Stochastic Hamiltonian systems with Lévy noises and singular potentials

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Based on on-going work with Jianhai Bao and Rongjuan Fang

the 17th Workshop on Markov Processes and Related Topics

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Stochastic Hamiltonian system

$$\begin{cases} \mathrm{d}X_t = Y_t \, \mathrm{d}t \\ \mathrm{d}Y_t = (-\nabla V(X_t) - Y_t) \, \mathrm{d}t + \sqrt{2} \, \mathrm{d}B_t. \end{cases}$$

- Invariant probability measure

$$\mu(dx, dy) = e^{-V(x)} \, dx \times e^{-|y|^2/2} \, dy.$$

- Three approaches:
  - Lyapunov function: Wu ('01); Mattingly-Stuart-Higham ('02). Adding a $c\langle x, y\rangle$ term into the Hamiltonian $H(x, y) = V(x) + |y|^2/2$.
  - Hypocoercivity: Villani ('09); Grothaus-Wang ('19). Functional inequalities for the symmetric and antisymmetric parts of the generator.
  - Coupling: Eberle-Guillin-Zimmer ('19). Reflection coupling with aid of coupling function (Chen-Wang).

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Why stochastic Hamiltonian system is important?

$$\begin{cases} \mathrm{d}X_t = Y_t \, \mathrm{d}t \\ \mathrm{d}Y_t = (-\nabla V(X_t) - Y_t) \, \mathrm{d}t + \sqrt{2} \, \mathrm{d}B_t. \end{cases}$$

- PDE: kinetic Fokker-Planck equation
- Probability: stochastic algorithms
  - Invariant measure

$$\mu(dx, dy) = C_1 e^{-V(x)} \, dx \times C_2 e^{-|y|^2/2} \, dy.$$

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Stochastic Hamiltonian system with singular potentials

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- $(\mathbf{X}_t, \mathbf{Y}_t)_{t\geq 0}$ takes values in $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$, and the potential energy is given by

$$V(\mathbf{x}) = \sum_{i=1}^N W(x_i) + \frac{1}{2N} \sum_{1\leq i\neq j\leq N} K(x_i - x_j).$$

- $W : \mathbb{R}^d \to \mathbb{R}$ is an external energy, growing fast enough at infinity, and satisfies $\langle \nabla W(x), x\rangle \asymp W(x)$ and $W(x) \succeq |x|^2$.
- $K : \mathbb{R}^d \to \mathbb{R}$ is an interacting energy. For example,
  - Lennard-Jones kernel: $K(x) = c_0|x|^{-12} - c_1|x|^{-6}$.
  - Coulomb kernel: $K(x) = |x|^{2-d}$ if $d \geq 3$, and $K(x) = -\log|x|$ if $d = 2$.

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Consider degenerate SDE for $(X_t, V_t)_{t\geq 0}$ on $\mathbb{R}^d \times \mathbb{R}^d$:

$$\begin{cases} dX_t = V_t\,dt, \\ dV_t = -\alpha V_t\,dt - \nabla U(X_t)\,dt + dL_t. \end{cases}$$

Background: fractional kinetic Fokker – Planck equation (Zhang ...).

(A1) There is a constant $K > 0$ such that

$$|\nabla U(x) - \nabla U(y)| \leq K|x-y|, \quad x, y \in \mathbb{R}^d.$$

(A2) There exist constants $\lambda_1, \lambda_2 > 0$ such that

$$\langle x, \nabla U(x)\rangle \geq \lambda_1 |x|^2 - \lambda_2, \quad x \in \mathbb{R}^d.$$

(A3) There are constants $\theta \in (0,1]$ and $c_0 > 0$ such that

$$\int_{\{|z|\geq 1\}} |z|^\theta\,\nu(dz) < \infty, \quad \nu(dz) \geq \frac{c_0}{|z|^{d+\theta/2}} 1_{\{0<z_1\leq 1\}}\,dz$$

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Stochastic Hamiltonian systems with Lévy noises

Theorem 1 (Bao-W., 22)

The process $(X_t, V_t)_{t\geq 0}$ *is exponentially ergodic in the sense that there are a unique invariant probability measure* μ *and a constant* $\lambda > 0$ *such that for all* $(x,v) \in \mathbb{R}^d \times \mathbb{R}^d$ *and* $t > 0$,

$$W_\Psi(P_t((x,v),\cdot),\mu) \leq C(x,v)e^{-\lambda t},$$

where $C(x,v) > 0$ *is independent of* t.

- Instead of $(X_t, V_t)_{t\geq 0}$, we will consider $(X_t, \tilde{V}_t)_{t\geq 0}$, where $\tilde{V}_t := X_t + \alpha^{-1}V_t$.

$$\begin{cases} dX_t = (-\alpha X_t + \alpha \tilde{V}_t)\,dt, \\ d\tilde{V}_t = -\nabla U(X_t)\,dt + dL_t. \end{cases}$$

- For any $x, x', v, v' \in \mathbb{R}^d$ and $\alpha_0 > 0$, we set

$$z := x - x', \quad w := v - v', \quad q := z + \alpha^{-1}w, \quad r := \alpha_0|z| + |q|.$$

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• Coupling function is not clear. How to metric the two points in the bounded subdomain of $\{(\mathbf{x},\mathbf{y}) : V(\mathbf{x}) + V(\mathbf{y}) \geq R\}$?

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where $\gamma > 0$, $U : \mathscr{D}(U) \to \mathbb{R}$ with $\mathscr{D}(U) := \{q \in \mathbb{R}^d : U(q) < \infty\}$. and $L(t)$ is a d-dimensional symmetric α-stable process.

- $$U(x) = A|x|^\alpha + B|x|^{-\beta},$$
  with $\alpha \geq 2$ and $\beta > 0$.
- $$U(x) = A|x|^\alpha + BK(|x|),$$
  where $\alpha \geq 2$ and $K(x)$ is the Coulomb kernel; that is, $K(x) = |x|^{2-d}$ if $d \geq 3$, and $K(x) = -\log|x|$ if $d = 2$.

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Main results

Theorem 2

Suppose that there exists a constant $C_U^* > 0$ *such that for all* $x \in \mathscr{D}(U)$,

$$\frac{U(x)}{|\nabla U(x)|^2}\left(1 + |\nabla^2 U(x)|\right) \le C_U^*,$$

where ∇^2 *stands for the Hessian operator. Then the process* $(X_t, V_t)_{t\ge 0}$ *is exponentially ergodic.*

- Villani ('09):

$$|\nabla^2 U| \le c(1 + |\nabla U|).$$

- Camrud-Herzog-Stoltz-Gordina ('22):

$$|\nabla^2 U| \le \varepsilon |\nabla U|^2 + C_\varepsilon, \quad \varepsilon > 0.$$

- Herzog-Mattingely ('19):

$$\frac{1}{|\nabla U|} + \frac{|\nabla^2 U|}{|\nabla U|^2} \to 0.$$

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$(\mathbf{H}_V)$ *For all* $x \in \mathbb{R}^d$,

$$C_V^*|x|^2 - M_V \le V(x), \quad C_V^* V(x) - M_V \le \langle \nabla V(x), x \rangle.$$

$(\mathbf{H}_K)$ $\{x \in \mathbb{R}^d : |x| \ge r\} \subset \mathscr{D}(K)$ *for all* $r > 0$, *and there exist constants* $r_K, C_K^* > 0$ *such that for all* $x \in \mathscr{D}(K)$ *with* $|x| \le r_K$,

$$K(x) \ge 0, \quad \frac{1}{|x|}\langle x, \nabla K(x) \rangle \le -C_K^* K(x).$$

and

$$\sup_{|x| \ge r_K} (|\nabla K(x)| \vee |\langle x, \nabla K(x) \rangle|) < \infty.$$

Then the process $(X_t, V_t)_{t \ge 0}$ *is exponentially ergodic.*

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Proof: Lyapunov approach

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$$V(x,v) := 1 + \frac{|v|^2}{2} + U(x) + \psi(x,v) \geq 1,$$

where

$$\psi(x,v) := \frac{\kappa\,U(x)}{|\nabla U(x)|^2}\langle v, \nabla U(x)\rangle.$$

Then, consider the function

$$\mathcal{V}(x,v) := V(x,v)^{\theta/2}$$

with $\theta \in (0,\alpha)$.

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• Irreducible property: Control-type arguments with aid of time-change idea due to Zhang ('13); Kulik ('22).

• Coulomb kernel:

$$V(x,v) = C^\star + \frac{1}{2}|v|^2 + V(x) + K(x) - \frac{\alpha}{|x|}\langle x, v\rangle + \beta\langle x, v\rangle$$

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Remark: invariant probability measure

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which corresponds to an invariant probability measure

$$\mu(dx, dy) = e^{-V(x)}\, dx \times e^{-|y|^2/2}\, dy.$$

- $$\begin{cases} \mathrm{d}X_t = \nabla W(Y_t)\,\mathrm{d}t \\ \mathrm{d}Y_t = (-\nabla V(X_t) - Y_t)\,\mathrm{d}t + \mathrm{d}L_t, \end{cases}$$

which corresponds to an invariant probability measure

$$\mu(dx, dy) = e^{-V(x)}\, dx \times e^{-W(y)}\, dy.$$

Note that here $e^{-W(y)}\, dy$ is a symmetric α-stable distribution, which is an invariant probability measure of

$$\mathrm{d}Y_t = -Y_t\,\mathrm{d}t + \mathrm{d}L_t.$$

Remark: invariant probability measure

- $$\begin{cases} \mathrm{d}X_t = Y_t\,\mathrm{d}t \\ \mathrm{d}Y_t = (-\nabla V(X_t) - Y_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t, \end{cases}$$

which corresponds to an invariant probability measure

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$$(V(x) + |v|^2 + c\langle x, v\rangle)^{\theta/2}$$

with $\theta \in (0, \alpha)$. Note that $(V(x) + W(y) + ...)^{\theta/2}$ does not work!

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see Simsekli-Zhu-Teh-Gürbüzbalaban ('20).

- Note that: $b \in C^{2-\alpha}_{\mathrm{loc}}(\mathbb{R}^d)$ and

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for large enough $|x|$; see Huang-Majka-W. ('21).

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Thank you!