Séminaire de Mathématiques Appliquées du CERMICS

École des Ponts
ParisTech

Ergodicity and Lyapunov functions for Langevin dynamics with singular potentials

David Herzog (Iowa State University)

21 novembre 2019

Ergodicity and Lyapunov functions for Langevin dynamics with singular potentials

David P. Herzog

CERMICS Seminar
Ecole des Ponts ParisTech
November 21st, 2019

Familiar setting

An ODE on $\mathbf{R}^d$:

$$\begin{aligned} \frac{dx(t)}{dt} &= b(x(t)) \\ x(0) &= x_0 \in \mathbf{R}^d. \end{aligned}$$

Familiar setting

An ODE on $\mathbf{R}^d$:

$$\begin{aligned} \frac{dx(t)}{dt} &= b(x(t)) \\ x(0) &= x_0 \in \mathbf{R}^d. \end{aligned}$$

- **Question**: How do you show that solutions exist for all times $t \geq 0$?

Familiar setting

An ODE on $\mathbf{R}^d$:

$$\begin{aligned} \frac{dx(t)}{dt} &= b(x(t)) \\ x(0) &= x_0 \in \mathbf{R}^d. \end{aligned}$$

- **Question**: How do you show that solutions exist for all times $t \geq 0$?
- **First Answer**: Apply iteration scheme and show it has a unique fixed point!

Familiar setting

An ODE on $\mathbf{R}^d$:

$$\begin{aligned} \frac{dx(t)}{dt} &= b(x(t)) \\ x(0) &= x_0 \in \mathbf{R}^d. \end{aligned}$$

- **Question**: How do you show that solutions exist for all times $t \geq 0$?
- **First Answer**: Apply iteration scheme and show it has a unique fixed point!
- **Problem**: This assumes b is *globally Lipschitz*, i.e., there exists $C > 0$ such that

$$|b(x) - b(y)| \leq C|x - y| \qquad \forall x, y \in \mathbf{R}^d.$$

Familiar setting

An ODE on $\mathbf{R}^d$:

$$\begin{aligned} \frac{dx(t)}{dt} &= b(x(t)) \\ x(0) &= x_0 \in \mathbf{R}^d. \end{aligned}$$

- **Question**: How do you show that solutions exist for all times $t \geq 0$?
- **First Answer**: Apply iteration scheme and show it has a unique fixed point!
- **Problem**: This assumes b is *globally Lipschitz*, i.e., there exists $C > 0$ such that

$$|b(x) - b(y)| \leq C|x - y| \qquad \forall x, y \in \mathbf{R}^d.$$

- **Solution**. Find a *Lyapunov function*.

Lyapunov functions

- Suppose that $V \in C^1(\mathbf{R}^d; [0,\infty))$ satisfies
  - $V(x) \to \infty$ as $|x| \to \infty$;
  - $b(x) \cdot \nabla V(x) \le CV(x)$ for some constant $C > 0$,

Lyapunov functions

- Suppose that $V \in C^1(\mathbf{R}^d; [0,\infty))$ satisfies
  - $V(x) \to \infty$ as $|x| \to \infty$;
  - $b(x) \cdot \nabla V(x) \le CV(x)$ for some constant $C > 0$,

Then

$$\frac{d}{dt} V(x(t)) \quad = \quad b(x(t)) \cdot \nabla V(x(t)) \le CV(x(t)).$$

Lyapunov functions

- Suppose that $V \in C^1(\mathbf{R}^d; [0,\infty))$ satisfies
  - $V(x) \to \infty$ as $|x| \to \infty$;
  - $b(x) \cdot \nabla V(x) \le CV(x)$ for some constant $C > 0$,

Then

$$\frac{d}{dt} V(x(t)) \quad = \quad b(x(t)) \cdot \nabla V(x(t)) \le CV(x(t)).$$

- Gronwall's inequality then implies

$$V(x(t)) \le V(x_0) e^{Ct}.$$

Lyapunov functions

- Suppose that $V \in C^1(\mathbf{R}^d; [0,\infty))$ satisfies
  - $V(x) \to \infty$ as $|x| \to \infty$;
  - $b(x) \cdot \nabla V(x) \le CV(x)$ for some constant $C > 0$,

Then

$$\frac{d}{dt} V(x(t)) \quad = \quad b(x(t)) \cdot \nabla V(x(t)) \le CV(x(t)).$$

- Gronwall's inequality then implies

$$V(x(t)) \le V(x_0) e^{Ct}.$$

- Therefore if we can find such a V, we are done.

Problems persist

- General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.

Problems persist

- General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.
- Even still, there is no known algorithm or procedure which would produce a Lyapunov function for a given ODE.

Problems persist

- General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.
- Even still, there is no known algorithm or procedure which would produce a Lyapunov function for a given ODE.
- Same problem exists in the context of *stochastic differential equations* AND every other type of dynamics.

Problems persist

- General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.
- Even still, there is no known algorithm or procedure which would produce a Lyapunov function for a given ODE.
- Same problem exists in the context of *stochastic differential equations* AND every other type of dynamics.

Goal: Make progress by studying *interesting* examples.

Problems persist

• General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.

• Even still, there is no known algorithm or procedure which would produce a Lyapunov function for a given ODE.

• Same problem exists in the context of *stochastic differential equations* AND every other type of dynamics.

<u>Goal</u>: Make progress by studying *interesting* examples.

<u>Singular stochastic Hamiltonian systems?</u>:

Problems persist

- General Lyapunov function theory is easy, but finding a Lyapunov function can be hard.
- Even still, there is no known algorithm or procedure which would produce a Lyapunov function for a given ODE.
- Same problem exists in the context of *stochastic differential equations* AND every other type of dynamics.

Goal: Make progress by studying *interesting* examples.

Singular stochastic Hamiltonian systems?: Noise in system forces particles to interact causing intermittent high-energy excursions.

Langevin dynamics

SDE on $(\mathsf{R}^k)^N \times (\mathsf{R}^k)^N$:

$$dq(t) = p(t)\,dt$$
$$dp(t) = -\gamma p(t)\,dt - \nabla U(q(t))\,dt + \sqrt{2\gamma T}\,dB(t).$$

- $q(t) = (q_1(t),\dots,q_N(t))$, $p(t) = (p_1(t),\dots,p_N(t)) \in (\mathsf{R}^k)^N$ are the position and momentum vectors;
- U is the potential function; $\gamma, T > 0$ are constants.
- B_t is a standard Brownian motion on $(\mathsf{R}^k)^N$.

Langevin dynamics

SDE on $(\mathbf{R}^k)^N \times (\mathbf{R}^k)^N$:

$$\begin{aligned} dq(t) &= p(t)\,dt \\ dp(t) &= -\gamma p(t)\,dt - \nabla U(q(t))\,dt + \sqrt{2\gamma T}\,dB(t). \end{aligned}$$

- $q(t) = (q_1(t), \dots, q_N(t))$, $p(t) = (p_1(t), \dots, p_N(t)) \in (\mathbf{R}^k)^N$ are the position and momentum vectors;
- U is the potential function; $\gamma, T > 0$ are constants.
- B_t is a standard Brownian motion on $(\mathbf{R}^k)^N$.

Main Assumption: U has singularities (e.g. Lennard-Jones).

Langevin dynamics

SDE on $(\mathbf{R}^k)^N \times (\mathbf{R}^k)^N$:

$$dq(t) = p(t)\,dt$$
$$dp(t) = -\gamma p(t)\,dt - \nabla U(q(t))\,dt + \sqrt{2\gamma T}\,dB(t).$$

- $q(t) = (q_1(t),\ldots,q_N(t))$, $p(t) = (p_1(t),\ldots,p_N(t)) \in (\mathbf{R}^k)^N$ are the position and momentum vectors;
- U is the potential function; $\gamma, T > 0$ are constants.
- B_t is a standard Brownian motion on $(\mathbf{R}^k)^N$.

Main Assumption: U has singularities (e.g. Lennard-Jones).

Main Questions: Relaxation to Gibbs measure? If so, in what sense and how fast?

Langevin dynamics

SDE on $(\mathbf{R}^k)^N \times (\mathbf{R}^k)^N$:

$$
\begin{aligned}
dq(t) &= p(t)\,dt \\
dp(t) &= -\gamma p(t)\,dt - \nabla U(q(t))\,dt + \sqrt{2\gamma T}\,dB(t).
\end{aligned}
$$

- $q(t) = (q_1(t),\ldots,q_N(t))$, $p(t) = (p_1(t),\ldots,p_N(t)) \in (\mathbf{R}^k)^N$ are the position and momentum vectors;
- U is the potential function; $\gamma, T > 0$ are constants.
- B_t is a standard Brownian motion on $(\mathbf{R}^k)^N$.

Main Assumption: U has singularities (e.g. Lennard-Jones).

Main Questions: Relaxation to Gibbs measure? If so, in what sense and how fast?

Point: Requires nontrivial understanding of how dissipation spreads through the system.

Langevin dynamics

Langevin equation:

$$\ddot{q}(t) = -\gamma\dot{q}(t) - \nabla U(q(t)) + \sqrt{2\gamma T}\,\dot{B}(t)$$

• Model for particle movement in fluids. Particles experience friction $\left(-\gamma\dot{q}(t)\right)$ and thermal fluctuations $\left(\sqrt{2\gamma k_B T}\,\dot{B}(t)\right)$. U encodes potential forces (e.g. presence of a wells/walls) and particle interactions.

Langevin dynamics

Langevin equation:

$$\ddot{q}(t) = -\gamma \dot{q}(t) - \nabla U(q(t)) + \sqrt{2\gamma T}\, \dot{B}(t)$$

- Model for particle movement in fluids. Particles experience friction $\left(-\gamma \dot{q}(t)\right)$ and thermal fluctuations $\left(\sqrt{2\gamma k_B T}\, \dot{B}(t)\right)$. U encodes potential forces (e.g. presence of a wells/walls) and particle interactions.
- Molecular dynamics simulation and Gibbs sampling:

$$\mu(dpdq) \propto e^{-\beta H(q,p)} dpdq, \qquad H(q,p) = \frac{|p|^2}{2} + U(q)$$

and $\beta = 1/T$.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Common examples:

(1) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x)$; $U_{\mathcal{I}}(x) = 0$ or $U_{\mathcal{I}}(x) \sim b|x|^{\ell}$.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Common examples:

(1) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = 0$ or $U_{\mathcal{I}}(x) \sim b|x|^{\ell}$.

(2) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = \frac{b}{|x|^{12}} - \frac{c}{|x|^{6}}$.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Common examples:

(1) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = 0$ or $U_{\mathcal{I}}(x) \sim b|x|^{\ell}$.

(2) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

(3) $U_{\mathcal{E}}(x) = \dfrac{a}{||x| - b|^{c}};\ \ U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Common examples:

(1) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = 0$ or $U_{\mathcal{I}}(x) \sim b|x|^{\ell}$.

(2) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x);\ \ U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

(3) $U_{\mathcal{E}}(x) = \dfrac{a}{||x| - b|^{c}};\ \ U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

Common examples:

(1) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x); \;\; U_{\mathcal{I}}(x) = 0$ or $U_{\mathcal{I}}(x) \sim b|x|^{\ell}$.

(2) $U_{\mathcal{E}}(x) = a|x|^{2j} + p_{2j-1}(x); \;\; U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

(3) $U_{\mathcal{E}}(x) = \dfrac{a}{||x| - b|^{c}}; \;\; U_{\mathcal{I}}(x) = \dfrac{b}{|x|^{12}} - \dfrac{c}{|x|^{6}}$.

Point: Mathematics literature almost exclusively restricted to potentials like those in (1). How does one handle potentials like (2) and (3)? How do (1)-(3) fit together? How is the dynamics different?

Langevin dynamics

Example: $k = N = \gamma = 1$, $U(q) = \frac{q^4}{4} + \frac{1}{2q^2}$, $q_0 = 8, p_0 = 1$, $T = 25$

Example: $k = 1$, $N = 2$, $\gamma = 1$, $T = 25$, $U_{\mathcal{Q}}(q) = q^2$, $U_{\mathcal{I}}(q) = \frac{1}{|q|^{1.3}}$

Langevin dynamics

Example: $k = 1$, $N = 3$, $\gamma = 1$, $T = 25$, $U_{\mathcal{E}}(q) = q^2$, $U_{\mathcal{I}}(q) = \frac{1}{|q|^{1.3}}$

History and Previous Work

Lots of papers. Here are highlights:

Lots of papers. Here are highlights:

Theorem (Mattingly, Stuart, Higham '02)
Suppose that $U \in C^\infty((\mathbf{R}^k)^N; (0,\infty))$ *satisfies the global bound*

$$\frac{1}{2}\nabla U(q)\cdot q \geq \beta U(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)}|q|^2 - \alpha$$

for some $\alpha > 0$ *and* $\beta \in (0,1)$. *Then for every* $\ell \geq 1$ *there exists* $C = C(\ell) > 0, \lambda = \lambda(\ell) > 0$ *such that*

$$\left|\mathbf{E}_{(q,p)}\phi(q(t),p(t)) - \int \phi \, d\mu\right| \leq CV(q,p)^\ell e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V^\ell$. *Here* $V \sim H+1$.

History and Previous Work

Lots of papers. Here are highlights:

Theorem (Mattingly, Stuart, Higham ′02)
Suppose that $U \in C^\infty((\mathbb{R}^k)^N;(0,\infty))$ *satisfies the global bound*

$$\frac{1}{2}\nabla U(q)\cdot q \geq \beta U(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)}|q|^2 - \alpha$$

for some $\alpha > 0$ *and* $\beta \in (0,1)$. *Then for every* $\ell \geq 1$ *there exists* $C = C(\ell) > 0, \lambda = \lambda(\ell) > 0$ *such that*

$$\left|\mathbb{E}_{(q,p)}\phi(q(t),p(t)) - \int \phi \, d\mu\right| \leq CV(q,p)^\ell e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V^\ell$. *Here* $V \sim H + 1$.

- Strengthens work of Tropper (′77).

History and Previous Work

Lots of papers. Here are highlights:

Theorem (Mattingly, Stuart, Higham ′02)
Suppose that $U \in C^\infty((\mathbf{R}^k)^N; (0,\infty))$ *satisfies the global bound*

$$\frac{1}{2}\nabla U(q)\cdot q \geq \beta U(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)}|q|^2 - \alpha$$

for some $\alpha > 0$ *and* $\beta \in (0,1)$. *Then for every* $\ell \geq 1$ *there exists* $C = C(\ell) > 0, \lambda = \lambda(\ell) > 0$ *such that*

$$\left|\mathsf{E}_{(q,p)}\phi(q(t),p(t)) - \int \phi \, d\mu\right| \leq CV(q,p)^\ell e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V^\ell$. *Here* $V \sim H + 1$.

- Strengthens work of Tropper (′77).
- (Talay ′02) Similar conclusion provided $U \in C^\infty((\mathbf{R}^k)^N; (0,\infty))$ is *essentially* a polynomial.

History and Previous Work: Langevin

Point: In both works, there is an explicit Lyapunov function V which satisfies

$$V(q,p) = H(q,p) + \psi(q,p)$$

where $\psi(q,p) = \epsilon p \cdot q$, $\epsilon > 0$ small.

History and Previous Work: Langevin

Point: In both works, there is an explicit Lyapunov function V which satisfies

$$V(q,p) = H(q,p) + \psi(q,p)$$

where $\psi(q,p) = \epsilon p \cdot q$, $\epsilon > 0$ small.

Theorem (Villani '06)
If $U \in C^2((\mathbf{R}^k)^N;(0,\infty))$ grows at least linearly at infinity and satisfies $|\nabla^2 U| \leq C(1+|\nabla U|)$, then there exist $C,\lambda > 0$ for which

$$\left\| \mathbf{E}_{(q,p)}\phi(q(t),p(t)) - \int \phi \, d\mu \right\|_{H^1(\mu)} \leq Ce^{-\lambda t}\|\phi\|_{H^1(\mu)}$$

for all $t \geq 0$, $\phi \in H^1(\mu)$.

History and Previous Work: Langevin

Point: In both works, there is an explicit Lyapunov function V which satisfies

$$V(q,p) = H(q,p) + \psi(q,p)$$

where $\psi(q,p) = \epsilon p \cdot q$, $\epsilon > 0$ small.

Theorem (Villani '06)
If $U \in C^2((\mathbf{R}^k)^N; (0,\infty))$ grows at least linearly at infinity and satisfies $|\nabla^2 U| \leq C(1 + |\nabla U|)$, then there exist $C, \lambda > 0$ for which

$$\left\| \mathbf{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right\|_{H^1(\mu)} \leq Ce^{-\lambda t} \|\phi\|_{H^1(\mu)}$$

for all $t \geq 0$, $\phi \in H^1(\mu)$.

- Builds off/strengthens work of Helffer and Nier ('05), Hérau ('06).

History and Previous Work: Langevin

- Hypocoercivity versus Lyapunov approach. Makes use of existence of an invariant measure, handles a different norm.

History and Previous Work: Langevin

- Hypocoercivity versus Lyapunov approach. Makes use of existence of an invariant measure, handles a different norm.
- Talay issues challenge in ′07 at AIM conference on Stochastic Simulation: Singular, Lennard-Jones U?

History and Previous Work: Langevin

- Hypocoercivity versus Lyapunov approach. Makes use of existence of an invariant measure, handles a different norm.
- Talay issues challenge in ′07 at AIM conference on Stochastic Simulation: Singular, Lennard-Jones U?
- (Conrad, Grothaus ′10 & ′15) Under appropriate growth of U and assuming

$$|\nabla^2 U| \leq C(1 + |\nabla U|^\alpha)$$

for some $C > 0$ and $\alpha \in [1,2)$, then there exists a constant $D > 0$ such that for all $t > 0$, $\phi \in L^2(\mu)$

$$\int \left(\frac{1}{t} \int_0^t \bar{\phi}(q(s), p(s))\, ds \right)^2 d\mu \leq \frac{D}{t} \|\bar{\phi}\|^2_{L^2(\mu)}.$$

In the above, $\bar{\phi} = \phi - \int \phi \, d\mu$.

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser $'10$) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser $'10$) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin $'13$) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery ($'85$).

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq C U^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq CU^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq CU^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:
    - A. Eberle, A. Guillen, R. Zimmer (Coupling methods);

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq CU^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:
  - A. Eberle, A. Guillen, R. Zimmer (Coupling methods);
  - G. Stoltz, B. Leimkuhler, M. Sachs (LD and adaptive Langevin);

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq CU^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:
  - A. Eberle, A. Guillen, R. Zimmer (Coupling methods);
  - G. Stoltz, B. Leimkuhler, M. Sachs (LD and adaptive Langevin);
  - (absence of friction in some directions) by J-P Eckmann, M. Hairer, L. Rey-Bellet, Mattingly, N. Cuneo.

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq C U^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:
    - A. Eberle, A. Guillen, R. Zimmer (Coupling methods);
    - G. Stoltz, B. Leimkuhler, M. Sachs (LD and adaptive Langevin);
    - (absence of friction in some directions) by J-P Eckmann, M. Hairer, L. Rey-Bellet, Mattingly, N. Cuneo.

History and Previous Work: Langevin

- (Dolbeault, Mouhot, Schmeiser ′10) New method for proving Hypocoercivity, nice parabolic scaling heuristic. Result does not apply in singular U case.
- (F. Baudoin ′13) Establishes connection between hypocoercivity and Gamma Calculus of Bakry-Emery (′85).
- (Cattiaux, Guillin, Monmarché, Zhang ′17) Geometric convergence to equilibrium in weighted $L^2(\mu)$ under

$$|\nabla^2 U| \leq C U^{2\eta} \leq C' U^{2\eta+1} \leq |\nabla U|^2.$$

- Numerous other results:
  - A. Eberle, A. Guillen, R. Zimmer (Coupling methods);
  - G. Stoltz, B. Leimkuhler, M. Sachs (LD and adaptive Langevin);
  - (absence of friction in some directions) by J-P Eckmann, M. Hairer, L. Rey-Bellet, Mattingly, N. Cuneo.

Question: Does a Lyapunov function exist in the singular case ? Can we improve convergence results? How does it all fit together?

Main Results

Theorem (Cooke, H., Mattingly, McKinley, Schmidler '17[1])
Suppose $N = k = 1$ and $U : (0,\infty) \to (0,\infty)$ is of the form

$$U(q) = \sum_{i=1}^{J} \beta_i q^{\alpha_i}$$

where $\beta_1, \beta_J > 0$, $\alpha_1 > \alpha_2 > \cdots > \alpha_J$, and $\alpha_1 > 2, \alpha_J < 0$. Then there exist constants $C, \lambda > 0$ such that

$$\left| \mathsf{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right| \le CV(q,p) e^{-\lambda t}$$

for all $t \ge 0$, $|\phi| \le V$. Here $V \sim \exp(\delta H)$ where $\delta < \beta$.

---

[1] *Comm. Math. Sci.* ***15*** *no. 7 pp. 1987-2025 (2017)*

Main Results

Theorem (Cooke, H., Mattingly, McKinley, Schmidler '17[1])
Suppose $N = k = 1$ and $U : (0,\infty) \to (0,\infty)$ is of the form

$$U(q) = \sum_{i=1}^{J} \beta_i q^{\alpha_i}$$

where $\beta_1, \beta_J > 0$, $\alpha_1 > \alpha_2 > \cdots > \alpha_J$, and $\alpha_1 > 2, \alpha_J < 0$. Then there exist constants $C, \lambda > 0$ such that

$$\left| \mathsf{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right| \leq CV(q,p)e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V$. Here $V \sim \exp(\delta H)$ where $\delta < \beta$.

- Result makes use of an explicit construction of a Lyapunov function of the form $V = H + \psi$, $\psi = o(H)$ as $H \to \infty$.

---

[1] *Comm. Math. Sci.* ***15*** *no. 7 pp. 1987-2025 (2017)*

Main Results

Theorem (Cooke, H., Mattingly, McKinley, Schmidler ′17[1])
Suppose $N = k = 1$ and $U : (0,\infty) \to (0,\infty)$ is of the form

$$U(q) = \sum_{i=1}^{J} \beta_i q^{\alpha_i}$$

where $\beta_1, \beta_J > 0$, $\alpha_1 > \alpha_2 > \cdots > \alpha_J$, and $\alpha_1 > 2, \alpha_J < 0$. Then there exist constants $C, \lambda > 0$ such that

$$\left| \mathbf{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right| \leq C V(q,p) e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V$. Here $V \sim \exp(\delta H)$ where $\delta < \beta$.

- Result makes use of an explicit construction of a Lyapunov function of the form $V = H + \psi$, $\psi = o(H)$ as $H \to \infty$.
- Works for two particles in $\mathbf{R}^1$. What about N particles on $\mathbf{R}^k$?

[1] *Comm. Math. Sci.* ***15*** *no. 7 pp. 1987-2025 (2017)*

Definition
Let $U : (\mathbb{R}^k)^N \to [0, +\infty]$ and $\mathcal{O} = \{q : U(q) < \infty\}$. We call U **admissible** if

- $\mathcal{O}$ is non-empty, open, connected. Moreover, for each $R > 0$ the set $\{q : U(q) < R\}$ has compact closure in $(\mathbb{R}^k)^N$.
- $U \in C^\infty(\mathcal{O})$ and $\int_{\mathcal{O}} e^{-\beta U(q)}\, dq < \infty$.
- For any sequence $\{q_k\} \subset \mathcal{O}$ for which $U(q_k) \to \infty$ as $k \to \infty$ we have

$$|\nabla U(q_k)| \to \infty \;\text{ and }\; \frac{|\nabla^2 U(q_k)|}{|\nabla U(q_k)|^2} \to 0$$

as $k \to \infty$.

Theorem (H., Mattingly '17[2])
Suppose $U : (\mathbb{R}^k)^N \to [0, +\infty]$ *is admissible. Then there exist constants* $C, \lambda > 0$ *such that*

$$\left| \mathbb{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right| \leq C V(q,p) e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V$. *Here* $V \sim \exp(\delta H)$, $\delta < \beta$.

[2] *Comm. Pure Appl. Math* **72** no. 10 pp. 2231-2255 (2019)

Main Results: Langevin

Theorem (H., Mattingly ′17[2])
Suppose $U : (\mathbf{R}^k)^N \to [0, +\infty]$ *is admissible. Then there exist constants* $C, \lambda > 0$ *such that*

$$\left| \mathbf{E}_{(q,p)} \phi(q(t), p(t)) - \int \phi \, d\mu \right| \leq CV(q,p) e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V$. *Here* $V \sim \exp(\delta H)$, $\delta < \beta$.

- Explicit Lyapunov function. Proof is relatively simple.
- Can relax regularity to $U \in C^2(\mathcal{O})$ in construction.
- Construction does not need apriori knowledge of the invariant measure.
- (Lu, Mattingly ′19) Extended to handle Coulomb interactions.

[2] *Comm. Pure Appl. Math* **72** no. 10 pp. 2231-2255 (2019)

Main Results

Let $\nabla_\zeta = \zeta^{-1}(\nabla_p, \nabla_q - c(\gamma)\nabla_p), c(\gamma) = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{2} + 1}$ and $H^1_{\zeta,W}$ denote the space of weakly differentiable functions $f : X \to \mathbf{R}$ with

$$\|f\|^2_{\zeta,W} = \int_X f^2 W \, d\mu + |\nabla_\zeta f|^2 \, d\mu < \infty.$$

Main Results

Let $\nabla_\zeta = \zeta^{-1}(\nabla_p, \nabla_q - c(\gamma)\nabla_p), c(\gamma) = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{2} + 1}$ and $H^1_{\zeta,W}$ denote the space of weakly differentiable functions $f : X \to \mathbf{R}$ with

$$\|f\|^2_{\zeta,W} = \int_X f^2 W \, d\mu + |\nabla_\zeta f|^2 \, d\mu < \infty.$$

Theorem (Baudoin, H., Gordina '19)
Suppose U is admissible. Then there is an explicit function $W \in C^\infty(X;[1,\infty)) \cap L^1(\mu)$ and explicit constants $\sigma, \zeta > 0$ such that for all $f \in H^1_{\zeta,W}$ with $\int_X f \, d\mu = 0$

$$\|P_t f\|^2_{\zeta,W} \le e^{-\sigma t} \|f\|^2_{\zeta,W} \qquad \forall t \ge 0.$$

Let $\nabla_\zeta = \zeta^{-1}(\nabla_p, \nabla_q - c(\gamma)\nabla_p), c(\gamma) = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{2} + 1}$ and $H^1_{\zeta,W}$ denote the space of weakly differentiable functions $f : X \to \mathbf{R}$ with

$$\|f\|^2_{\zeta,W} = \int_X f^2 W \, d\mu + |\nabla_\zeta f|^2 \, d\mu < \infty.$$

Theorem (Baudoin, H., Gordina '19)
Suppose U is admissible. Then there is an explicit function $W \in C^\infty(X; [1,\infty)) \cap L^1(\mu)$ and explicit constants $\sigma, \zeta > 0$ such that for all $f \in H^1_{\zeta,W}$ with $\int_X f \, d\mu = 0$

$$\|P_t f\|^2_{\zeta,W} \le e^{-\sigma t} \|f\|^2_{\zeta,W} \qquad \forall t \ge 0.$$

Corollary
For singular interaction and polynomial confining well: $\sigma \ge c/(\rho \vee N^p)$ where $\rho > 0$ is a local Poincaré constant for μ and $c > 0$ and $p \ge 1$ are independent of N.

Heuristics and Proof

Propagation of dissipation

Goal: Need to see how energy dissipates.

Propagation of dissipation

Goal: Need to see how energy dissipates.

If $H(q,p) = \frac{|p|^2}{2} + U(q)$ and $x_0 = (q_0, p_0)$, then

$$\mathbf{E}_{x_0} H(q(t), p(t)) - H(x_0) = \mathbf{E}_{x_0} \int_0^t \underbrace{-\gamma |p(s)|^2 + \gamma k_B T k N}_{\mathcal{L}H(q(s),p(s))} \, ds.$$

Propagation of dissipation

Goal: Need to see how energy dissipates.

If $H(q,p) = \frac{|p|^2}{2} + U(q)$ and $x_0 = (q_0, p_0)$, then

$$\mathbf{E}_{x_0} H(q(t),p(t)) - H(x_0) = \mathbf{E}_{x_0} \int_0^t \underbrace{-\gamma |p(s)|^2 + \gamma k_B T k N}_{\mathcal{L}H(q(s),p(s))} \, ds.$$

Problem: H is NOT pointwise contractive.

- $\mathcal{L}H(q,p) > 0$ for $|p|^2 > 0$ small enough. Is dissipation possible?
- Yes, but must be due to averaging effects:

$$A_{p^2}(x_0, t, R) := \frac{1}{t} \int_0^t |p(s)|^2 \mathbf{1}\{H(q(s),p(s)) \geq R\} \, ds$$

where for fixed x_0, t and $R \gg 1$ we hope

$$\frac{1}{2} A_{p^2}(x_0, t, R) \gg 1.$$

Averaging

Example: $k = N = \gamma = 1$, $U(q) = \frac{q^4}{4} + \frac{1}{2q^2}$, $q_0 = 8, p_0 = 1$, $T = 25$

Averaging

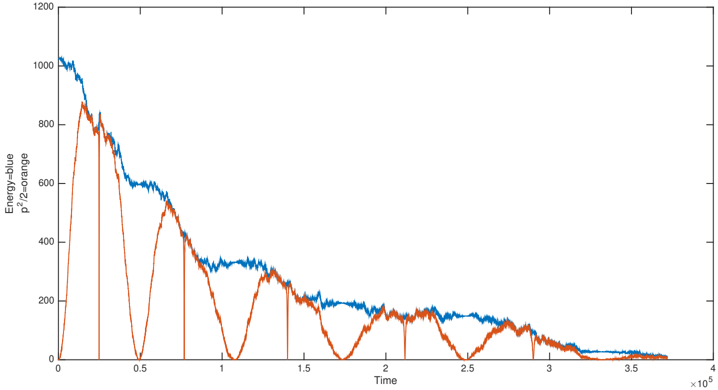

Figure 1: $H(q(t), p(t))$ and $\frac{p^2(t)}{2}$ plotted for $t \in [0, 4]$. We have $A_H((8,1), 10, 8) \approx 82.04$ and $\frac{1}{2} A_{p^2}((8,1), 10, 8) \approx 53.62$

Averaging ($N = 2$, $T = 25$, $U_{\mathcal{E}}(q) = q^2$, $U_{\mathcal{I}}(q) = \frac{1}{|q|^{1.3}}$)

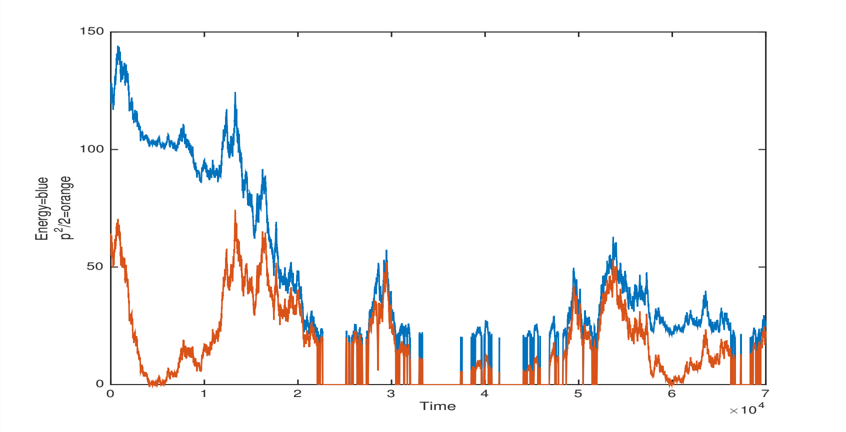

Figure 2: $H(q(t), p(t))$ and $\frac{p^2(t)}{2}$ plotted for $t \in [0, 70]$. We have $A_H((8, -8, 1, .5), 70, 20) \approx 3.94$ and $\frac{1}{2}A_{p^2}((8, -8, 1, .5), 70, 20) \approx 1.58$

Construction

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q,p) \le -\kappa \qquad \text{for} \qquad H \ge R$$

for some constants $\kappa > 2\gamma k_B TkN, R \gg 1$.

Construction

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q,p) \leq -\kappa \qquad \text{for} \qquad H \geq R$$

for some constants $\kappa > 2\gamma k_B TkN, R \gg 1$.

Set $V = H + \psi$ and note $V \approx H$ and

$$\mathcal{L}V(q,p) \leq -\gamma|p|^2 - \gamma k_B TkN \qquad \text{for} \qquad H \geq R.$$

Construction

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q,p) \leq -\kappa \qquad \text{for} \qquad H \geq R$$

for some constants $\kappa > 2\gamma k_B TkN, R \gg 1$.

Set $V = H + \psi$ and note $V \approx H$ and

$$\mathcal{L}V(q,p) \leq -\gamma|p|^2 - \gamma k_B TkN \qquad \text{for} \qquad H \geq R.$$

- Great in and of itself already. Implies expected returns to center of space are finite.

Construction

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q,p) \leq -\kappa \qquad \text{for} \qquad H \geq R$$

for some constants $\kappa > 2\gamma k_B TkN, R \gg 1$.

Set $V = H + \psi$ and note $V \approx H$ and

$$\mathcal{L}V(q,p) \leq -\gamma |p|^2 - \gamma k_B TkN \qquad \text{for} \qquad H \geq R.$$

- Great in and of itself already. Implies expected returns to center of space are finite.
- Does not (immediately) imply geometric convergence, however!

Construction

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q,p) \leq -\kappa \qquad \text{for} \qquad H \geq R$$

for some constants $\kappa > 2\gamma k_B TkN, R \gg 1$.

Set $V = H + \psi$ and note $V \approx H$ and

$$\mathcal{L}V(q,p) \leq -\gamma|p|^2 - \gamma k_B TkN \qquad \text{for} \qquad H \geq R.$$

- Great in and of itself already. Implies expected returns to center of space are finite.
- Does not (immediately) imply geometric convergence, however!
- Existence of invariant measure (if we perturb γ and noise coefficients within reason) follows immediately.

Defining ψ

For simplicity: Set $k = N = 1$ and $U(q) = q^{\alpha} + 1/q^{\beta}$ for $q > 0$ where $\alpha > 1, \beta > 0$.

Defining ψ

For simplicity: Set $k = N = 1$ and $U(q) = q^\alpha + 1/q^\beta$ for $q > 0$ where $\alpha > 1, \beta > 0$.

Note:

$$\mathcal{L}H(q,p) = -\gamma p^2 + \gamma k_B T$$

Defining ψ

For simplicity: Set $k = N = 1$ and $U(q) = q^\alpha + 1/q^\beta$ for $q > 0$ where $\alpha > 1, \beta > 0$.

Note:

$$\begin{aligned} \mathcal{L}H(q,p) &= -\gamma p^2 + \gamma k_B T \\ &\leq -\kappa \qquad \text{for} \qquad p^2 \geq \frac{\kappa + \gamma k_B T}{\gamma}. \end{aligned}$$

Defining ψ

For simplicity: Set $k = N = 1$ and $U(q) = q^\alpha + 1/q^\beta$ for $q > 0$ where $\alpha > 1, \beta > 0$.

Note:

$$\begin{aligned} \mathcal{L}H(q,p) &= -\gamma p^2 + \gamma k_B T \\ &\leq -\kappa \qquad \text{for} \qquad p^2 \geq \frac{\kappa + \gamma k_B T}{\gamma}. \end{aligned}$$

Conclusion: We don't need ψ if p^2 is large enough. Need to analyze the behavior of process at large energies when p^2 is bounded (i.e. p^2 is bounded while $U(q)$ is large).

Defining ψ

Note:

$$\begin{aligned}\mathcal{L} &= p\partial_q - U'(q)\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &= p\partial_q - (\alpha q^{\alpha-1} - \beta q^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2.\end{aligned}$$

Defining ψ

Note:

$$\begin{aligned}\mathcal{L} &= p\partial_q - U'(q)\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &= p\partial_q - (\alpha q^{\alpha-1} - \beta q^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2.\end{aligned}$$

Large U asymptotics: U is large when $q \gg 1$ or when $q \approx 0$, so consider the scalings

$$q = \lambda Q_\infty \qquad \text{and} \qquad q = \lambda^{-1} Q_0$$

for $\lambda \gg 1$.

Defining ψ

Note:

$$\begin{aligned}\mathcal{L} &= p\partial_q - U'(q)\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &= p\partial_q - (\alpha q^{\alpha-1} - \beta q^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2.\end{aligned}$$

Large U asymptotics: U is large when $q \gg 1$ or when $q \approx 0$, so consider the scalings

$$q = \lambda Q_\infty \qquad \text{and} \qquad q = \lambda^{-1} Q_0$$

for $\lambda \gg 1$.

Q_∞ scaling:

$$\mathcal{L} = \lambda^{-1} p\partial_{Q_\infty} - (\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1} - \lambda^{-\beta-1} Q_\infty^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2$$

Defining ψ

Note:

$$\begin{aligned}\mathcal{L} &= p\partial_q - U'(q)\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &= p\partial_q - (\alpha q^{\alpha-1} - \beta q^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2.\end{aligned}$$

Large U asymptotics: U is large when $q \gg 1$ or when $q \approx 0$, so consider the scalings

$$q = \lambda Q_\infty \qquad \text{and} \qquad q = \lambda^{-1} Q_0$$

for $\lambda \gg 1$.

Q_∞ **scaling:**

$$\begin{aligned}\mathcal{L} &= \lambda^{-1} p\partial_{Q_\infty} - (\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1} - \lambda^{-\beta-1} Q_\infty^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &\approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1}\partial_p.\end{aligned}$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1}\partial_p.$$

Q_0 scaling:

$$\mathcal{L} = \lambda p \partial_{Q_0} - (\alpha\lambda^{-\alpha+1} Q_0^{\alpha-1} - \lambda^{\beta+1} Q_0^{-\beta-1})\partial_p - \gamma p \partial_p + \gamma k_B T \partial_p^2$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1}\partial_p.$$

Q_0 scaling:

$$\begin{aligned}\mathcal{L} &= \lambda p \partial_{Q_0} - (\alpha\lambda^{-\alpha+1} Q_0^{\alpha-1} - \lambda^{\beta+1} Q_0^{-\beta-1})\partial_p - \gamma p \partial_p + \gamma k_B T \partial_p^2 \\ &\approx \lambda^{\beta+1} Q_0^{-\beta-1}\partial_p.\end{aligned}$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1}\partial_p.$$

Q_0 scaling:

$$\begin{aligned} \mathcal{L} &= \lambda p \partial_{Q_0} - (\alpha\lambda^{-\alpha+1} Q_0^{\alpha-1} - \lambda^{\beta+1} Q_0^{-\beta-1})\partial_p - \gamma p \partial_p + \gamma k_B T \partial_p^2 \\ &\approx \lambda^{\beta+1} Q_0^{-\beta-1}\partial_p. \end{aligned}$$

Summary: If p^2 is bounded and $U(q)$ is large

$$\mathcal{L} \approx -U'(q)\partial_p.$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1}\partial_p.$$

Q_0 scaling:

$$\begin{aligned}\mathcal{L} &= \lambda p \partial_{Q_0} - (\alpha\lambda^{-\alpha+1} Q_0^{\alpha-1} - \lambda^{\beta+1} Q_0^{-\beta-1})\partial_p - \gamma p \partial_p + \gamma k_B T \partial_p^2 \\ &\approx \lambda^{\beta+1} Q_0^{-\beta-1}\partial_p.\end{aligned}$$

Summary: If p^2 is bounded and $U(q)$ is large

$$\mathcal{L} \approx -U'(q)\partial_p.$$

Solve:

$$-U'(q)\partial_p\psi(q,p) = -\kappa$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1} Q_\infty^{\alpha-1} \partial_p.$$

Q_0 scaling:

$$\begin{aligned} \mathcal{L} &= \lambda p \partial_{Q_0} - (\alpha\lambda^{-\alpha+1} Q_0^{\alpha-1} - \lambda^{\beta+1} Q_0^{-\beta-1})\partial_p - \gamma p \partial_p + \gamma k_B T \partial_p^2 \\ &\approx \lambda^{\beta+1} Q_0^{-\beta-1} \partial_p. \end{aligned}$$

Summary: If p^2 is bounded and $U(q)$ is large

$$\mathcal{L} \approx -U'(q)\partial_p.$$

Solve:

$$\begin{aligned} -U'(q)\partial_p \psi(q,p) &= -\kappa \\ \Longrightarrow \qquad \psi(q,p) &= \kappa \frac{p}{U'(q)} + f(q). \end{aligned}$$

Defining ψ

Recall the Q_∞ scaling:

$$\mathcal{L} \approx -\alpha\lambda^{\alpha-1}Q_\infty^{\alpha-1}\partial_p.$$

Q_0 scaling:

$$\begin{aligned}\mathcal{L} &= \lambda p\partial_{Q_0} - (\alpha\lambda^{-\alpha+1}Q_0^{\alpha-1} - \lambda^{\beta+1}Q_0^{-\beta-1})\partial_p - \gamma p\partial_p + \gamma k_B T\partial_p^2 \\ &\approx \lambda^{\beta+1}Q_0^{-\beta-1}\partial_p.\end{aligned}$$

Summary: If p^2 is bounded and $U(q)$ is large

$$\mathcal{L} \approx -U'(q)\partial_p.$$

Solve:

$$\begin{aligned}-U(q)\partial_p\psi(q,p) &= -\kappa \\ \implies \psi(q,p) &= \kappa\frac{p}{U'(q)} + \cancelto{0}{f(q)}.\end{aligned}$$

Faster return times?

Point: Should be the case that $W = e^{\delta(H+\psi)} \approx e^{\delta H}$ satisfies

$$\mathcal{L}W(q,p) \leq -cW + D$$

for some constants $c, D > 0$.

Faster return times?

Point: Should be the case that $W = e^{\delta(H+\psi)} \approx e^{\delta H}$ satisfies

$$\mathcal{L}W(q,p) \leq -cW + D$$

for some constants $c, D > 0$.

Why? For $H \geq R$

$$\begin{aligned}\mathcal{L}W(q,p) &= \delta W(q,p) \times \left[\mathcal{L}V(q,p) + \delta\gamma k_B T |\nabla_p(V)|^2\right] \\ &\leq \delta W(q,p) \times \left[-\gamma \|p\|^2 - \gamma k_B T k N + \delta\gamma k_B T \|p\|^2 + \delta o(1)\right]\end{aligned}$$

Faster return times?

Point: Should be the case that $W = e^{\delta(H+\psi)} \approx e^{\delta H}$ satisfies

$$\mathcal{L}W(q,p) \leq -cW + D$$

for some constants $c, D > 0$.

Why? For $H \geq R$

$$\begin{aligned}\mathcal{L}W(q,p) &= \delta W(q,p) \times \left[\mathcal{L}V(q,p) + \delta\gamma k_B T|\nabla_p(V)|^2\right] \\ &\leq \delta W(q,p) \times \left[-\gamma\|p\|^2 - \gamma k_B TkN + \delta\gamma k_B T\|p\|^2 + \delta o(1)\right]\end{aligned}$$

Conclusion: Exponentiate δV and control quadratic variation terms by picking $0 < \delta < 1/(k_B T)$.

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

is a viable perturbation.

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

  is a viable perturbation.
- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

  is a viable perturbation.
- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.
- Relationship to ϵpq? $\psi = \epsilon p \frac{U(q)}{U'(q)} \approx \epsilon pq$.

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

  is a viable perturbation.
- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.
- Relationship to ϵpq? $\psi = \epsilon p \frac{U(q)}{U'(q)} \approx \epsilon pq$.
- Condition $|\nabla^2 U|$ dominated by $|\nabla U|^2$ for large U?

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

  is a viable perturbation.
- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.
- Relationship to ϵpq? $\psi = \epsilon p \frac{U(q)}{U'(q)} \approx \epsilon pq$.
- Condition $|\nabla^2 U|$ dominated by $|\nabla U|^2$ for large U?

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

  is a viable perturbation.

- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.
- Relationship to ϵpq? $\psi = \epsilon p \frac{U(q)}{U'(q)} \approx \epsilon pq$.
- Condition $|\nabla^2 U|$ dominated by $|\nabla U|^2$ for large U?

$$p\partial_q\left(\kappa \frac{p}{U'(q)}\right) = -\kappa p^2 \frac{U''(q)}{(U'(q))^2}$$

Concluding remarks

- For general k, N, one can repeat the analysis to conclude

$$\psi = \frac{p \cdot \nabla U}{|\nabla U|^2}$$

is a viable perturbation.

- Why is it so easy? Finding the right equation to solve IS the hardship because ∇U does not scale homogeneously with U.
- Relationship to ϵpq? $\psi = \epsilon p \frac{U(q)}{U'(q)} \approx \epsilon pq$.
- Condition $|\nabla^2 U|$ dominated by $|\nabla U|^2$ for large U?

$$p\partial_q\left(\kappa \frac{p}{U'(q)}\right) = -\kappa p^2 \frac{U''(q)}{(U'(q))^2}$$

$\implies$ competition with $-\gamma p^2$ unless condition is satisfied.