Uncertainty Relations and Diffusion Processes

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Outline of the talk

1. Introduction:
2. Controlled diffusions
   - Schrödinger diffusion problem
     - A Kolmogorov interludio
   - Explicit form of the optimal control problem
3. Refined second law
   - Schrödinger diffusion: alternative formulation
   - Solvable cases
     - Equilibrium
     - Langevin–Smoluchowski limit
     - Gaussian boundary conditions
4. Conclusions

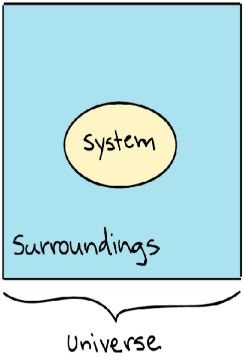
Micro- and sub-micro systems

- Here comes something

1st block 1st column

2nd block 1st column

- Times long with respect to the relaxation time of the reservoir.
- Markovian approximation.



Schrödinger question

Let the probability to find the particle in a certain position be assigned not only at time t_o but also at a second time instant $t_1 > t_0$:

$$w(x, t_0) = w_0(x); \qquad w(x, t_1) = w_1(x)$$

What is the probability for

$$w(x, t)$$

intermediate times, i.e., for any t such that

$$t_0 \le t \le t_1 \qquad ?$$

Langevin–Kramers dynamics

$$d\chi_t = \left(\mathsf{J} - \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\, dt + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2}\, d\boldsymbol{W}_t$$

$\chi_t \mapsto \boldsymbol{x} = [\boldsymbol{q}\,,\boldsymbol{p}]^\dagger \in \mathbb{R}^{2d}$ with $\boldsymbol{q}\,,\boldsymbol{p} \in \mathbb{R}^d$

$$\lim_{dt\downarrow 0} \mathrm{E}_{\boldsymbol{x},t}\frac{f(\chi_{t+dt}) - f(\chi_t)}{dt} =$$

$$\Big\{ \underbrace{(\partial_{\boldsymbol{x}} H)\cdot \mathsf{J}^\dagger \cdot \partial_{\boldsymbol{x}}}_{\text{Symplectic structure}} + \underbrace{\frac{m}{\tau}\left(-(\partial_{\boldsymbol{x}} H)\cdot \mathsf{S}_g \cdot \partial_{\boldsymbol{x}} + \frac{1}{\beta}\mathsf{S}_g : \partial_{\boldsymbol{x}} \otimes \partial_{\boldsymbol{x}}\right)}_{\text{Dissipative structure}} \Big\} f(\boldsymbol{x})$$

Zwanzig, R. Journal of Statistical Physics, 1973, 9, 215-220
Cépas, O. & Kurchan, J. EPJ B: Condensed Matter and Complex Systems, 1998, 2, 221-223

Langevin–Kramers dynamics

Wiener increment

$$d\chi_t = \left(\mathsf{J} - \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\, dt + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2}\, d\boldsymbol{W}_t$$

$$H = \frac{\|\boldsymbol{p}\|^2}{2} + U(\boldsymbol{q}, t) \qquad \mathsf{J} = \begin{bmatrix} 0 & 1_d \\ -1_d & 0 \end{bmatrix} \qquad \mathsf{S}_g = \begin{bmatrix} \frac{g\,\tau^2}{m^2} 1_d & 0 \\ 0 & 1_d \end{bmatrix}$$

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Abnormal fluctuation

Normal diffusion

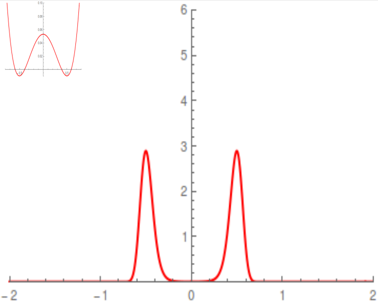
- Fix initial data
- Fix final data

Final data (abnormal)

- observed first a normal distribution
- observed later an anomalous fluctuation
- anomalous fluctuation brought into beiing by reverting the sign of the diffusion current!

Evolution of probability densities

Double well in one dimension



Initial state= $\mathrm{p}(\boldsymbol{x}, t_{\mathrm{o}})$

Markovian dynamics

Final state

Given the Hamiltonian H the transition probability density $\mathrm{p}(\boldsymbol{x}, t_{\mathrm{f}} \,|\, \boldsymbol{y}, t_{\mathrm{o}})$ is fixed

$$\mathrm{p}(\boldsymbol{x}, t_{\mathrm{f}}) = \int_{\mathbb{R}^{2\,d}} \mathrm{d}^d\boldsymbol{y}\, \mathrm{p}(\boldsymbol{x}, t_{\mathrm{f}} \,|\, \boldsymbol{y}, t_{\mathrm{o}})\, \mathrm{p}(\boldsymbol{y}, t_{\mathrm{o}})$$

Asymptotic state of probability densities

For any choice of the parameters:

- Einstein relation:
  The covariance of the noise is aligned with the matrix S_g appearing in the dissipative force $\mathsf{S}_g \partial_{\boldsymbol{x}} H$.
- H theorem.
- Boltzmann equilibrium: if the potential energy is confining

$$\mathrm{p}_{\infty}(\boldsymbol{x}) \propto \exp - \beta \left(\frac{\|\boldsymbol{p}\|^2}{2\,m} + U(\boldsymbol{q}) \right)$$

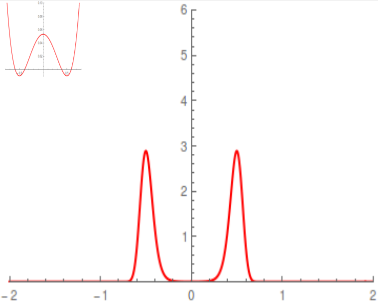
Schrödinger diffusion problem (1931)

**Schrödinger, "Über die Umkehrung der Naturgesetze"
Sitz.-Ber. d Preuss. Akad. d. Wiss., Phys.-math. Klasse, 1931**

- end states given
- the drift steering the transition along the path of a diffusion is unknown
- how to choose it?

Transition between two assigned states in a finite time

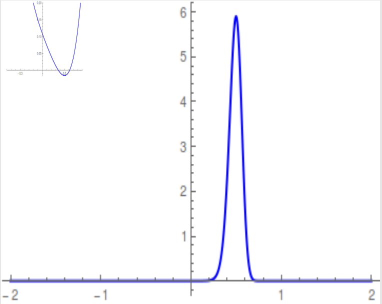
Double well in one dimension



Initial state

Controlled

Markovian dynamics



Final state

Schrödinger, “Über die Umkehrung der Naturgesetze”

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The 1931 idea

Minimize a Kullback–Leibler divergence (introduced in 1951)

$$\text{drift} = \operatorname{argmin}_{u \in \mathbb{A}} \int \mathrm{dP}[u] \, \ln \frac{\mathrm{dP}[u]}{\mathrm{d}\bar{\mathrm{P}}}$$

Kullback, S. & Leibler, R. Annals of Mathematical Statistics, 1951, 22, 79-86
Aebi, R. *Schrödinger Diffusion Processes* Birkhäuser, 1996, 186
Chung, K. L. & Zambrini, J.-C. *Introduction to random time and quantum randomness* World Scientific, 2003, 1, 211

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- $\bar{\mathrm{P}}$ measure of a fixed reference diffusion process.

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- $\bar{\mathrm{P}}$ measure of a fixed reference diffusion process.
- P measure of a diffusion process matching the boundary data.

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- $\bar{\mathrm{P}}$ measure of a fixed reference diffusion process.
- P measure of a diffusion process matching the boundary data.
- u drift of a diffusion process matching the boundary data.
- $\mathbb{A}$ space of admissible drifts.

Kullback, S. & Leibler, R. Annals of Mathematical Statistics, 1951, 22, 79-86
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Kolmogorov 1936

Zur Theorie der Markoffschen Ketten.

Von

A. Kolmogoroff in Moskau.

Die nachfolgenden Betrachtungen scheinen mir, trotz ihrer Einfachheit, neu und nicht ohne Interesse für gewisse physikalische Anwendungen zu sein, insbesondere für die Analyse der Umkehrbarkeit der statistischen Naturgesetze, welche Herr Schrödinger im Falle eines speziellen Beispiels durchgeführt hat[1]). In der ganzen weiteren Darstellung ist es gleichgültig, welche der beiden folgenden Voraussetzungen über die in Betracht kommenden Werte der Zeitkoordinate t gemacht wird: entweder durchläuft t alle reellen Werte, oder man beschränkt sich auf die Heranziehung der ganzzahligen Werte von t. Der klassischen Auffassung Markoffscher Ketten entspricht die zweite Möglichkeit.

1. Begriff der Markoffschen Kette.

Wir betrachten ein physikalisches System, welches sich in jedem Zeitmoment t in einem der endlich vielen verschiedenen Zustände E_1, $E_2, \ldots, E_N$ befinden kann. Wir setzen dabei voraus, daß für je zwei Zustände E_i und E_j und je zwei Zeitmomente t und s, $t \leq s$, eine bestimmte bedingte Wahrscheinlichkeit $P_{ij}(t, s)$ dafür existiert, daß unter der Voraussetzung des Zustandes E_i im Zeitmoment t der Zustand E_j im Zeitmoment s auftreten wird. Eine wesentliche, nicht immer mit genügender Klarheit hervorgehobene weitere Voraussetzung bildet die Unabhängigkeit der bedingten Wahrscheinlichkeit $P_{ij}(t, s)$ von beliebigen Kenntnissen über die Vorgeschichte des Systems vor dem Zeitmoment t. Auf dieser Voraussetzung beruht wesentlich die Ableitung der fundamentalen Gleichung der Theorie der Markoffschen Ketten:

$$P_{ik}(s, t) = \sum_j P_{ij}(s, u)\, P_{jk}(u, t), \qquad s \leq u \leq t. \tag{1}$$

Außer der Fundamentalgleichung (1) erwähnen wir die Formeln

$$P_{ij}(t, s) \geq 0, \tag{2}$$

$$\sum_j P_{ij}(t, s) = 1, \tag{3}$$

$$P_{ij}(t, t) = \delta_{ij}, \tag{4}$$

wobei δ_{ij} gleich 0 oder 1 ist, je nachdem $i \neq k$, oder $i = k$ ist.

[1]) Berliner Berichte 1931, S. 144.

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Kolmogorov 1937

Zur Umkehrbarkeit der statistischen Naturgesetze.

Von

A. Kolmogoroff in Moskau.

§ 1.

Die Problemstellung.

Es wird eine n-dimensionale differentialgeometrische Mannigfaltigkeit R betrachtet. Sei $f(t, x, y)\, d y_1\, d y_2 \ldots d y_n$ die Wahrscheinlichkeit des Überganges, im Laufe der Zeit $t > 0$, aus dem Punkte x in einen Punkt η, dessen Koordinaten η_i die Ungleichungen $y_i < \eta_i < y_i + d y_i$ befriedigen. Wir setzen voraus, daß $f(t, x, y)$ Ableitungen bis zu einer genügend hohen Ordnung besitzt und den folgenden Bedingungen genügt [1]):

$$f(t, x, y) \geqq 0, \tag{1}$$

$$\int\int \ldots \int_R f(t, x, y)\, d y_1\, d y_2 \ldots d y_n = 1, \tag{2}$$

$$f(s + t, x, y) = \int\int \ldots \int_R f(s, x, z)\, f(t, z, y)\, d z_1\, d z_2 \ldots d z_n, \tag{3}$$

$$\begin{cases} \int\int \ldots \int_G f(t, x, y)\, d y_1\, d y_2 \ldots d y_n \to 1, \\ \text{mit } t \to 0, \text{ falls } x \text{ innerhalb des Gebietes } G \text{ liegt.} \end{cases} \tag{4}$$

Ist die Funktion $f(t, x, y)$ gegeben, so definiert die Funktion $p(x)$ dann und nur dann eine mit $f(t, x, y)$ verträgliche *stationäre Wahrscheinlichkeitsverteilung*, wenn die Bedingungen:

$$p(x) \geqq 0, \tag{5}$$

$$\int\int \ldots \int_R p(x)\, d x_1\, d x_2 \ldots d x_n = 1, \tag{6}$$

$$p(y) = \int\int \ldots \int_R p(x)\, f(t, x, y)\, d x_1\, d x_2 \ldots d x_n \tag{7}$$

erfüllt sind.

Die stationäre Verteilung ist *ergodisch*, falls, bei beliebigen x und y, die Relation $f(t, x, y) \to p(y)$ mit $t \to \infty$ stattfindet. Es folgt aus der Formel (7), daß eine ergodische stationäre Verteilung immer auch die einzige stationäre Verteilung ist, d. h.: sobald eine ergodische stationäre Verteilung $p_0(x)$

[1]) Vgl. A. Kolmogoroff: a) Über die analytischen Methoden in der Wahrscheinlichkeitsrechnung, Math. Annalen 104 (1931), S. 415—458. b) Zur Theorie der stetigen zufälligen Prozesse, Math. Annalen 108 (1933), S. 149—160.

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Divergence between two mechanical systems

$$
\begin{aligned}
\mathrm{d}\boldsymbol{\xi}_t &= \left(\frac{\boldsymbol{\psi}_t}{m} - \frac{\tau\, g}{m}\,\partial_{\boldsymbol{\xi}_t} U\right)\mathrm{d}t + \sqrt{\frac{2\, g\, \tau}{m\, \beta}}\mathrm{d}\boldsymbol{w}_t \\
\mathrm{d}\boldsymbol{\psi}_t &= -\left(\frac{\boldsymbol{\psi}_t}{\tau} + \partial_{\boldsymbol{\xi}_t} U\right)\mathrm{d}t + \sqrt{\frac{2\, m}{\tau\, \beta}}\mathrm{d}\boldsymbol{\omega}_t
\end{aligned}
$$

$\mathrm{d}\boldsymbol{w}_t$, $\mathrm{d}\boldsymbol{\omega}_t$ independent d-dimensional Wiener processes

Divergence between two mechanical systems

Compare two systems with potentials $U^{(i)}$ for $i = 1, 2$

$$\mathrm{d}\boldsymbol{\xi}_t{}^{(i)} = \left(\frac{\boldsymbol{\psi}_t}{m} - \frac{\tau\, g}{m}\, \partial_{\boldsymbol{\xi}_t} U^{(i)} \right) \mathrm{d}t + \sqrt{\frac{2\, g\, \tau}{m\, \beta}} \mathrm{d}\boldsymbol{w}_t$$

$$\mathrm{d}\boldsymbol{\psi}_t{}^{(i)} = - \left(\frac{\boldsymbol{\psi}_t}{\tau} + \partial_{\boldsymbol{\xi}_t} U^{(i)} \right) \mathrm{d}t + \sqrt{\frac{2\, m}{\tau\, \beta}} \mathrm{d}\boldsymbol{\omega}_t$$

$\mathrm{d}\boldsymbol{w}_t$, $\mathrm{d}\boldsymbol{\omega}_t$ independent d-dimensional Wiener processes

Kullback–Leibler divergence for a transition for $t \in [t_{\mathrm{o}}\,, t_{\mathrm{f}}]$

$$\mathrm{K}(\mathrm{P}^{(2)} \| \mathrm{P}^{(1)}) = \frac{\beta\, \tau\, (1 + g)}{4\, m} \int_{t_{\mathrm{o}}}^{t_{\mathrm{f}}} \mathrm{d}t \; \mathrm{E}_{\mathrm{P}^{(2)}} \, \| \partial_{\boldsymbol{\xi}_t} (U^{(1)} - U^{(2)}) \|^2$$

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Fluctuation relations, time reversal and entropy production

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Kullback–Leibler as indicator of irreversibility

Forward process with measure P_F: t increases from t_o to t_f

$$\mathrm{d}\chi_t = \left(\mathsf{J} - \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\,\mathrm{d}t + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2}\mathrm{d}\boldsymbol{W}_t \quad \& \quad \chi_{t_\mathrm{o}} \overset{\text{law}}{=} \mathrm{p}_{t_\mathrm{o}}$$

Backward process with measure P_B: t decreases from t_f to t_o

$$\mathrm{d}\chi_t = \left(\mathsf{J} + \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\,\mathrm{d}t + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2}\mathrm{d}\boldsymbol{W}_t \quad \& \quad \chi_{t_\mathrm{f}} \overset{\text{law}}{=} \mathrm{p}_{t_\mathrm{f}}$$

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Kullback–Leibler as indicator of irreversibility

Forward process with measure P_F: t increases from t_{o} to t_{f}

$$d\chi_t = \left(\mathsf{J} - \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\, dt + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2} d\boldsymbol{W}_t \quad \& \quad \chi_{t_{\mathrm{o}}} \overset{\text{law}}{=} \mathrm{p}_{t_{\mathrm{o}}}$$

Backward process with measure P_B: t decreases from t_{f} to t_{o}

$$d\chi_t = \left(\mathsf{J} + \frac{m}{\tau}\mathsf{S}_g\right)\partial_{\chi_t} H\, dt + \sqrt{\frac{2\,m}{\beta\,\tau}}\,\mathsf{S}_g^{1/2} d\boldsymbol{W}_t \quad \& \quad \chi_{t_{\mathrm{f}}} \overset{\text{law}}{=} \mathrm{p}_{t_{\mathrm{f}}}$$

Entropy production during the transition

$$\mathrm{K}(\mathrm{P}_F \| \mathrm{P}_B) = \int d\mathrm{P}_F \, \ln \frac{d\mathrm{P}_F}{d\mathrm{P}_B}$$

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Explicit form of the cost functional

Dynamics

$$\mathrm{d}\boldsymbol{\xi}_t = \left(\frac{\boldsymbol{\psi}_t}{m} - \frac{\tau\, g}{m}\,\partial_{\boldsymbol{\xi}_t} U\right)\mathrm{d}t + \sqrt{\frac{2\, g\, \tau}{m\,\beta}}\mathrm{d}\boldsymbol{w}_t$$

$$\mathrm{d}\boldsymbol{\psi}_t = -\left(\frac{\boldsymbol{\psi}_t}{\tau} + \partial_{\boldsymbol{\xi}_t} U\right)\mathrm{d}t + \sqrt{\frac{2\, m}{\tau\,\beta}}\mathrm{d}\boldsymbol{\omega}_t$$

Boundary conditions

$$\mathrm{p}_\iota(\boldsymbol{q},\boldsymbol{p}) \propto \exp -\beta\left(\frac{\|\boldsymbol{p}\|^2}{2\,m} + U_\iota(\boldsymbol{q})\right)$$

$$\mathrm{p}_f(\boldsymbol{q},\boldsymbol{p}) \propto \exp -\beta\left(\frac{\|\boldsymbol{p}\|^2}{2\,m} + U_f(\boldsymbol{q})\right)$$

Kullback–Leibler divergence for a transition for $t \in [t_\mathrm{o}\,,\, t_\mathrm{f}]$

$$\mathrm{K}(\mathrm{P}_F \,\|\, \mathrm{P}_B) = \text{Gibbs–Shannon entropy change} - \frac{t_\mathrm{f} - t_\mathrm{o}}{\tau} d$$

$$+ \int_{t_\mathrm{o}}^{t_\mathrm{f}} \frac{\mathrm{d}t}{\tau}\, \mathrm{E}_{\mathrm{P}_F}\left\{\frac{\|\boldsymbol{\psi}_t\|^2}{m} + \frac{g\,\tau^2}{m}\left(\|\partial_{\boldsymbol{\xi}_t} U\|^2 - \frac{1}{\beta}\partial^2_{\boldsymbol{\xi}_t} U\right)\right\}$$

Vanishes at equilibrium !

Equilibrium

Maxwell–Boltzmann equilibrium

$$\mathrm{p_i}(\boldsymbol{x}) = \mathrm{p_f}(\boldsymbol{x}) \propto \exp\left\{-\beta\left(\frac{\|\boldsymbol{p}\|^2}{2\,m} + \bar{U}(\boldsymbol{q})\right)\right\}$$

The equations preserve equilibrium.

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Overdamped expansion

The typical length scale L of U_ι, U_f defines a characteristic time

$$L^2 = \frac{\tau\,\tau_L}{\beta\, m}$$

The overdamped limit

$$\varepsilon \equiv \frac{\tau}{\tau_L} \ll 1 \qquad \tau \sim \text{momentum equilibration time scale}$$

We may look for a control strategy of the form

$$H(\boldsymbol{q},\boldsymbol{p},t) = \frac{\|\boldsymbol{p}\|^2}{2\,m} + \sum_n \varepsilon^{n/2}\, U_n\left(\sqrt{\varepsilon}\,\boldsymbol{q}, t, \sqrt{\varepsilon}\,t, \varepsilon\,t \dots\right)$$

$$V(\boldsymbol{q},\boldsymbol{p},t) \equiv \sum_n \varepsilon^{n/2}\, V_n(\boldsymbol{p}, \sqrt{\varepsilon}\boldsymbol{q}, t, \sqrt{\varepsilon}\,t, \varepsilon\,t, \dots)$$

$$\mathrm{p}(\boldsymbol{p},\boldsymbol{q}_1,t,t_1,t_2) \equiv \sum_n \varepsilon^{n/2}\, \mathrm{p}_n(\boldsymbol{p}, \sqrt{\varepsilon}\,\boldsymbol{q}, t, \sqrt{\varepsilon}\,t, \varepsilon\,t, \dots)$$

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Configuration space dynamics in the overdamped limit

$$V(\boldsymbol{p},\boldsymbol{q},t)=\frac{(t_{\mathrm{f}}-t_0)\,d}{\beta\,\tau}+\frac{\|\boldsymbol{p}\|^2}{2\,m}+V_{0:1}\left(\sqrt{\varepsilon}\boldsymbol{q},\varepsilon\,t\right)+O(\sqrt{\varepsilon})$$

$$\mathrm{p}(\boldsymbol{p},\boldsymbol{q},t)=\left(\frac{\beta}{2\,\pi\,m}\right)^{d/2}e^{-\frac{\beta\,\|\boldsymbol{p}\|^2}{2\,m}}\,\mathrm{p}_{0:1}(\sqrt{\varepsilon}\boldsymbol{q},\varepsilon t)+O(\sqrt{\varepsilon})$$

Overdamped solution: $\mathrm{p}(\boldsymbol{q},t)=e^{-S(\boldsymbol{q},t)}$ & $\boldsymbol{q}_1=\sqrt{\varepsilon}\,\boldsymbol{q}$ & $t_2=\varepsilon\,t$

$$\partial_{t_2}S-\frac{\tau\,(1+g)}{m}(\partial_{\boldsymbol{q}_1}\tilde{U})\cdot\partial_{\boldsymbol{q}_1}S+\frac{\tau\,(1+g)}{m}\partial^2_{\boldsymbol{q}_1}\tilde{U}=0$$ mass conservation

$$\partial_{t_2}\tilde{U}-\frac{\tau\,(1+g)}{2\,m}\|\partial_{\boldsymbol{q}_1}\tilde{U}\|^2=0$$ HJB equation

$$V_{0:1}-U=U-\frac{1}{\beta}\tilde{S}=\tilde{U}$$ extremal condition

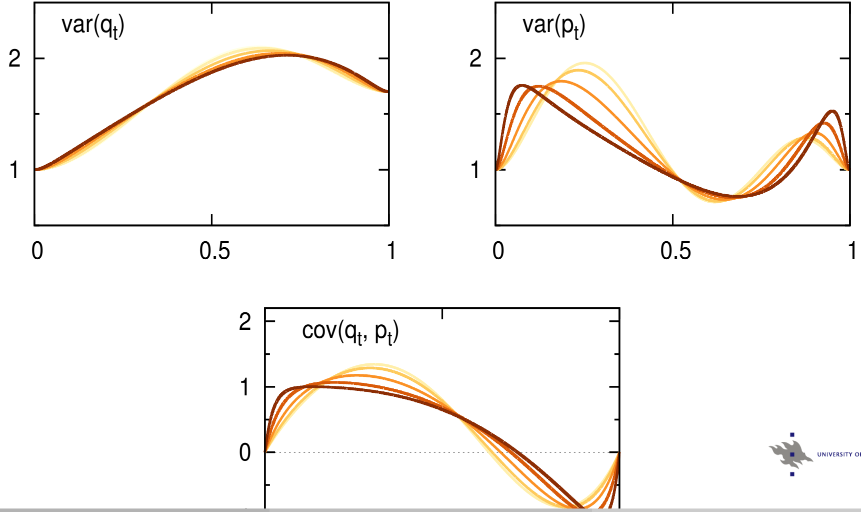
Gaussian case

Solvable for $g > 0$

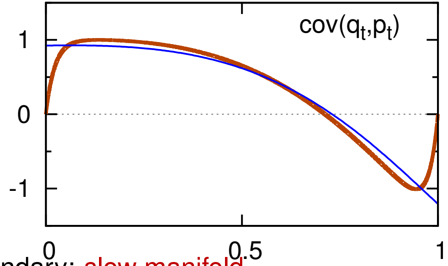
- Optimal control equation reduce to a finite dimensional kinetic hierarchy.
- Cumulants obey a finite set of ordinary differential equations.

Exact solution in the Gaussian case: covariance matrix

covariances as $g \to 0$



Slow Manifold for $g = 0$



- Away from boundary: slow manifold

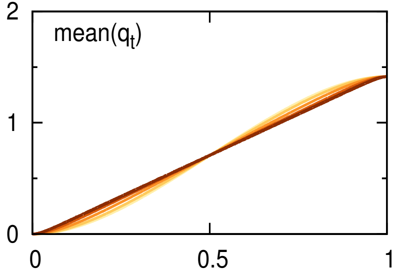
$$\boldsymbol{f}_p = \int_{\mathbb{R}^d} \mathrm{d}^d p \, \frac{\mathrm{p}(\boldsymbol{q},\boldsymbol{p},t)}{\tilde{\mathrm{p}}(\boldsymbol{q},t)} \, \partial_{\boldsymbol{p}} V(\boldsymbol{q},\boldsymbol{p},t) = 0$$

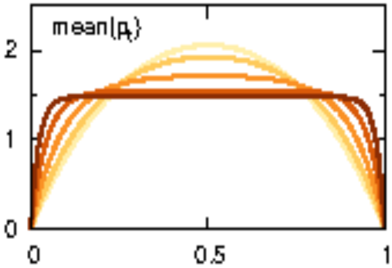
  Fokker-Planck + dynamic programming for $g = 0$

- At the boundary: $g \downarrow 0$ exponentially connects the slow manifold and boundary conditions

Exact solution in the Gaussian case: mean values

mean as $g \to 0$





Summary

- Symplectic structure introduces non local constraint.
- Optimal protocol (when they exist) describe transitions between non-equilibrium states
- Lower bound for accelerated equilibration.
- As we decrease the effect of thermal fluctuations we recover optimal control by Langevin–Smoluchowski dynamics.
- What beyond the overdamped limit?

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THANK YOU !

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