ASYMPTOTIC ANALYSIS FOR THE GENERALIZED LANGEVIN EQUATION

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- Goal: study of qualitative properties of solutions to the Generalized Langevin equation (GLE) in $\mathbb{R}^d$

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

- 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)

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

- Here β 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 assosicated Markov semigroup.
  - Homogenization theorem when $V(q)$ is periodic, estimates on the diffusion coefficient, subdiffusive phenomena.
  - Convergence to the (Markovian) Langevin dynamics.

- 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

$$H(Q,P;q,p) = H_{BP}(Q,P) + H_{HB}(q,p) + H_I(Q,q), \tag{3}$$

- $\{Q, P\}$ 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.

- See, e.g. Givon, Kupferman, Stuart, Nonlin, 17, 2004, pp R55-R127 or Cortes, West, Lindenberg, J. Chem. Phys. **82**(6) 1985 pp. 2708–2717.
- Consider a harmonic heat bath and of linear coupling:

$$H(Q_N, P_N, q, p) = \frac{P_N^2}{2} + V(Q_N) + \sum_{n=1}^{N} \frac{p_n^2}{2m_n} + \frac{1}{2}k_n(q_n - \lambda Q_N)^2. \quad (4$$

- 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 $\{Q_0, P_0\}$:

$$\mu_\beta(dpdq) = Z^{-1} e^{-\beta H(q,p)} \, dqdp, \tag{5}$$

where β is the inverse temperature.

- In order to choose the initial conditions according to $\mu_\beta(dpdq)$ we can take

$$q_n(0) = \lambda Q_0 + \sqrt{\beta^{-1} k_n^{-1}}\xi_n, \quad p_n(0) = \sqrt{m_n \beta^{-1}}\eta_n, \qquad (6)$$

where the ξ_n η_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:

$$\ddot{Q}_N + V'(Q_N) = \sum_{n=1}^{N} k_n(\lambda q_n - \lambda^2 Q_N), \qquad (7a)$$

$$\ddot{q}_n + \omega_n^2(q_n - \lambda Q_N) = 0, \quad n = 1, \dots N, \qquad (7b)$$

where $\omega_n^2 = k_n/m_n$, which is taken to be a random variable.

- We solve (7b) and substitute this in equation (7a) 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 with different memory kernels $R(t)$ and noise processes $F(t)$:

$$\ddot{Q} = -V'(Q) - \lambda^2 \int_0^t \gamma(t-s)\dot{Q}(s)\,ds + \lambda F(t). \tag{8}$$

- The parameter λ measures the strength of the coupling between the Brownian particle and the heat bath.

- 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

$$f^2(\omega) = \frac{2\alpha/\pi}{\alpha^2+\omega^2} \tag{9}$$

- 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:

$$\frac{dF}{dt} = -\alpha F + \sqrt{2\beta^{-1}\alpha}\frac{dW}{dt}, \quad F(0) \sim \mathcal{N}(0, \beta^{-1}). \tag{10}$$

- We can rewrite (8) with an exponential memory kernel as a system of SDEs:

$$\frac{dQ}{dt} = P, \tag{11a}$$

$$\frac{dP}{dt} = -V'(Q) + \lambda Z, \tag{11b}$$

$$\frac{dZ}{dt} = -\alpha Z - \lambda P + \sqrt{2\alpha\beta^{-1}}\frac{dW}{dt}, \tag{11c}$$

- 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.

- See L. Rey-Bellet, *Open classical systems*, in Lecture Notes in Math., 1881, Springer, Berlin, 2006 and the references therein.
- 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.

$$\partial_t^2 \phi(t,x) = \partial_x^2 \phi(t,x). \tag{12}$$

- The Hamiltonian of this system is

$$\mathcal{H}_{HB}(\phi,\pi) = \int \left(|\partial_x \phi|^2 + |\pi(x)|^2 \right). \tag{13}$$

- $\pi(x)$ 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 β.

- We assume that the coupling between the particle and the field is linear (dipole approximation):

$$H_I(q,\phi) = \lambda q \int \partial_x \phi(x) \rho(x) \, dx. \tag{14}$$

- The full Hamiltonian is

$$H(q,p,\phi,\pi) = H_{BP}(p,q) + \mathcal{H}(\phi,\pi) + \lambda q \int \rho(x) \partial_q \phi(x) \, dx. \tag{15}$$

- By integrating out the heat bath variables we obtain the GLE

$$\ddot{q} = -\partial_q V(q) - \lambda^2 \int_0^t \gamma(t-s) \dot{q}(s) \, ds + \lambda F(t), \tag{16}$$

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

$$\langle F(t) F(s) \rangle = \beta^{-1} \gamma(t-s) = \int |\widehat{\rho}(k)|^2 e^{ik(t-s)} \, dk,$$

- Notice that the spectral density of the autocorrelation function of the noise process is the square of the Fourier trannsform of the density $\rho(x)$ which controls the coupling between the particle and the heat bath.
- The GLE (16) is equivalent to the original infinite dimensional Hamiltonian system with random initial conditions.
- Proving ergodicity, convergence to equilibrium etc for (16) implies ergodicity and convergence to equilibrium for the "particle + heat bath" system.

- Ergodic properties of (16) 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

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

- 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 (16) 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 (16) 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 can be constructed as solutions of linear stochastic differential equations.
- Assume that $|\widehat{\rho}(k)|^2 = \frac{1}{|p(k)|^2}$ 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 $|\widehat{\rho}(k)|^2$ 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 (16) is equivalent to

$$\begin{aligned}
\frac{dq}{dt} &= p, \\
\frac{dp}{dt} &= -V'(q) + \lambda z, \\
\frac{dz}{dt} &= -\alpha z - \lambda p + \sqrt{2\alpha\beta^{-1}}\frac{dW}{dt}.
\end{aligned}$$

- We will consider the GLE

$$\ddot{q} = -V'(q) - \int_0^t \gamma(t-s)\dot{q}\, ds + F(t) \tag{18}$$

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

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

- We will consider the case where the memory kernel is given by the sum of exponentials:

$$\gamma(t) = \sum_{j=1}^{N} \lambda_j^2 e^{-\alpha_j |t|}, \tag{19}$$

where $\lambda_j > 0$, $j = 1, \dots, N$ are coupling constants.

- Under this assumption (18) is equivalent to the $N+2$-dimensional Markovian system

$$
\begin{aligned}
dq &= p\,dt, && (20a)\\
dp &= -V'(q)\,dt + \sum_{j=1}^{N} \lambda_j z_j\,dt, && (20b)\\
dz_j &= -\alpha_j z_j\,dt - \lambda_j p\,dt + \sqrt{2\alpha_j \beta^{-1}}\,dW_j, && (20c)
\end{aligned}
$$

- for $j = 1, \dots, N$ and where $q(0) = q_0$, $p(0) = p_0$ and $z_j \sim \mathcal{N}(0, \beta^{-1})$.

- It is more customary in non-equilibrium statistical mechanics to approximate the Laplace transform of the memory kernel through a truncated continued fraction expansion (Mori's method, 1965).
- This approximation leads to a system of SDEs which is slightly different than (20).
- This system can be transformed to (20) through an orthogonal transformation.
- The coefficients $\{\alpha_j, \lambda_j\}_{j=1}^N$ can be obtained, in principle, from the "microscopic dynamics".
- The Markovian finite dimensional stochastic system (20) is more amenable to analysis than the original infinite dimensional GLE (16). We can study, e.g., the rate of convergence to equilibrium, estimates on the derivatives of the Markov semigroup, homogenization (central limit theorem) results, asymptotic limits etc.

- The Process $\{q(t), p(t), z_1(t), \dots z_N(t)\}$ is Markovian with generator

$$-\mathcal{L} = p\partial_q - V'(q)\partial_p + \left(\sum_{j=1}^{N} \lambda_j z_j\right)\partial_p + \sum_{j=1}^{N}\left(-\alpha_j z_j \partial_{z_j} - \lambda_j p \partial_{z_j} + \beta^{-1}\alpha_j \partial_{z_j}^2\right). \quad (21)$$

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

- Invariant distributions are solutions to the stationary Fokker-Planck equation

$$\mathcal{L}^* \rho = 0.$$

- A solution to this equation is

$$\rho_\beta(q, p, \mathbf{z}) = \frac{1}{Z} e^{-\beta(H(q,p) + \frac{1}{2}\|\mathbf{z}\|^2)}, \qquad (22)$$

- where $\mathbf{z} := \{z_1, \dots z_N\}$.
- Notice that ρ_β is independent of the coefficients $\{\alpha_j, \lambda_j\}_{j=1}^N$.
- The invariant measure $\mu_\beta(dq, dp, d\mathbf{z}) = \rho_\beta(q, p, \mathbf{z}) dq dp d\mathbf{z}$ is unique.
- This follows from Markov chain-type arguments, together with the hypoellipticity of the generator $\mathcal{L}$ (minorization condition + Lypunov function). L. Rey-Bellet and L. Thomas Comm. Math. Phys. 225 (2002), no. 2, 305–329.

- The right function space to study the Markov process $x(t) := \{q(t), p(q), \mathbf{z}(t)\}$ is the weighted L^2 space $L^2_\rho := L^2(\mathbb{R}^{2+N}; \mu_\beta(dqdpd\mathbf{z}))$. 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_ρ-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

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

- 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 hypocercivity 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 λ.

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

$$\|h\|_{\mathcal{H}^1}^2 = \|h\|^2 + \sum_{j=0}^{N_c} \|C_j h\|^2.$$

- Set $N = 1$, $\alpha = \lambda = \beta = 1$. The first two commutators are

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

- 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 $x(t) = \{q(t), p(t), \mathbf{z}(t)\} \in \mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$. Then there exist constants C, $\lambda > 0$ such that

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

Remark

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

$$H(\rho_t|\rho_\infty) \leq Ce^{-\lambda t} H(\rho_0|\rho_\infty),$$

where ρ_t is the law of the process at time t and $H(f|h) = \int f \log(f/h)$.

2. *We can obtain estimates on the spectral gap as a function of the parameters $\{\alpha_j, \lambda_j\}_{j=1}^N$.*

Convergence to Equilibrium

- Set $\beta = 1$ and consider the case $N = 1$. Define the creation and annihilation operators

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

- The generator of the process $\mathbf{x}(t) = \{q(t), p(t), z(t)\}$ 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 $P_t = e^{-\mathcal{L}t}$ 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 estimates on the derivatives of P_t using an appropriate Lyapunov function. See G.P. and Hairer, J. Stat. Phys. **131**(1) (2008), 175–202 and F. Herau J. Funct. Anal. **244**(1) (2007), 95–118.
- It is possible to prove similar estimates for the GLE.

Theorem

The Markov semigroup $P_t = e^{-t\mathcal{L}}$ satisfies the bounds

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

Proof.

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

$$\begin{aligned} F(t) &= a_0 t\|Au\|^2 + a_1 t^3 \|C_1 u\|^2 + a_2 t^5 \|C_2 u\|^2 \\ &\quad + + b_0 t^2 (Au, C_1 u) + t^4 b_1 (C_1 u, C_2 u) + b_2 \|u\|^2 . \end{aligned}$$

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 $C_j^{\sharp} e^{-L^{\flat} t}$ where $\sharp, \flat$ are either nothing or $\star$ (i.e. the $\mathcal{L}^2_{\rho}$–adjoint).*
- *An appropriate Lyapunov function can be constructed for more general hypocoercive operators of the form $\mathcal{L} = A^{\star} A + B$.*

- Consider the Smoluchowski and Langevin dynamics

$$\dot{q} = -V'(q) + \sqrt{2\beta^{-1}}\dot{W} \tag{26}$$

and

$$\ddot{q} = -V'(q) - \gamma\dot{q} + \sqrt{2\gamma\beta^{-1}}\dot{W} \tag{27}$$

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_{γ}, 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))

$$\frac{D^{\star}}{\gamma} \leq D_{\gamma} \leq \frac{D_V}{\gamma}, \quad \gamma \in (0, +\infty). \tag{28}$$

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

Theorem

Let $\{q(t), p(t), \mathbf{z}(t)\}$ *on* $\mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$ *be the solution of* (20) *with* $V(q) \in C^\infty(\mathbb{T})$ *with stationary initial conditions. Then the rescaled process* $q^\epsilon(t) := \epsilon q(t/\epsilon^2)$ *converges weakly on* $C([0,T], \mathbb{R})$ *to a Brownian motion with diffusion coefficient* D *given by*

$$D = \int_0^{+\infty} \langle p(t)p(0) \rangle \, dt = \beta^{-1} \sum_{j=1}^N \alpha_j^{-1} \|\partial_{z_j} \phi\|^2 \tag{29}$$

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

$$\mathcal{L}\phi = p, \tag{30}$$

on $\mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$*. Furthermore, we have the estimates* $0 < D \leq \frac{4}{\beta} \sum_{i=1}^N \frac{\alpha_i}{\lambda_i^2}$.

Proof.

- Prove existence and uniqueness and estimates for (30), and use the Martingale CLT:
  - Apply Itô's formula to $\phi(x(t))$ to obtain

$$\begin{aligned} q^\epsilon(t) &= \epsilon q(0) - \epsilon\big(\phi(x(t/\epsilon^2)) - \phi(x(0))\big) \\ &\quad + \sum_{j=1}^{N} \sqrt{2\beta^{-1}\alpha_j \epsilon} \int_0^{t/\epsilon^2} \partial_{z_j}\phi \, dW_j \\ &=: R_\epsilon(t) + \epsilon \sum_{j=1}^{N} M^j_{t/\epsilon^2}. \end{aligned}$$

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

$$\lim_{\epsilon \to 0} \langle M^j_{t/\epsilon^2}, M^j_{t/\epsilon^2} \rangle = 2\beta^{-1}\alpha_j \|\partial_{z_j}\phi\|^2 \, t, \quad \text{a.s.}$$

$\square$

- 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:

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

- Consider the Langevin equation (27). When $\gamma \gg 1$, the momentum "thermalizes" much faster than the position and the dynamics can be described by the Smoluchowski equation, after elimination of the momentum variable.
- Similarly, we can obtain the Langevin equation (and a formula for the friction coefficient) from the GLE, after appropriate rescaling.

- Rescale $\lambda_j \to \frac{\lambda_j}{\epsilon}$, $\alpha_j \to \frac{\alpha_j}{\epsilon^2}$ (i.e. consider the noise process $F^\epsilon(t) = \frac{1}{\epsilon}F(t/\epsilon^2)$.)
- Eqn. (20) becomes

$$
\begin{aligned}
dq^\epsilon &= p^\epsilon \, dt, && \text{(31a)} \\
dp^\epsilon &= -V'(q^\epsilon)\, dt + \sum_{j=1}^{N} \frac{\lambda_j}{\epsilon} z_j^\epsilon \, dt, && \text{(31b)} \\
dz_j^\epsilon &= -\frac{\alpha_j}{\epsilon^2} z_j^\epsilon \, dt - \frac{\lambda_j}{\epsilon} p^\epsilon \, dt + \sqrt{\frac{2\alpha_j \beta^{-1}}{\epsilon^2}}\, dW_j, && \text{(31c)}
\end{aligned}
$$

- In the limit as $\epsilon \to 0$ we obtain a closed equation for $q^\epsilon(t)$, $p^\epsilon(t)$.

Proposition

Let $\{q^\epsilon(t), p^\epsilon(t), \mathbf{z}^\epsilon(t)\}$ on $\mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$ be the solution of (31) with $V(q) \in C^\infty(\mathbb{T})$ with stationary initial conditions. Then $\{q^\epsilon(t), p^\epsilon(t)\}$ converge strongly to the solution of the Langevin equation

$$dq = p\,dt, \quad dp = -V'(q)\,dt - \gamma p\,dt + \sqrt{2\gamma\beta^{-1}}dW, \tag{32}$$

where the friction coefficient is given by the formula

$$\gamma = \int_0^\infty \gamma(t)\,dt = \sum_{j=1}^N \frac{\lambda_j^2}{\alpha_j}. \tag{33}$$

- We can study formally this limit for the diffusion coefficient. Let D^{ϵ}_{GLE} denote the diffusion coefficient for the rescaled GLE (31). Then, when $\epsilon \ll 1$ (and for $N = 1$)

$$D^{\epsilon}_{GLE} = D_{\gamma} + \epsilon^2 \int_{\mathbb{T}\times\mathbb{R}} \psi p \rho_{\beta}(p, q) \, dpdq + \mathcal{O}(\epsilon^3),$$

- where D_{γ} is the diffusion coefficient for the Langevin equation, $\rho_{\beta}(p, q) = \frac{1}{Z} e^{-\beta H(p,q)}$, and ψ is the unique (up to constants) solution of

$$-\mathcal{L}_L \psi = \frac{\gamma}{\alpha} c^{+} b^{-} \phi.$$

- We don't know whether $D_{GLE} \leq D_{\gamma}$ or not.

- Consider the three models

$$\dot{q} = -V'(q) + \sqrt{2}\dot{W}, \tag{34a}$$
$$\ddot{q} = -V'(q) - \gamma\dot{q} + \sqrt{2\gamma}\dot{W}, \tag{34b}$$
$$\dot{q} = p, \ \dot{p} = -V'(q) + \lambda z, \ \dot{z} = -\alpha z - \lambda p + \sqrt{2\alpha}\dot{W}. \tag{34c}$$

- All these three models can be used in order to sample from $Z^{-1}e^{-V(q)}$.
- Notice that there are not control parameters in (34a), 1 (the friction coefficient) in (34b) and 2 (α and λ) in (34c).
- We would like to choose (α, λ) in (34c) in order to optimize the rate of convergence to equilibrium.
- Recent related work by Parrinello et. al (PhD thesis of M. Ceriotti).

- For quadratic potentials we can compute the spectrum of the generator of (34c) and obtain very detailed information on the rate of convergence to equilibrium (joint work with K. Pravda-Starov and M. Ottobre).
- Formulas for the spectrum have also been obtained in Metafune, Pallara and Priola, J. Func. Analysis 196 (2002), pp. 40-60.
- 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 (34c).

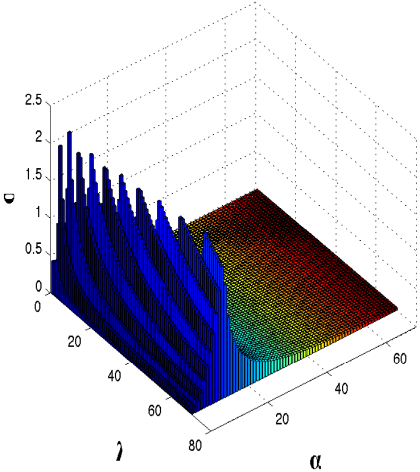

Figure: Spectral gap as a function of α and λ.

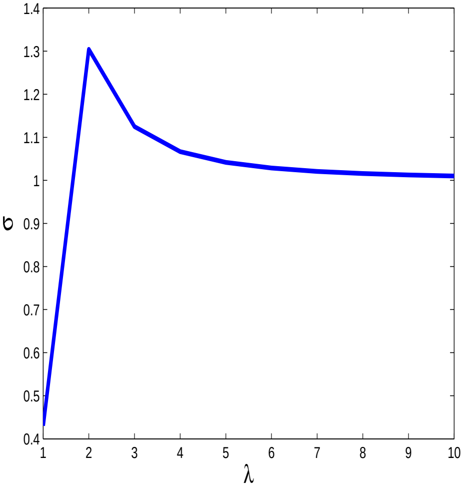

Figure: Spectral gap as a function of λ with $\gamma = \frac{\lambda^2}{\alpha}$ fixed.

- *Asymptotic Analysis of the Green-Kubo Formula* (G.P., IMA Applied Mathematics, to appear 2010)
- *Asymptotic Analysis of the Generalized Langevin Equation*, (M. Ottobre and G. P.), Submitted to Nonlinearity (2010).
- *Exponential Return to Equilibrium for Hypoeliptic Quadratic Systems* (M. Ottobre, G.P and K. Pravda-Starov, preprint 2010.
- *From ballistic to diffusive behavior in periodic potentials* (M. Hairer and G.P.), J. Stat. Phys. 131(1) 175-202 (2008).
- *Periodic homogenization for hypoelliptic diffusions* (M. Hairer and G.P.), J. Stat. Phys. 117 no. 1/2 (2004), 261-279.
- *Multiscale Methods: Homogenization and Averaging* (G.P. and A.M. Stuart), Vol. 53 in Springer series *Texts in Applied Mathematics*.