LONG TIME ASYMPTOTICS FOR NON-MARKOVIAN LANGEVIN EQUATIONS

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Coarse-graining of many-body systems: analysis, computations and applications
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Goal: study of qualitative properties of solutions to the Generalized Langevin equation (GLE) in $\mathbb{R}^d$

$$\ddot{q} = -\nabla V(q) - \int_0^t \gamma(t-s) \dot{q}(s) \, ds + F(t),$$  \hspace{1cm} (1)

where $V(q)$ is a smooth potential (confining or periodic), $F(t)$ a mean zero stationary Gaussian process with autocorrelation function $\gamma(t)$ (fluctuation-dissipation theorem)

$$\langle F(t) \otimes F(s) \rangle = \beta^{-1} \gamma(t-s) I.$$  \hspace{1cm} (2)

Here $\beta$ stands for the inverse temperature and $I$ for the identity matrix.
In particular, under the assumption of a "Markovian heat bath", we want to study:

- Ergodicity, exponentially fast convergence to equilibrium, estimates on the exponent (earlier work by Eckmann, Pillet, Rey-Bellet, Hairer, Thomas, Mattingly,.....)
- Estimates on derivatives of the associated Markov semigroup.
- Homogenization theorem when $V(q)$ is periodic, estimates on the diffusion coefficient.
- Calculation of the spectrum of the generator for quadratic potentials.
One of the standard models of non-equilibrium statistical mechanics is that of a particle (Brownian particle) in contact with a heat bath.

The dynamics of the particle-reservoir system can be described through a Hamiltonian of the form

\[ H(Q, P; q, p) = H_{BP}(Q, P) + H_{HB}(q, p) + H_i(Q, q), \]  

\( \{Q, P\} \) are the coordinates of the Brownian particle and \( \{q, p\} \) of the heat bath particles.

The initial conditions of the Brownian particle are taken to be fixed, whereas the "environment" is assumed to be initially at equilibrium (Gibbs distribution).
The equations of motion for (3) are a system of ODEs with random initial conditions.

By integrating out the heat bath variables we can obtain a stochastic integrodifferential equation.

This equation is non-Markovian.

Consider a harmonic heat bath and of linear coupling:

$$H(Q_N, P_N, q, p) = \frac{P_N^2}{2} + V(Q_N) + \sum_{n=1}^{N} \frac{p_n^2}{2m_n} + \frac{1}{2} k_n(q_n - \lambda Q_N)^2.$$ 

The initial conditions of the Brownian particle \( \{ Q_N(0), P_N(0) \} := \{ Q_0, P_0 \} \) are taken to be deterministic.

The initial conditions of the heat bath particles are distributed according to the Gibbs distribution, conditional on the knowledge of \( \{ Q_0, P_0 \} \):

$$\mu_\beta(dpdq) = Z^{-1} e^{-\beta H(q,p)} dqdp,$$ 

where \( \beta \) is the inverse temperature.
In order to choose the initial conditions according to \( \mu_\beta(dpdq) \) we can take

\[
q_n(0) = \lambda Q_0 + \sqrt{\beta^{-1} k_n^{-1}} \xi_n, \quad p_n(0) = \sqrt{m_n \beta^{-1}} \eta_n, \quad (5)
\]

where the \( \xi_n, \eta_n \) are mutually independent sequences of i.i.d. \( \mathcal{N}(0, 1) \) random variables.

Notice that we actually consider the Gibbs measure of an effective (renormalized) Hamiltonian.

Hamilton’s equations of motion are:

\[
\ddot{Q}_N + V'(Q_N) = \sum_{n=1}^{N} k_n (\lambda q_n - \lambda^2 Q_N), \quad (6a)
\]

\[
\ddot{q}_n + \omega_n^2 (q_n - \lambda Q_N) = 0, \quad n = 1, \ldots N, \quad (6b)
\]

where \( \omega_n^2 = k_n/m_n \), which is taken to be a random variable.
We solve (6b) and substitute this in equation (6a) to obtain the GLE and the fluctuation-dissipation theorem.

The noise $F_N(t)$ (which depends only on the initial conditions of the heat bath) is a mean zero stationary Gaussian process with correlation function $\gamma_N(t)$.

Let $a \in (0, 1)$, $2b = 1 - a$ and set $\omega_n = N^a \zeta_n$ where $\{\zeta_n\}_{n=1}^{\infty}$ are i.i.d. with $\zeta_1 \sim \mathcal{U}(0, 1)$. Choose the spring constants according to $k_n = \frac{f^2(\omega_n)}{N^{2b}}$.

We can pass to the thermodynamic limit as $N \to +\infty$ and obtain the GLE:

$$\ddot{Q} = -V'(Q) - \lambda^2 \int_0^t \gamma(t - s) \dot{Q}(s) \, ds + \lambda F(t). \quad (7)$$

The parameter $\lambda$ measures the strength of the coupling between the Brownian particle and the heat bath.
The Kac-Zwanzig Model

- The memory kernel (and, consequently, the noise $F(t)$) are determined by the function $f(\omega)$:

$$
\gamma(t) = \int_{0}^{+\infty} f^2(\omega) \cos(\omega t) \, d\omega.
$$

- Ex: Consider the Lorentzian function

$$
f^2(\omega) = \frac{2\alpha/\pi}{\alpha^2 + \omega^2}
$$

with $\alpha > 0$. Then

$$
\gamma(t) = e^{-\alpha |t|}.
$$

- The noise process $F(t)$ is a mean zero stationary Gaussian process with continuous paths and, exponential autocorrelation function.

- Hence, $F(t)$ is the stationary Ornstein-Uhlenbeck process:

$$
\frac{dF}{dt} = -\alpha F + \sqrt{2\beta^{-1}\alpha} \frac{dW}{dt}, \quad F(0) \sim \mathcal{N}(0, \beta^{-1}).
$$
We can rewrite (7) with an exponential memory kernel as a system of SDEs:

\[
\begin{align*}
\frac{dQ}{dt} &= P, \\
\frac{dP}{dt} &= -V'(Q) + \lambda Z, \\
\frac{dZ}{dt} &= -\alpha Z - \lambda P + \sqrt{2\alpha\beta^{-1}} \frac{dW}{dt},
\end{align*}
\]

where \( Z(0) \sim \mathcal{N}(0, \beta^{-1}) \).

The process \( \{Q(t), P(t), Z(t)\} \in \mathbb{R}^3 \) is Markovian.

It is a degenerate Markov process: noise acts directly only on one of the 3 degrees of freedom.
Open Classical Systems

- The environment is modeled through a classical linear field theory (i.e. the wave equation). This means that we consider an ideal reservoir, i.e. there are no interactions between the particles in the heat bath.

\[ \partial_t^2 \phi(t, x) = \partial_x^2 \phi(t, x). \]  

(11)

- The Hamiltonian of this system is

\[ \mathcal{H}_{HB}(\phi, \pi) = \int \left( |\partial_x \phi|^2 + |\pi(x)|^2 \right). \]  

(12)

- \( \pi(x) \) denotes the conjugate momentum field.
- The initial conditions are distributed according to the Gibbs measure (which in this case is a Gaussian measure) at inverse temperature \( \beta \).
We assume that the coupling between the particle and the field is linear (dipole approximation):

$$H_{I}(q, \phi) = \lambda q \int \partial x \phi(x) \rho(x) \, dx. \quad (13)$$

The full Hamiltonian is

$$H(q, p, \phi, \pi) = H_{BP}(p, q) + \mathcal{H}(\phi, \pi) + \lambda q \int \rho(x) \partial q \phi(x) \, dx. \quad (14)$$

By integrating out the heat bath variables we obtain the GLE

$$\ddot{q} = -\partial q V(q) - \lambda^2 \int_{0}^{t} \gamma(t - s) \dot{q}(s) \, ds + \lambda F(t), \quad (15)$$

where (for a Gibbs initial distribution) $F(t)$ is a mean zero stationary Gaussian process with autocorrelation function

$$\langle F(t)F(s) \rangle = \beta^{-1} \gamma(t - s) = \int |\hat{\rho}(k)|^2 e^{ik(t-s)} \, dk,$$
Notice that the spectral density of the autocorrelation function of the noise process is the square of the Fourier transform of the density $\rho(x)$ which controls the coupling between the particle and the heat bath.

The GLE (15) is equivalent to the original infinite dimensional Hamiltonian system with random initial conditions.

Proving ergodicity, convergence to equilibrium etc for (15) implies ergodicity and convergence to equilibrium for the "particle + heat bath" system.
Ergodic properties of (15) were studied by V. Jaksic and C.-A. Pillet ($\approx$ 1997 – 98).

Under the assumption $\|(−\Delta + |x|^2)^s \rho\| < \infty$, $s > 3/2$ we have global existence and uniqueness of solutions.

Under the additional assumption that there exist $C, \nu > 0$ so that

$$|\hat{\rho}(k)| \geq \frac{C}{(1 + |k|)^\nu},$$

the process $\{q, p = \dot{q}\}$ is mixing with respect to the measure

$$\mu_\beta(dqdp) = \frac{1}{Z_\beta} e^{-\beta H_{BP}(q,p)} dqdp.$$

Nothing is known about the rate of convergence to equilibrium.
For general coupling functions $\rho(x)$ the GLE (15) describes a non-Markovian system. It can be represented as a Markovian system only if we add an infinite number of additional variables.

However, under appropriate assumptions on the coupling function $\rho(x)$ the GLE (15) is equivalent to a Markovian process in a **finite dimensional** extended phase space.

This follows from the fact that all finite dimensional mean zero Gaussian stationary stochastic processes with an exponential autocorrelation function can be constructed as solutions of linear stochastic differential equations.
Assume that $|\hat{\rho}(k)|^2 = \frac{1}{|p(k)|^2}$ where $p(k) = \sum_{m=1}^{M} c_m(-k)^m$ is a polynomial with real coefficients and roots in the upper half plane. Then the Gaussian process with spectral density $|\hat{\rho}(k)|^2$ is the solution of the SDE

$\left( p \left( -i \frac{d}{dt} \right) x_t \right) = \frac{dW_t}{dt}$.
For example, when $p(k) \sim (ik + \alpha)$, then (15) is equivalent to

\[
\begin{align*}
\frac{dq}{dt} &= p, \\
\frac{dp}{dt} &= -V'(q) + \lambda z, \\
\frac{dz}{dt} &= -\alpha z - \lambda p + \sqrt{2\alpha \beta^{-1}} \frac{dW}{dt}.
\end{align*}
\]
In order to approximate the non-Markovian dynamics (15) by a finite dimensional Markovian system, we need to approximate the noise $F(t)$ by a finite dimensional Markovian Gaussian stationary process.

We will approximate the memory kernel by a sum of exponentials:

$$\gamma(t) \approx \sum_{j=1}^{N} \lambda_j^2 e^{-\alpha_j t} =: \gamma_N(t).$$

We can also approximate the Fourier transform of $\gamma(t)$ by a rational function (Padè approximation).

We can also approximate the Laplace transform of $\gamma(t)$ by a continued fraction expansion (Mori’s method, 1965).
We will consider the GLE

$$\ddot{q} = -V'(q) - \int_0^t \gamma(t - s) \dot{q} \, ds + F(t)$$  \hspace{1cm} (17)

where $F(t)$ is a mean zero, Gaussian stationary process with covariance

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

and the memory kernel is given by a sum of exponentials:

$$\gamma(t) = \sum_{j=1}^{N} \lambda_j^2 e^{-\alpha_j |t|},$$  \hspace{1cm} (18)

where $\lambda_j > 0$, $\alpha_j > 0$, $j = 1, \ldots, N$. 
Under this assumption the GLE (17) is equivalent to the $N + 2$-dimensional Markovian system

\[ dq = p \, dt, \quad (19a) \]
\[ dp = -V'(q) \, dt + \sum_{j=1}^{N} \lambda_j z_j \, dt, \quad (19b) \]
\[ dz_j = -\alpha_j z_j \, dt - \lambda_j p \, dt + \sqrt{2\alpha_j/\beta^{-1}} \, dW_j, \quad (19c) \]

for $j = 1, \ldots, N$ and where $q(0) = q_0$, $p(0) = p_0$ and $z_j \sim \mathcal{N}(0, \beta^{-1})$. 
Different approximations of the memory kernel lead to different SDEs for the noise and the auxiliary variables. For example, the continued fraction expansion of the Laplace transform of $\gamma(t)$ leads to the SDEs (with $N=2$):

\[
\begin{align*}
 dq &= p \, dt, \\
 dp &= -V'(q) \, dt + \lambda Z_1 \, dt, \\
 dZ_1 &= (-\alpha_1 Z_1 + Z_2) \, dt, \\
 dZ_2 &= (-\alpha_2 Z_2 - \lambda p) \, dt + \sqrt{2\beta^{-1}\alpha_2} \, dW.
\end{align*}
\]

Notice that there is "less" noise in (20) than in (19).

Connection with gentle thermostats (B. Leimkuhler, E. Noorizadeh, F. Theil 2009).

We can use either (20) or (19) to sample from $\frac{1}{Z}e^{-\beta H(q,p)}$. 
Consider the approximation

\[ \gamma(t) \approx \sum_{j=1}^{N} \lambda_j^2 e^{-\alpha_j t} =: \gamma_N(t). \]

The (positive) coefficients \( \{\alpha_j, \lambda_j\}_{j=1}^{N} \) should be obtained from "first principles". This is a problem in approximation theory.

Under appropriate assumptions on \( \{\alpha_j, \lambda_j\}_{j=1}^{N} \), the dynamics (19) is well defined for \( N = +\infty \) (related work on the Rouse chain model from polymer theory by S.A. McKinley).

Assuming that \( \|\gamma_N(t) - \gamma(t)\| \to 0 \) we can prove that \( \|q_N(t) - q(t)\| + \|p_N(t) - p(t)\| \to 0 \) over finite time intervals.
The Process \( \{q(t), p(t), z_1(t), \ldots z_N(t)\} \) is Markovian with generator

\[
-L = p \partial_q - V'(q) \partial_p + \left( \sum_{j=1}^{N} \lambda_j z_j \right) \partial_p \\
+ \sum_{j=1}^{N} \left( -\alpha_j z_j \partial z_j - \lambda_j p \partial z_j + \beta^{-1} \alpha_j \partial^2 z_j \right). \tag{21}
\]

This is the generator of a degenerate diffusion process: noise acts directly only to the heat bath variables \( \{z_j\}_{j=1}^{N} \).

There is, however, sufficient interaction between the different degrees of freedom so that noise gets transmitted to all variables.
Proposition

The generator $-\mathcal{L}$ is **hypoelliptic**: the transition probability of the process $\{q(t), p(t), z_1(t), \ldots, z_N(t)\}$ has a smooth density wrt Lebesgue.

Proof.

Use Hörmander’s theorem.

Proposition

The generator $-\mathcal{L}$ generates a contraction semigroup.

Proof.

Use the Lumer-Phillips theorem together with an appropriate family of cut-off functions and a priori estimates.
Invariant distributions are solutions to the stationary Fokker-Planck equation

\[ \mathcal{L}^\ast \rho = 0. \]

A solution to this equation is

\[ \rho_\beta(q, p, z) = \frac{1}{Z} e^{-\beta(H(q,p)+\frac{1}{2}\|z\|^2)}, \]

(22)

where \( z := \{z_1, \ldots, z_N\} \).

Notice that \( \rho_\beta \) is independent of the coefficients \( \{\alpha_j, \lambda_j\}_{j=1}^N \).

The invariant measure \( \mu_\beta(dq, dp, dz) = \rho_\beta(q, p, z)dqdpdz \) is unique.

The right function space to study the Markov process
\[ x(t) := \{ q(t), p(q), z(t) \} \]
is the weighted \( L^2 \) space \( L^2_\rho := L^2(\mathbb{R}^{2+N} ; \mu_\beta(dqdpdz)) \). In this space the generator takes the form
\[
- \mathcal{L} = -B - \sum_{j=1}^{N} A_j^* A_j, \tag{23}
\]
where
\[
A_j = \sqrt{\beta^{-1} \alpha_j} \partial z_j, \quad A_j^* = \sqrt{\beta^{-1} \alpha_j} (-\partial z_j + z_j)
\]
and
\[
B = -p \partial q + V'(q) \partial p - \left( \sum_{j=1}^{N} \lambda_j z_j \right) \partial p - p \sum_{j=1}^{N} \lambda_j \partial z_j.
\]
\( A_j^* \) is the \( L^2_\rho \)-adjoint of \( A_j \) and \( B^* = -B \).
The operator $\mathcal{L}$ given by (23) is of the form

$$\mathcal{L} = B + A^* A,$$

for which C. Villani’s theory of **hypocoercivity** (AMS 2009) applies:

- Let $\mathcal{L}$ be an unbounded operator on $\mathcal{H}$ with kernel $\mathcal{K}$ and let $\tilde{\mathcal{H}}$ be continuously and densely embedded in $\mathcal{K}^\perp = \mathcal{H}/\mathcal{K}$.

- $\mathcal{L}$ is **coercive** on $\tilde{\mathcal{H}}$ if and only if

  $$\| e^{-t\mathcal{L}} h_0 \|_{\tilde{\mathcal{H}}} \leq e^{-\lambda t} \| h_0 \|_{\tilde{\mathcal{H}}} \quad \forall h_0 \in \tilde{\mathcal{H}}, \ t \geq 0.$$ 

- $\mathcal{L}$ is **hypocoercive** on $\tilde{\mathcal{H}}$ provided that there exists a constant $C \geq 1$ such that

  $$\| e^{-t\mathcal{L}} h_0 \|_{\tilde{\mathcal{H}}} \leq C e^{-\lambda t} \| h_0 \|_{\tilde{\mathcal{H}}} \quad \forall h_0 \in \tilde{\mathcal{H}}, \ t \geq 0.$$
Hypocoercivity is invariant under change of equivalent norms on $\tilde{\mathcal{H}}$, whereas coercivity is not.

The basic idea for proving exponentially fast convergence to equilibrium: find an appropriate inner product that induces a norm on $\mathcal{K}^\perp = \mathcal{H}/\mathcal{K}$ that is equivalent to the $\mathcal{H}$ norm and wrt which $\mathcal{L}$ is coercive. Use then the invariance of hypocoercivity under change of equivalent norm to show exponentially fast convergence to equilibrium.

This modified inner product involves "mixed derivatives".

This methodology also leads to systematic techniques for obtaining bounds on the constants $C$ and $\lambda$. 
Theorem (Villani)

Define $C_0 = A$, $C_{j+1} = [C_j, B]$, $j = 0, 1, \ldots$, $C_{N_c+1} = 0$ for some $N_c$. If the operator $\sum_{j=0}^{N_c+1} C_j^* C_j$ is coercive and the commutators between $A$, $A^*$ and $C_j$ satisfy appropriate bounds, then

$$\| e^{-t\mathcal{L}} \|_{\mathcal{H}^1/\mathcal{K}} = \mathcal{O}(e^{-\lambda t}).$$

where $\mathcal{K} = \text{Ker}(\mathcal{L})$ and

$$\| h \|_{\mathcal{H}^1}^2 = \| h \|^2 + \sum_{j=0}^{N_c} \| C_j h \|^2.$$
The decomposition of the generator of the Markov process into a symmetric and antisymmetric part *in the right function space* is quite natural from the point of view of statistical Mechanics:

- The antisymmetric part describes the deterministic dynamics—it is the generator of the Hamiltonian unitary group (Stone’s theorem).
- The symmetric part describes the dissipative part of the dynamics/heat bath—it is the generator of a Markov semigroup (Hille-Yosida, Lumer-Phillips etc).
- The interaction between the conservative and dissipative parts of the dynamics is expressed through the non-commutativity between the symmetric and antisymmetric parts of the generator.
- The theory of hypocoercivity enables us to study convergence to equilibrium for systems of this form in an abstract functional analytic setting.
Set $N = 1$, $\alpha = \lambda = \beta = 1$. The first two commutators are

$$C_1 = [A, B] = \partial_p \quad \text{and} \quad C_2 = [C_1, B] = \partial_q - \partial_p. \quad (24)$$

We can check that

$$P = A^* A + C_1^* C_1 + C_2^* C_2$$

is coercive.

**Theorem**

Let $V(q) \in C^\infty(\mathbb{T})$ and consider

$$x(t) = \{q(t), p(t), z(t)\} \in \mathbb{T} \times \mathbb{R} \times \mathbb{R}^N. \quad \text{Then there exist}$$

constants $C, \lambda > 0$ such that

$$\|e^{t\mathcal{L}}\|_{\mathcal{H}^1 \to \mathcal{H}^1} \leq Ce^{-\lambda t}.$$
Remark

1. We can also prove exponentially fast convergence to equilibrium in relative entropy

\[ H(\rho_t | \rho_\infty) \leq C e^{-\lambda t} H(\rho_0 | \rho_\infty), \]

where \( \rho_t \) is the law of the process at time \( t \) and
\[ H(f | h) = \int f \log(f/h), \text{ assuming that } H(\rho_0 | \rho_\infty) < +\infty. \]
Set $\beta = 1$ and consider the case $N = 1$. Define the creation and annihilation operators

$$
\begin{align*}
a^- &= \partial_z, & a^+ &= -\partial_z + z, \\
b^- &= \partial_p, & b^+ &= -\partial_p + p, \\
c^- &= \partial_q, & c^+ &= -\partial_q + \partial_q V.
\end{align*}
$$

The generator of the process $x(t) = \{q(t), p(t), z(t)\}$ can be written in the form

$$
-\mathcal{L} = -\alpha a^+ a^- + \lambda (a^+ b^- - b^+ a^-) + (b^+ c^- - c^+ b^-).
$$

This form is very useful for doing perturbation theory and for calculating the eigenvalues/eigenfunctions when the potential is quadratic.
For the semigroup $P_t = e^{-Lt}$ generated by the Langevin equation

$$
\dot{q} = p, \quad \dot{p} = -\nabla V(q) - \gamma p + \sqrt{2\gamma\beta^{-1}} \dot{W},
$$


It is possible to prove similar estimates for the GLE.

**Theorem**

*The Markov semigroup $P_t = e^{-tL}$ satisfies the bounds*

$$
\| C_k P_t \|_{L^2_\rho \to L^2_\rho} \leq C \left( 1 + \frac{1}{t^{1+2k}} \right), \quad k = 0, 1, 2. \tag{25}
$$
Proof.

Let $u = e^{-Lt}u_0$ (i.e. the solution of the backward Kolmogorov equation) and use the Lyapunov function

$$F(t) = a_0 t \|Au\|^2 + a_1 t^3 \|C_1 u\|^2 + a_2 t^5 \|C_2 u\|^2 + b_0 t^2 (Au, C_1 u) + t^4 b_1 (C_1 u, C_2 u) + b_2 \|u\|^2.$$

We calculate $\partial_t F$ and choose the constants so that $\partial_t F$ is negative.
Remark

- Estimate (25) is sharp.
- Similar bounds hold for $C_j^\# e^{-L^b t}$ where $\#$, $b$ are either nothing or $\star$ (i.e. the $\mathcal{L}_\rho^2$ adjoint).
- An appropriate Lyapunov function can be constructed for more general hypocoercive operators of the form $\mathcal{L} = A^*A + B$.
- Similar (in fact pointwise) estimates can also be obtained for more general diffusion processes (work in progress with M. Ottobre, B. Zegarlinski, V. Kontis).
Consider the Smoluchowski and Langevin dynamics
\[ \dot{q} = -V'(q) + \sqrt{2\beta^{-1}} \dot{W} \] (26)
and
\[ \ddot{q} = -V'(q) - \gamma \dot{q} + \sqrt{2\gamma\beta^{-1}} \dot{W} \] (27)
in a periodic or random potential. Under the diffusive rescaling \( q^\epsilon(t) = \epsilon q(t/\epsilon^2) \), solutions to (26) and (27) converge weakly to a Brownian motion with diffusion coefficients \( D_V \) and \( D_\gamma \), respectively.

Furthermore, we have estimates of the form (see P. and Hairer, J. Stat. Phys. 131(1) (2008), 175–202, see also Benabu, CMP 266, 699-714 (2006))
\[ \frac{D^*}{\gamma} \leq D_\gamma \leq \frac{D_V}{\gamma}, \quad \gamma \in (0, +\infty). \] (28)

We can prove a homogenization theorem and obtain estimates on the diffusion coefficient for the GLE.
Theorem

Let \( \{q(t), p(t), z(t)\} \) on \( \mathbb{T} \times \mathbb{R} \times \mathbb{R}^N \) be the solution of (19) with \( V(q) \in C^\infty(\mathbb{T}) \) with stationary initial conditions. Then the rescaled process \( q^\varepsilon(t) := \varepsilon q(t/\varepsilon^2) \) converges weakly on \( C([0, T], \mathbb{R}) \) to a Brownian motion with diffusion coefficient \( D \) given by

\[
D = \int_0^{+\infty} \langle p(t)p(0) \rangle \, dt = \beta^{-1} \sum_{j=1}^N \alpha_j^{-1} \| \partial z_j \phi \|^2
\]

(29)

where \( \phi \in L^2_\rho \) is the unique (up to a constant) solution of the Poisson equation

\[
\mathcal{L}\phi = p,
\]

(30)
on \( \mathbb{T} \times \mathbb{R} \times \mathbb{R}^N \). Furthermore, we have the estimates

\[
0 < D \leq \frac{4}{\beta} \sum_{i=1}^N \frac{\alpha_i}{\chi_i^2}.
\]
Proof.

Prove existence and uniqueness and estimates for (30), and use the Martingale CLT:

- Apply Itô's formula to \( \phi(x(t)) \) to obtain

\[
q^\varepsilon(t) = \varepsilon q(0) - \varepsilon \left( \phi(x(t/\varepsilon^2)) - \phi(x(0)) \right) \\
+ \sum_{j=1}^{N} \sqrt{2\beta^{-1}} \alpha_j \varepsilon \int_{0}^{t/\varepsilon^2} \partial z_j \phi \, dW_j \\
=:\ R_\varepsilon(t) + \varepsilon \sum_{j=1}^{N} M^j_{t/\varepsilon^2}.
\]

- Our estimates on \( \phi \) imply that \( \mathbb{E}|R_\varepsilon(t)|^2 = o(1) \).
- From the ergodicity of the process \( x(t) \) we deduce

\[
\lim_{\varepsilon \to 0} \langle M^j_{t/\varepsilon^2}, M^j_{t/\varepsilon^2} \rangle = 2\beta^{-1} \alpha_j \| \partial z_j \phi \|^2 t, \quad \text{a.s.}
\]
Proposition

Let \( f \in L^2_\rho \cap C^\infty(X) \) with \( \int_X f \mu_\beta(dx) = 0 \). Then the Poisson equation \( \mathcal{L} u = f \) has a unique smooth mean zero solution \( u \in L^2_\rho \cap C^\infty(X) \).

This follows from:

Proposition

The generator \( \mathcal{L} \) has compact resolvent.

Proof.

Use the estimates on the derivatives of the Markov semigroup and the fact that the resolvent of \( \mathcal{L} \) is given by the Laplace transform of the semigroup.
The homogenization result is proved for $N$ (number or auxiliary processes $z_j$) arbitrary but finite.

Subdiffusive behavior is possible in the limit as $N \to +\infty$.

Consider the "free particle", i.e. set $V(q) \equiv 0$. In this case we can solve the Poisson equation (30) to calculate the diffusion coefficient:

$$D = \beta^{-1} \frac{1}{\sum_{k=1}^{N} \frac{\lambda_k^2}{\alpha_k}}.$$

In the limit as $N \to +\infty$ the diffusion coefficient can become 0:

$$\lim_{N \to +\infty} D = \begin{cases} \beta^{-1} C & \text{if } \sum_{k=1}^{+\infty} \frac{\lambda_k^2}{\alpha_k} = C^{-1}, \\ 0 & \text{if } \sum_{k=1}^{+\infty} \frac{\lambda_k^2}{\alpha_k} = +\infty, \end{cases}$$
Consider the three models

\[ \dot{q} = -V'(q) + \sqrt{2}\dot{W}, \]
(31a)

\[ \ddot{q} = -V'(q) - \gamma \dot{q} + \sqrt{2\gamma} \dot{W}, \]
(31b)

\[ \dot{q} = p, \quad \dot{p} = -V'(q) + \lambda z, \quad \dot{z} = -\alpha z - \lambda p + \sqrt{2\alpha} \dot{W}. \]
(31c)

All these three models can be used in order to sample from the distribution $Z^{-1} e^{-V(q)}$.

Notice that there are no control parameters in (31a), 1 (the friction coefficient) in (31b) and 2 ($\alpha$ and $\lambda$) in (31c).

We would like to choose ($\alpha$, $\lambda$) in (31c) in order to optimize the rate of convergence to equilibrium.

Recent related work by Parrinello et. al (PhD thesis of M. Ceriotti).
When the potential $V(q)$ is quadratic, equations (31c) become linear. The generator $\mathcal{L}$ of a linear SDE

$$dX_t = AX_t \, dt + B \, dW_t$$

has the form

$$\mathcal{L} = \frac{1}{2} \text{Tr} \left( QD^2 \right) + \langle Bx, \nabla \rangle$$

(32)

where $A, B \in \mathbb{R}^{n \times n}$, $D^2$ denotes the Hessian and $Q = BB^T$.

$Q$ can be degenerate (e.g. Langevin, GLE).

The spectrum of the generator of a linear SDE in $L^p_\mu$ has been calculated in Metafune, Pallara and Priola, J. Func. Analysis 196 (2002), pp. 40-60. See also L. Lorenzi and M. Bertoldi, Analytical Methods for Markov Semigroups.

For all $p > 1$ the spectrum consists of integer linear combinations of the drift matrix. It is independent of the diffusion matrix.
The generator of the Langevin SDE in a quadratic potential can be written in the form

$$
\mathcal{L} = -\gamma a^+ a^- - \omega_0 (b^+ a^- - a^+ b^-).
$$

(33)

We can find a change of variables that transforms this operator to the Schrödinger operator for the two-dimensional harmonic oscillator (Risken 1984):

$$
\mathcal{L} = -\lambda_1 c^+ c^- - \lambda_2 d^+ d^-,
$$

(34)

where $\lambda_1, \lambda_2$ are the eigenvalues of the drift matrix.

The eigenvalues of $\mathcal{L}$ consist of integer linear combinations of the eigenvalues of the drift matrix. The eigenfunctions are Hermite polynomials.
- The spectrum of quadratic pseudodifferential hypoelliptic operators can be computed explicitly and very detailed information on the rate of convergence to equilibrium can be obtained (joint work with K. Pravda-Starov and M. Ottobre).

\[
\frac{\partial u}{\partial t}(t, x) + q^w(x, D_x)u(t, x) = 0, \quad u(t, x)|_{t=0} = u_0 \in L^2(\mathbb{R}^n),
\]

where

\[
q^w(x, D_x)u(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^{2n}} e^{i(x-y)\cdot \xi} q\left(\frac{x+y}{2}, \xi\right)u(y)dyd\xi,
\]

and \(q(x, \xi)\) is a complex valued quadratic form.

- The computation of the spectrum of the generator of a linear SDE follows as a particular case of this result.
If we study the spectrum of (32) in $L^p$ spaces weighted by the invariant measure of the SDE, then the spectrum becomes independent of the diffusion matrix for all $p > 1$.

The calculation of the spectrum reduces to the calculation of the eigenvalues of the drift matrix $B$.

The calculation of the spectrum requires the solution of an algebraic equation of $N + 2$ degree, where $N$ is the number of additional OU processes in (31c).
Figure: Spectral gap as a function of $\alpha$ and $\lambda$. 
Figure: Spectral gap as a function of $\lambda$ with $\gamma = \frac{\lambda^2}{\alpha}$ fixed.


