Nonequilibrium Markov processes conditioned on large deviations

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New Frontiers in Non-equilibrium Physics of Glassy Materials
Kyoto, JAPAN
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- Work with Hugo Touchette (Stellenbosch, South Africa)
- PRL 2013 and Ann. Henri Poincaré 2014
- New paper: arxiv:1506.05291

Heuristic of Large Deviation

"Improbable events permit themselves the luxury of occurring."
C.Chan 1928

- Random variable A_T which converges typically toward $\langle a \rangle$

Large Deviation

How improbable for A_T to converge towards a which is different from the typical value $\langle a \rangle$ (rare events) :

$$\text{LDP:} \quad \mathbb{P}\left(\mathbf{A_T \approx a}\right) \asymp \mathbf{exp(-TI(a))}$$

- $I(a)$: rate function (or fluctuation functional).
- Large deviation theory: 1 Prove the LDP and 2 calculate the rate function.

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Conditioning Problem

Physical

- Nonequilibrium process: $\{X_t\}_{t=0}^{T}$
- Observable: $A_T[x]$
- Consider trajectories leading to the constraint $A_T = a$
- Construct effective Markov process for forget the constraint

Mathematical

- Markov process: $\{X_t\}_{t=0}^{T}$
- Conditioned process: $X_t | A_T = a$
- "Deconditionning" :

$$\underbrace{X_t \,|\, A_T = a}_{\text{conditioned}} \quad \overset{T\to\infty}{\cong} \quad \underbrace{Y_t}_{\text{Equivalent Markovian process}}$$

Exemple Jump Process : the mercantile view of the scientific life

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Historial Work on "Deconditionning"

In Probability : Doob 1957

- $\{W_t \mid \text{ to go outside } [0, L] \text{ via } L\} \equiv \underbrace{Y_t}_{\text{EQN: } \frac{dY_t}{dt} = \frac{1}{Y_t} + \frac{dW_t}{dt}}$
- Brownian bridge : $\{W_t \mid W_T = 0\} \equiv \underbrace{Y_t}_{\text{EQN: } \frac{dY_t}{dt} = -\frac{Y_t}{T-t} + \frac{dW_t}{dt}}$
- Quasi-stationary distributions (Deroch-Seneta 1967):
  $\underbrace{X_t}_{\text{absorbing}} \mid \text{not reaching absorbing state} \equiv \underbrace{Y_t}_{\text{non-absorbing}}$

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But First : in Physics with Schrödinger 1931

E. Schrödinger

Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique

Annales de l'I. H. P., tome 2, n° 4 (1932), p. 269-310.

<http://www.numdam.org/item?id=AIHP_1932__2_4_269_0>

libre. Imaginez que vous observez un système de particules en diffusion, qui soient en équilibre thermodynamique. Admettons qu'à un instant donné t_0 vous les ayez trouvées en répartition à peu près uniforme et qu'à $t_1 > t_0$ vous ayez trouvé un écart spontané et *considérable* par rapport à cette uniformité. On vous demande de quelle manière cet écart s'est produit. Quelle en est la manière la plus probable ?

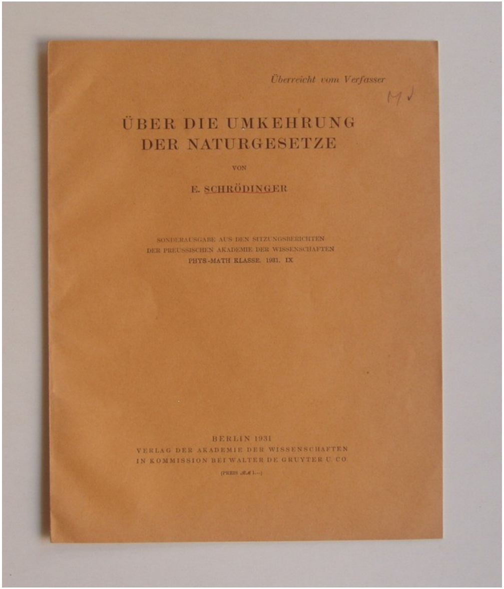
VII. — **Une analogie entre la mécanique ondulatoire et quelques problèmes de probabilités en physique classique**

Le sujet que je vais aborder maintenant n'est pas intimement lié aux questions dont il s'est agi dans les chapitres précédents. Tout d'abord vous aurez l'impression de choses qui ne sont pas du tout liées. Il s'agit d'un problème classique : problème de probabilités dans la théorie du mouvement brownien. Mais en fin de compte, il *ressortira* une analogie avec la mécanique ondulatoire, qui fut si frappante pour moi lorsque je l'eus trouvée, qu'il m'est difficile de la croire purement accidentelle.

A titre d'introduction, je voudrais vous citer une remarque que j'ai trouvée dans les « Gifford lectures » de A. S. EDDIGTON (Cambridge, 1928, p. 216 et sqq). EDDINGTON, en parlant de l'interprétation de la mécanique ondulatoire, fait dans une note au bas de la page la remarque suivante :

« The whole interpretation is very obscure, but it seems to depend on whether you are considering the probability *after you know what has happened* or the probability for the purposes of prediction. The $\psi\psi^*$ is obtained by introducing two symmetrical systems of ψ waves travelling in opposite directions in time ; one of these must presumably correspond to probable inference from what is known (or is stated) to have been the condition at a later time. »

Les recherches que je vais exposer ne forment nullement une théorie nette et complètement achevée [1]. Le lien commun, un peu lâche d'ailleurs, qui les rattache les unes aux autres, la source commune dont elles dérivent, est le mécontentement que l'on éprouve quand on considère l'état présent de la théorie et surtout celui de l'*interprétation physique actuelle* de la mécanique quantique. Je voudrais


Überreicht vom Verfasser
ÜBER DIE UMKEHRUNG DER NATURGESETZE
VON
E. SCHRÖDINGER
SONDERAUSGABE AUS DEN SITZUNGSBERICHTEN
DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN
PHYS.-MATH. KLASSE. 1931. IX
BERLIN 1931
VERLAG DER AKADEMIE DER WISSENSCHAFTEN
IN KOMMISSION BEI WALTER DE GRUYTER U. CO.

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, $t \leqq s$, 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:

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

Außer der Fundamentalgleichung (1) erwähnen wir die Formeln

$$(2) \qquad P_{ij}(t, s) \geqq 0,$$

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

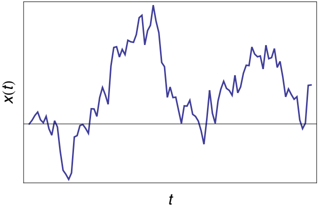
$$(4) \qquad P_{ij}(t, t) = \delta_{ij},$$

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

Diffusion Process

- SDE: (with additive noise here for simplicity)

$$dX_t = F(X_t)dt + \sigma dW_t$$



- One or many particles
- Equilibrium or nonequilibrium
- Includes external forces, reservoirs
- Generator:

$$\partial_t E_x[f(X_t)] = E_x[Lf(X_t)], \qquad \partial_t p(x,t) = L^\dagger p(x,t)$$

$$L = F \cdot \nabla + \frac{D}{2}\nabla^2, \qquad D = \sigma\sigma^T$$

- Path distribution: $\mathbb{P}_{[0,T]}[x]$

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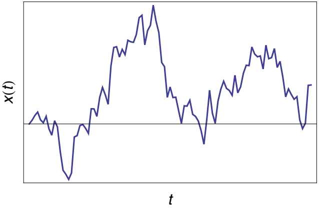

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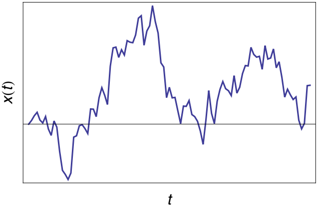

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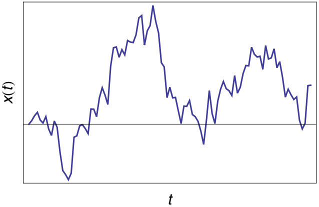
Observable - random variable

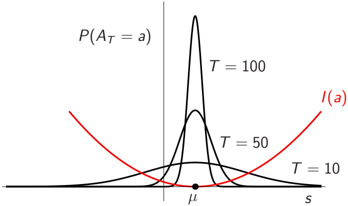
- Path x_t over $[0, T]$
- General observable:

$$A_T = \frac{1}{T}\int_0^T f(X_t)\,dt + \frac{1}{T}\int_0^T g(X_t)\circ dX_t$$



- Large deviation principle (LDP):

$$\mathbb{P}(A_T = a) \approx e^{-T I(a)}, \quad T \to \infty$$



Examples

- Occupation time, mean speed, empirical drift
- Work, heat, probability current, entropy production
- Jump process: current, activity

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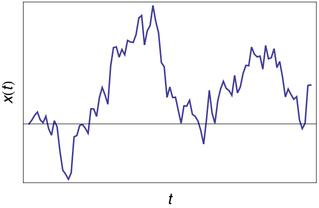

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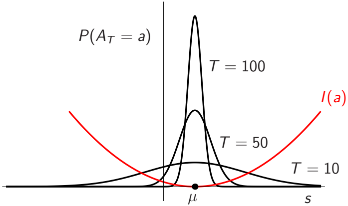

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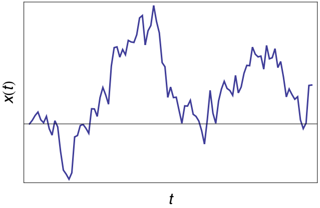

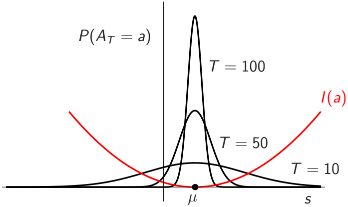

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Conditioned process

- Path microcanonical ensemble :

$$\mathbb{P}^{micro}_{a,[0,T]}[x] \equiv \mathbb{P}([x]/A_T = a) = \frac{\mathbb{P}_{[0,T]}[x]\,\delta(A_T[x] - a)}{\mathbb{P}(A_T = a)}$$

- Intermediate : Path Canonical Ensemble

$$\mathbb{P}^{cano}_{k,[0,T]}[x] \equiv \frac{\mathbb{P}_{[0,T]}[x]\exp(kTA_T)}{\mathbb{E}_{\mathbb{P}}(\exp(kTA_T))}$$

- Motivation in Physics for the Thermodynamics of Trajectories :
  - Conditioned view to Sheared Fluids (M.Evans).
  - Dynamical Phase transition for Kinetically constrained models (V.Lecomte, F.Van Wijland,...).
  - Rare trajectories of Glassy phases (D.Chandler, J.P Garrahan...)

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Driven process

- Tilted (Feynman-Kac) generator:

$$\mathcal{L}_k = F \cdot (\nabla + kg) + \frac{D}{2}(\nabla + kg)^2 + kf, \qquad k \in \mathbb{R}$$

- Dominant (Perron-Frobenius) eigenvalue: Λ_k
- right Eigenfunction: $r_{k(x)}$ and left Eigenfunction: $l_{k(x)}$

Generator

$$L_k = {r_k}^{-1}\mathcal{L}_k r_k - {r_k}^{-1}(\mathcal{L}_k r_k)$$

- Generalized Doob transform
- Driven SDE:

$$d\hat{X}_t = F_k(\hat{X}_t)dt + \sigma dW_t$$

- Modified drift:

$$F_k = F + D(kg + \nabla \ln r_{k)}$$

- Associated Path distribution $\mathbb{P}_k^{\text{driven}}[x]$

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Main result

Hypotheses

- A_T satisfies LDP
- Rate function $I(a)$ convex
- Other properties (spectral gap, regular r_k)

Result : Equivalent Markovian process

$$X_t | A_T = a \quad \overset{T\to\infty}{\cong} \quad Y_t$$

$$\mathbb{P}^{micro}_{a,[0,T]}[x] \quad \approx \quad \mathbb{P}^{\text{driven}}_{k(a)}[x] \text{ si } \; k(a) = I'(a)$$

$$B_T \to b^* \quad \Longleftrightarrow \quad B_T \to b^*$$

Pause $\frac{1}{T}\int_0^T dt\delta(X_t - .) \to r_{k(a)} l_{k(a)} \quad \Leftarrow \quad \frac{1}{T}\int_0^T dt\delta(X_t - .) \to r_{k(a)} l_{k(a)}$

- Same typical states but different fluctuations in general
- Precursor Work : Jack-Sollich 2010 understood the path canonical ensemble associated to Pure Jump process

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Simple applications

- Modified drift: $F_k = F + D(kg + \nabla \ln r_k)$

Brownian motion

$$W_t | W_T = aT \qquad \to \qquad \hat{X}_t = W_t + at$$

Ornstein-Uhlenbeck process

$$dX_t = -\gamma X_t dt + \sigma dW_t$$

- Empirical drift/area:

$$A_T = \frac{1}{T}\int_0^T X_t dt \qquad \to \qquad F_{k(a)}(x) = -\gamma x + \frac{a}{\gamma}$$

- Empirical variance:

$$A_T = \frac{1}{T}\int_0^T X_t^2 dt \qquad \to \qquad F_{k(a)}(x) = -\frac{\sigma^2}{2a}x$$

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$$A_T = \frac{1}{T} \int_0^T X_t^2 dt \qquad \longrightarrow \qquad F_{k(a)}(x) = -\frac{\sigma^2}{2a} x$$

Conclusion

$$\underbrace{X_t \,|\, A_T = a}_{\text{conditioned microcanonical}} \quad \overset{T\to\infty}{\cong} \quad \underbrace{Y_t}_{\text{Equivalent process}}$$

- Process (ensemble) equivalence
- Effective Markov dynamics for fluctuations
- Optimal (asymptotic) change of measures
- Also works for Markov chains, jump processes, mixed processes

Other links/applications

- Variational principles : Rayleigh-Ritz, Donsker-Varadhan, Nemoto-Sasa
- Stochastic optimal control : Flemming-Sheu

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- Nonequilibrium maxent
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Practical interest ? Maybe

Physics is like ♡ : sure, it may give practical results,
but that is not why we do it. Richard Feynman (1918 - 1988)