ASYMPTOTIC PROBLEMS FOR NON-MARKOVIAN LANGEVIN EQUATIONS

G.A. Pavliotis
Department of Mathematics Imperial College London
Joint Work with M. Ottobre (IC) and M. Hairer (Warwick/Courant)

SPDE09 TU DARMSTADT
27/08/09

Contents

- Particle coupled to a heat bath models and the Generalized Langevin Equation (GLE).
- The Markovian Approximation.
- Analysis of the GLE: Ergodicity, homogenization and white noise limits.
- Weak friction asymptotics for the Langevin equation.

- 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

$$H(Q,P;q,p) = H_{BP}(Q,P) + H_{HB}(q,p) + H_I(Q,q), \qquad (1)$$

- $\{Q,\ P\}$ 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 (1) are a system of ODEs with random initial conditions.
- By integrating out the heat bath variables we can obtain a "stochastic differential equation".
- This equation is non-Markovian.

- Consider a harmonic heat bath and of linear coupling:

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

- 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 $\{Q_0,\ P_0\}$:

$$\mu_\beta(dpdq) = Z^{-1} e^{-\beta H(q,p)}\, dqdp, \quad (3)$$

where β is the inverse temperature.

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

$$q_n(0) = \lambda Q_0 + \sqrt{\beta^{-1} k_n^{-1}}\xi_n, \quad p_n(0) = \sqrt{m_n \beta^{-1}}\eta_n, \qquad (4)$$

  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:

$$\begin{aligned} \ddot{Q}_N + V'(Q_N) &= \sum_{n=1}^{N} k_n(\lambda q_n - \lambda^2 Q_N), & (5a) \\ \ddot{q}_n + \omega_n^2(q_n - \lambda Q_N) &= 0, \quad n = 1, \ldots N, & (5b) \end{aligned}$$

  where $\omega_n^2 = k_n/m_n$.

The solution of (5b) is

$$\begin{aligned} q_n(t) &= q_n(0)\cos(\omega_n t) + \frac{p_n(0)}{m_n\omega_n}\sin(\omega_n t) + \lambda Q_N(t) \\ &\quad -\lambda Q_N(0)\cos(\omega_n t) - \lambda\int_0^t \cos(\omega_n(t-s))\dot{Q}_N(s)\,ds. \end{aligned}$$

We substitute this in equation (5a) to obtain the GLE

$$\ddot{Q}_N = -V'(Q_N) - \lambda^2\int_0^t R_N(t-s)\dot{Q}_N(s)\,ds + \lambda F_N(t), \tag{6}$$

where the **memory kernel** is

$$R_N(t) = \sum_{n=1}^{N} k_n \cos(\omega_n t) \tag{7}$$

and the **noise process** is

$$F_N(t) = \sum_{n=1}^{N} k_n\left(q_n(0) - \lambda Q_0\right)\cos(\omega_n t) + \frac{k_n p_n(0)}{m_n\omega_n}\sin(\omega_n t)$$

1. The noise $F(t)$ is a mean zero Gaussian process.
2. The noisy and random term are related through the **fluctuation-dissipation theorem**:

$$\begin{aligned}\langle F_N(t)F_N(s)\rangle &= \beta^{-1}\sum_{n=1}^{N} k_n\big(\cos(\omega_n t)\cos(\omega_n s) \\ &\quad + \sin(\omega_n t)\sin(\omega_n s)\big) \\ &= \beta^{-1}R_N(t-s). \end{aligned} \tag{9}$$

3. The parameter λ measures the strength of the coupling between the Brownian particle and the heat bath.
4. By choosing the frequencies ω_n and spring constants $k_n(\omega)$ of the heat bath particles appropriately we can pass to the limit as $N \to +\infty$ and obtain the GLE with different memory kernels $R(t)$ and noise processes $F(t)$.

- 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 $\zeta_1 \sim \mathcal{U}(0,1)$. Furthermore, we choose the spring constants according to

$$k_n = \frac{f^2(\omega_n)}{N^{2b}},$$

- where the function $f(\omega_n)$ decays sufficiently fast at infinity.
- We can rewrite the dissipation and noise terms in the form

$$R_N(t) = \sum_{n=1}^{N} f^2(\omega_n) \cos(\omega_n t)\, \Delta\omega$$

and

$$F_N(t) = \sum_{n=1}^{N} f(\omega_n) \left(\xi_n \cos(\omega_n t) + \eta_n \sin(\omega_n t)\right) \sqrt{\Delta\omega},$$

- where $\Delta\omega = N^a/N$.

- Using now properties of Fourier series with random coefficients/frequencies and of weak convergence of probability measures we can pass to the limit:

$$R_N(t) \rightarrow R(t) \quad \text{in} \;\; L^1[0, T],$$

- for a.a. $\{\zeta_n\}_{n=1}^{\infty}$ and

$$F_N(t) \rightarrow F(t) \quad \text{weakly in} \;\; C([0, T], \mathbb{R}).$$

- The time $T > 0$ if finite but arbitrary.
- The limiting kernel and noise satisfy the fluctuation-dissipation theorem (9):

$$\langle F(t)F(s) \rangle = \beta^{-1} R(t-s). \tag{10}$$

- $Q_N(t)$, the solution of (6) converges weakly to the solution of the limiting GLE

$$\ddot{Q} = -V'(Q) - \lambda^2 \int_0^t R(t-s)\dot{Q}(s)\,ds + \lambda F(t). \tag{11}$$

- The properties of the limiting dissipation and noise are determined by the function $f(\omega)$.
- Ex: Consider the Lorentzian function

$$f^2(\omega) = \frac{2\alpha/\pi}{\alpha^2 + \omega^2} \tag{12}$$

- with $\alpha > 0$. Then

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

- The noise process $F(t)$ is a mean zero stationary Gaussian process with continuous paths and, from (10), exponential correlation function:

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

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

$$\frac{dF}{dt} = -\alpha F + \sqrt{2\beta^{-1}\alpha}\frac{dW}{dt}, \tag{13}$$

with $F(0) \sim \mathcal{N}(0, \beta^{-1})$.

- The GLE (11) becomes

$$\ddot{Q} = -V'(Q) - \lambda^2 \int_0^t e^{-\alpha|t-s|} \dot{Q}(s)\, ds + \lambda^2 F(t), \qquad (14)$$

- where $F(t)$ is the OU process (13).

- We can rewrite (14) as a system of SDEs:

$$
\begin{aligned}
\frac{dQ}{dt} &= P, && (15a)\\
\frac{dP}{dt} &= -V'(Q) + \lambda Z, && (15b)\\
\frac{dZ}{dt} &= -\alpha Z - \lambda P + \sqrt{2\alpha\beta^{-1}}\frac{dW}{dt}, && (15c)
\end{aligned}
$$

- 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.

- When studying the Kac-Zwanzing model we considered a one dimensional Hamiltonian system coupled to a finite dimensional Hamiltonian system with random initial conditions (the harmonic heat bath) and then passed to the theromdynamic limit $N \to \infty$.
- We can also consider a small Hamiltonian system coupled to its environment which we model as an infinite dimensional Hamiltonian system with random initial conditions.

- The environment is modeled through a classical linear field theory (i.e. the wave equation)

$$\partial_t^2 \phi(t,x) = \partial_x^2 \phi(t,x). \tag{16}$$

- The Hamiltonian of this system is

$$\mathcal{H}_{HB}(\phi,\pi) = \int \left(|\partial_x \phi|^2 + |\pi(x)|^2 \right). \tag{17}$$

- $\pi(x)$ 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:

$$H_I(q, \phi) = \lambda q \int \partial_q \phi(x) \rho(x) \, dx. \tag{18}$$

- The full Hamiltonian is

$$H(q, p, \phi, \pi) = H_{BP}(p, q) + \mathcal{H}(\phi, \pi) + \lambda q \int \rho(x) \phi(x) \, dx + \frac{\lambda^2}{6} |q|^2. \tag{19}$$

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

$$\ddot{q} = -\nabla V_{eff}(q) - \int_0^t R(t-s) \dot{q}(s) + F(t), \tag{20}$$

- where

$$D(t) = -\dot{C}(t) = \frac{1}{3} \int |\widehat{\rho}(k)|^2 |k| \sin(|k| t) dk.$$

- Ergodic properties of (20) were studied by V. Jaksic and C.-A. Pillet.
- 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

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

- No information about the rate of convergence to equilibrium.

- Under appropriate assumptions on the coupling function $\rho(x)$ the GLE (20) is equivalent to a Markovian process in an extended phase space. Assume that

$$|\widehat{\rho}(k)| = \frac{1}{|p(k)|^2}, \tag{21}$$

- where $p(\cdot)$ is a polynomial with real coefficients and roots in the upper half plane.
- Then (20) can be rewritten as a Markovian system with the addition of a finite number of additional variables.
- For example, when $p(k) \sim (ik + \alpha)$, then (20) 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

$$\ddot{q} = -V'(q) - \int_0^t \gamma(t-s)\dot{q}\, ds + F(t) \qquad (23)$$

- 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:

$$\gamma(t) = \sum_{j=1}^{N} \lambda_j^2 e^{-\alpha_j |t|}, \qquad (24)$$

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

- Under this assumption (23) is equivalent to the $N+2$-dimensional Markovian system

$$
\begin{aligned}
dq &= p\,dt, && \text{(25a)}\\
dp &= -V'(q)\,dt + \sum_{j=1}^{N} \lambda_j z_j\,dt, && \text{(25b)}\\
dz_j &= -\alpha_j z_j\,dt - \lambda_j p\,dt + \sqrt{2\alpha_j \beta^{-1}}\,dW_j, && \text{(25c)}
\end{aligned}
$$

- 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).
- This approximation leads to a system of SDEs which is slightly different than (25).
- This system can be transformed to (25) 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 (25) is more amenable to analysis than the original infinite dimensional GLE (20). 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

$$\mathcal{L} = p\partial_q - V'(q)\partial_p + \left(\sum_{j=1}^N \lambda_j z_j\right)\partial_p + \sum_{j=1}^N \left(-\alpha_j z_j \partial_{z_j} - \lambda_j p \partial_{z_j} + \beta^{-1}\alpha_j \partial^2_{z_j}\right). \quad (26)$$

- 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

$$\rho_\beta(q, p, \mathbf{z}) = \frac{1}{Z} e^{-\beta\left(H(q,p) + \frac{1}{2}\|\mathbf{z}\|^2\right)}, \tag{27}$$

- 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). A similar argument has been used for a related problem by L. Rey-Bellet and L. Thomas.

- 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

$$\mathcal{L} = B - \sum_{j=1}^{N} A_j^* A_j, \tag{28}$$

- 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 generator $\mathcal{L}$ given by (28) is of the form

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

for which C. Villani's theory of **hypocoercivity** applies:

  - Define $C_0 = A,\ C_{j+1} = [C_j, B], j = 0, 1, \dots,\ C_{N_c+1} = 0$ 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

$$\|e^{tL}\|_{\mathcal{H}^1 \to \mathcal{H}^1} = \mathcal{O}(e^{-\lambda t}).$$

  - where

$$\|h\|^2_{\mathcal{H}^1} = \|h\|^2 + \sum_j \|C_j h\|^2.$$

- The basic idea is to use an appropriate "skewed" Hilbert space and the fact hypocoercivity remains invariant under change of norms.

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

$$C_1 = [A, B] = \partial_p \quad \text{and} \quad C_2 = [C_1, B] = \partial_q - \partial_p. \tag{29}$$

- 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

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

Remark

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

$$H(\rho_t|\rho_\infty) \leq H(\rho_0|\rho_\infty),$$

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 $\{\alpha_j, \lambda_j\}_{j=1}^N$.*

Theorem

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

$$\|C_k P_t\|_{L^2_\rho \to L^2_\rho} \leq C\Big(1 + \frac{1}{t^{1+2k}}\Big), \quad k = 0, 1, 2. \tag{30}$$

Proof.

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 nonpositive. □

Theorem

Let $\{q(t), p(t), \mathbf{z}(t)\}$ *on* $\mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$ *be the solution of* (25) *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*

$$D = \beta^{-1} \sum_{j=1}^{N} \alpha_j^{-1} \|\partial_{z_j} \phi\|^2 \tag{31}$$

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

$$-\mathcal{L}\phi = p, \tag{32}$$

on $\mathbb{T} \times \mathbb{R} \times \mathbb{R}^N$*.*

Proof.

- Prove existence and uniqueness and estimates for (32), 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 $\|R_{\epsilon}(t)\| = o(1)$.
  - From the stationarity of the process $x(t)$ we deduce

$$\frac{1}{t}\mathbb{E}\langle M^j_{t/\epsilon^2}, M^j_{t/\epsilon^2}\rangle = 2\beta^{-1}\alpha_j \|\partial_{z_j}\phi\|^2$$

□

- Rescale $\lambda_j \to \frac{\lambda_j}{\epsilon}$, $\alpha_j \to \frac{\alpha_j}{\epsilon^2}$
- Eqn. (25) becomes

$$dq^\epsilon = p^\epsilon \, dt, \tag{33a}$$

$$dp^\epsilon = -V'(q^\epsilon)\, dt + \sum_{j=1}^{N} \frac{\lambda_j}{\epsilon} z_j^\epsilon \, dt, \tag{33b}$$

$$dz_j^\epsilon = -\frac{\alpha_j}{\epsilon^2} z_j^\epsilon \, dt - \frac{\lambda_j}{\epsilon} p^\epsilon \, dt + \sqrt{\frac{2\alpha_j \beta^{-1}}{\epsilon^2}} \, dW_j, \tag{33c}$$

- 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* (33) *with* $V(q) \in C^\infty(\mathbb{T})$ *with stationary initial conditions. Then* $\{q^\epsilon(t), p^\epsilon(t)\}$ *converge weakly to the solution of the Langevin equation*

$$dq = p\,dt, \quad dp = -V'(q)\,dt - \gamma p\,dt + \sqrt{2\gamma\beta^{-1}}\,dW, \tag{34}$$

where the friction coefficient is given by the formula

$$\gamma = \sum_{j=1}^{N} \frac{\lambda_j^2}{\alpha_j}. \tag{35}$$

Remark

It is possible to prove a strong convergence theorem and to obtain error estimates.

- For the Langevin equation (34) is it known that
  - The unique invariant measure is $\mu_\beta = Z^{-1} e^{-\beta H(q,p)}\, dqdp$.
  - The convergence to equilibrium is exponentially fast in relative entropy.
  - The rescaled particle position $q^\epsilon(t)$ converges weakly to $\sqrt{2D_\gamma} W(t)$ where

$$D_\gamma = \int \phi p \mu_\beta \tag{36}$$

  - where $\phi \in L^2(\mathbb{T} \times \mathbb{R}; \mu_\beta)$ is the solution of the Poisson equation

$$-L\phi = p, \tag{37}$$

  - with periodic boundary conditions in q. See Papanicolaou and Varadhan 1985, Kozlov 1989.
- We can obtain more detailed estimates on the weak friction asymptotics of solutions to the Langevin equation.

- We can obtain a two-sided bound on the diffusion coefficient.

Proposition

The diffusion coefficient satisfies the lower and upper bounds

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

with explicit formulas for D^* and D_V. Furthermore,

$$\lim_{\gamma \to 0} \gamma D_\gamma = D^* \quad \textit{and} \quad \lim_{\gamma \to \infty} \gamma D_\gamma = D_V.$$

Remark

- *Both D^* and D_V can be obtained through the solution of a two-point boundary value problem. The results are (period of potential 2π, critical energy $E_0 = 1$):*

$$D^* = \frac{8\pi^2}{Z_\beta \beta} \int_1^{+\infty} \frac{e^{-\beta z}}{S(z)}\, dz \approx \frac{\pi}{2\beta} e^{-2\beta}, \quad \beta \gg 1, \qquad (38)$$

- *and*

$$D_V = \frac{4\pi^2}{\beta Z \widehat{Z}} \approx 2\pi e^{-2\beta}, \quad \beta \gg 1,$$

- *where $Z = \int_{-\pi}^{\pi} \exp(-\beta V(q))\, dq$, $\widehat{Z} = \int_{-\pi}^{\pi} \exp(\beta V(q))\, dq$. (The large β asymptotic results are for $V(q) = -\cos(q)$.)*

- To prove the upper/lower bounds we write the weak formulation of the Poisson equation $-L\phi = p$ and use appropriate test functions:

$$(\mathcal{A}\psi, \phi)_\beta + \gamma\beta^{-1}(\partial_p\psi, \partial_p\phi)_\beta = (\psi, p)_\beta.$$

- The test functions that we use are, essentially, the limits of the solution to the Poisson equation as $\gamma \to 0$ and $\gamma \to +\infty$.
- The upper bound on D_γ is also true in higher dimensions.
- It is not clear that the lower bound is true in arbitrary dimensions and for arbitrary smooth periodic potentials.

- The particle position, appropriately rescaled, converges in the limit as $\gamma \to 0$ to a Brownian motion:

Theorem

Let

$$q^{\gamma}(t) = \gamma^{1+\alpha} q(t/\gamma^{1+2\alpha})$$

and assume stationary initial conditions. Then

$$\lim_{\gamma \to 0} q^{\gamma}(t) = \sqrt{2D^*}\, W(t)$$

for every $\alpha \in \left(\frac{1}{2}, +\infty\right)$, *where* D^* *is the FW diffusion coefficient.*

Remark

1. *This is NOT the CLT rescaling!*
2. *The diffusion coefficient of the limiting process is independent of the exponent α.*
3. *The case $\alpha = 0$ corresponds to the FW rescaling–for which the limiting process is not a Brownian motion. We believe that the result is true for every $\alpha > 0$.*
4. *Similar result for the large γ limit:*

$$\lim_{\gamma \to \infty} \gamma^{-\alpha} q(t\gamma^{1+2\alpha}) = \sqrt{2D_V}\, W(t)$$

5. *weakly on $C([0, T], \mathbb{R})$ for every $\alpha > 0$.*

- For the proof of our results we need to study properties of a singularly perturbed hypoelliptic operator:

$$\mathcal{L} = p\partial_q - \partial_q V(q)\partial_p + \gamma\left(-p\partial_p + \beta^{-1}\partial_p^2\right) =: \mathcal{A} + \gamma\mathcal{L}_0 \quad (39)$$

on $\mathbb{T} \times \mathbb{R}$.

- $\mathcal{A}$ is the (backward) Liouville operator, the generator of the Hamiltonian unitary group and $\mathcal{L}_0$ is the Ornstein-Uhlenbeck operator, the generator of the OU semigroup.
- We need estimates on $\mathcal{L}^{-1}$ (i.e. $e^{\mathcal{L}t}$) valid at $\gamma \ll 1$.
- Notice that $\mathcal{L}^*(\exp(-\beta H)) = 0$. The natural space to work is

$$L^2(\mu_\beta), \quad \mu_\beta(dp\,dq) = Z^{-1}\exp(-\beta H(p,q))\,dp\,dq.$$

- More convenient to work with the rescaled operator

$$L_\gamma = \gamma^{-1}\mathcal{A} + \mathcal{L}_0.$$

Theorem

There exist constants C_1, C_2 *independent of* γ *such that*

$$C_1\|f\| \leq \|L_\gamma^{-1} f\| \leq C_2\|f\| \,, \tag{40}$$

holds for every $\gamma < 1$, *and every* $f \in L^2(\mu_\beta)$ *such that* $\int_{\mathbb{T}\times\mathbb{R}} f \, \mu_\beta(dp\, dq) = 0$. *Let now* $\phi_\gamma \in L^2(\mu_\beta)$, *periodic in* q *with* $\int_{\mathbb{T}\times\mathbb{R}} \phi_\gamma \, \mu_\beta(dp\, dq) = 0$, *be the solution to* $-L_\gamma\phi_\gamma = p$. *Then there exists a constant* C *which is independent of* γ *such that*

$$\|\phi_\gamma\|^2+\|\partial_p\phi_\gamma\|^2+\|\partial_q\phi_\gamma\|^2+\gamma\Big(\|\partial_p^2\phi_\gamma\|^2+\|\partial_p\partial_q\phi_\gamma\|^2+\|\partial_q^2\phi_\gamma\|^2\Big) \leq C.$$

Furthermore, $\partial_p\phi_\gamma$ *is an element of* $L^4(\mu_\beta)$ *and*

$$\|\partial_p\phi_\gamma\|_{L^4(\mu_\beta)} \leq C(1+\gamma^{-1/4}) \,. \tag{41}$$

- The proof of Theorem 5 is based on the commutator techniques of C. Villani (hypocoercivity): work in an appropriately "skewed" Hilbert space and obtain estimates on the vector fields

$$
\begin{aligned}
A &= \beta^{-1/2}\partial_p\,, \quad A^* = -\beta^{-1/2}\partial_p + \beta^{1/2}p\,, \\
B &= p\partial_q - V'(q)\partial_p\,, \quad B^* = -B\,,
\end{aligned}
$$

- (notice that $L_\gamma = -A^*A + \gamma^{-1}B$) and their commutators

$$
\begin{aligned}
&\widehat{C} = [A,B] = \beta^{-1/2}\partial_q\,, \\
&R = [[A,B],B] = -\beta^{-1/2}V''(q)\partial_p = -V''(q)A\,.
\end{aligned}
$$

- The Hilbert space is defined though the bilinear form

$$
\langle\langle f,f\rangle\rangle = a\langle f,f\rangle + \gamma\Big(b\langle Af,Af\rangle + 2\,\Re\langle Af,\widehat{C}f\rangle + b\langle \widehat{C}f,\widehat{C}f\rangle\Big)\,.
$$

- The upper bound on (40) follows from the corresponding bound on the semigroup:

$$\|e^{L_\gamma t} f\| \leq C e^{-\alpha t} \|f\|, \quad \int_{\mathbb{T}\times\mathbb{R}} f \, \mu_\beta(dpdq) = 0.$$

- The lower bound follows from the formula

$$\|L_\gamma^{-1}\| = \left(\inf_{f \in \mathcal{D}(L_\gamma) \, : \, \langle 1, f \rangle = 0} \frac{\|L_\gamma f\|}{\|f\|} \right)^{-1}$$

- and the use of the Hamiltonian as as a test function.
- For the $L^4(\mu)$–estimate we need to work on the scale of spaces

$$L^2(\mu_\delta), \quad \mu_\delta = Z_\delta^{-1} \exp(-\delta H(p,q)) \, dp \, dq, \quad \delta \in (0, \beta]$$

Proof of Theorem 4

- We apply Itô's formula to $\phi_\gamma(p(t), q(t))$:

$$
\begin{aligned}
q^\gamma(t) &= \gamma^{1+\alpha} q(0) - \gamma^\alpha \Big(\phi_\gamma(p(t/\gamma^{1+2\alpha}), q(t/\gamma^{1+2\alpha})) \\
&\quad - \phi_\gamma(p(0), q(0)) \Big) \\
&\quad + \sqrt{2\gamma^{1+2\alpha}\beta^{-1}} \int_0^{t/\gamma^{1+2\alpha}} \partial_p \phi_\gamma(p(s), q(s))\, dW(s) \\
&=: \gamma^{1+\alpha} q(0) + R^\gamma + M^\gamma,
\end{aligned}
$$

- Our estimates on ϕ_γ imply that

$$R^\gamma = o(1).$$

- We need to prove that $\lim_{\gamma \to 0} M^\gamma(t) = \sqrt{2D^*}\, W(t)$.

- According to the Martingale CLT, it is enough to prove convergence of the quadratic variation to $2D^* t$ in $L^1(\mu)$. Let

$$\bar{f}_\gamma := 2\beta^{-1}\|\partial_p \phi_\gamma\|^2 \to D^*.$$

- We have that

$$\begin{aligned}
\mathbb{E}\left(\sup_{s\in[0,t/\gamma^{1+2\alpha}]} |\langle M^\gamma\rangle_s - \bar{f}_\gamma s|\right) &\leq C\left(\|\partial_p\phi_\gamma\|^2_{L^4(\mu)}\gamma^\alpha \tau^{-1/2}\right. \\
&\quad \left. + \|\partial_p\phi_\gamma\|^2 \tau\right) \\
&\leq C\left(\gamma^{\alpha-1/2}\tau^{-1/2} + \tau\right).
\end{aligned}$$

- where $\tau = \gamma^\zeta$, $\zeta > 0$ arbitrarily small. Convergence follows since $\alpha > 1/2$.

- *Asymptotic Analysis of the Generalized Langevin Equation*, (M. Ottobre and G. P.), preprint (2009).
- *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.
- *Diffusive Transport in Periodic Potentials: Underdamped dynamics* (G.P. and T. Vogiannou), Fluct. Noise Lett., 8(2) L155-L173 (2008).
- *Homogenization for Inertial Particles in a Random Flow.* (With A.M. Stuart and K.C. Zygalakis), Comm. Math. Sci., 5(3) 507-531 (2007).
- *Multiscale Methods: Homogenization and Averaging* (G.P. and A.M. Stuart), Vol. 53 in Springer series *Texts in Applied Mathematics*.