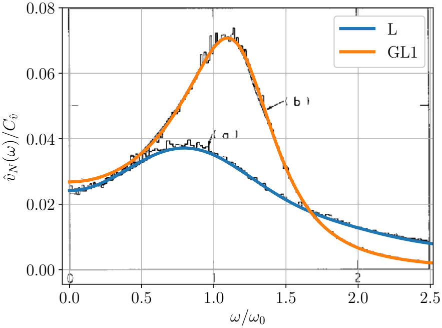
Comparison with previous literature

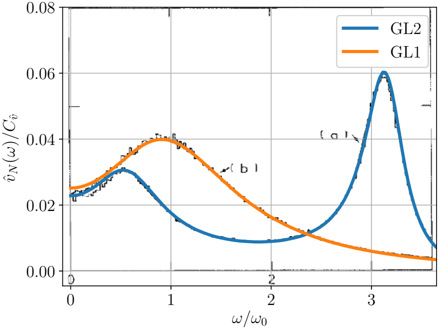
A Fourier/Hermite discretization can also be used to calculate the velocity autocorrelation.

$$\begin{cases} \dfrac{\partial v_N}{\partial t} = (\Pi_N \, \mathcal{L} \, \Pi_N) v_N, \\ v_N(0) = \Pi_N p. \end{cases}$$

Its spectrum is

$$\hat{v}_N(\omega) := \int_{\mathbf{R}} \langle v_N(t), \Pi_N p \rangle \, \mathrm{e}^{-i\omega t} \, \mathrm{d}t.$$





Dependence of D on γ

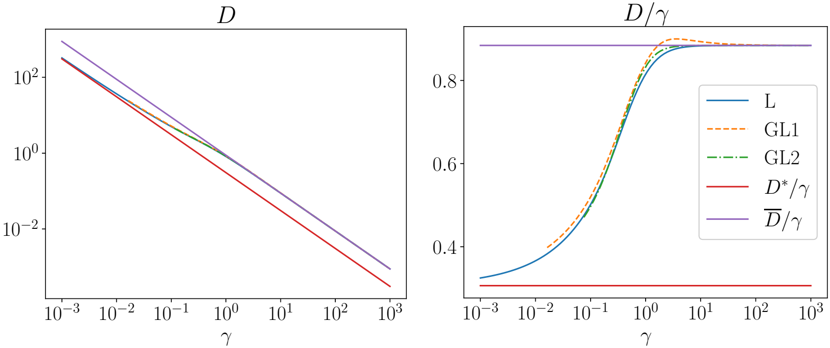


Figure: Diffusion coefficient as a function of γ, when $\nu = \alpha = 1$.

Dependence of D on ν and α

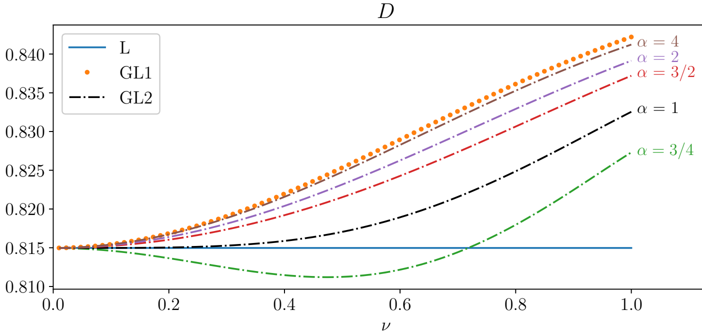


Figure: Effective diffusion coefficient against ν, for fixed values $\beta = \gamma = 1$.

Dependence of D on ν and α

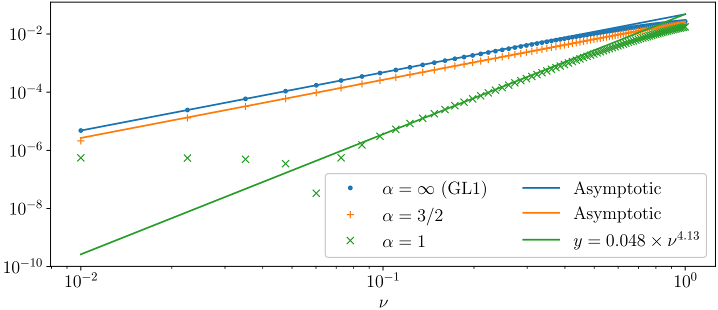


Figure: Deviation of the effective diffusion coefficient from its limiting value as $\nu \to 0$, for fixed values $\beta = \gamma = 1$.