Fluctuation relations for diffusion processes

Raphael CHETRITE

Weakly non-equilibrium dynamics :

- Fluctuation dissipation theorem
- Green-Kubo relations
- Onsager relations

Far from equilibrium equilibrium dynamics :

FLUCTUATION RELATIONS

→ Robust identities for non-equilibrium systems and reducing close to equilibrium to the previous relations.

Fluctuation relations for diffusion processes. R.Chetrite, K.Gawedzki,
arXiv:0707.2725, appear in CMP

Mathematical setup for this talk:
Diffusion processes

Vincent Doeblin, soldat téléphoniste, automne 1939

$$\frac{dx}{dt} = u_t(x) + v_t(x)$$

$$\left\langle v_t^i(x) v_{t'}^j(x') \right\rangle = \delta(t - t') D_t^{ij}(x, x')$$

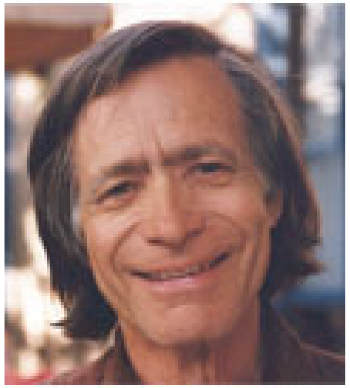
Stratonovich convention

ITO (1915-)

The **density** $\exp(-\varphi_t(x))$ of x_t satisfies the continuity equation (Focker-Planck) :

$$\partial_t \rho_t + \partial_i J_t^i = 0$$

Exemple1 : Kraichnan model



Kraichnan

$$\frac{dx}{dt} = v_t(x)$$

where solutions x_t represent trajectories of fluid particles with **no inertia** in a synthetic random flow.

Exemple 2 : Deterministic dynamics

$$\frac{dx}{dt} = u_t(x)$$

Example 3 : Langevin equation

$$\frac{dx}{dt} = -\Gamma\nabla H_t + \Pi\nabla H_t + G_t(x) + \eta_t$$

Dissipative term

Hamiltonian term

Non-Conservative force

White noise

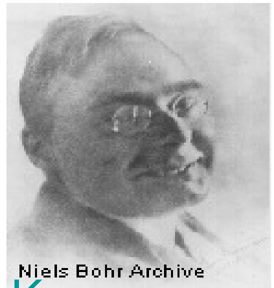
Langevin Paul(1872-1946)

$$\langle \eta_t^i \eta_{t'}^j \rangle = \frac{2}{\beta}\Gamma^{ij}\delta(t-t')$$

Einstein relation

Special case : **Kramers model**

- $H_t(q,p) = \frac{p^2}{2m} + V_t(q)$
- $\Gamma = \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix}$
- $\Pi = \begin{pmatrix} 0 & Id \\ -Id & 0 \end{pmatrix}$
- $G(t) = \begin{pmatrix} 0 \\ f(t,q) \end{pmatrix}$



Kramers Hendrik (1894-1952)

$$\Rightarrow \quad m\frac{d^2q}{d^2t} = -\gamma\frac{dq}{dt} - \nabla V_t(q) + f_t(q) + \eta_t$$

Langevin model I : $$\frac{dx}{dt} = -\Gamma \nabla H + \eta(t)$$

The **density current** associated to the **Gibbs density** vanishes and we have the **detailed balance (DB) :**

$$\exp(-\beta H(x))P^T(x \rightarrow y) = \exp(-\beta H(y))P^T(y \rightarrow x)$$

⇨ Strong equilibrium

Langevin-Kramer model II : $$\frac{dx}{dt} = -\Gamma\nabla H + \Pi\nabla H + \eta_t$$

The **density current** associated to the **Gibbs density** is not zero so the **detailed balance** is broken but we have the **modified detailed balance(MDB)** :

$$\exp(-\beta H(q_1, p_1))P^T(q_1, p_1 \rightarrow q_2, p_2) = \exp(-\beta H(q_2, p_2))P^T(q_2, -p_2 \rightarrow q_1, -p_1)$$

⇨ equilibrium

What we can say if we add an external force and an explicit dependence in time?

Langevin-Kramers model III

$$\frac{dx}{dt} = -\Gamma \nabla H + \Pi \nabla H + G + \eta(t)$$

The **Gibbs density** is no invariant, there may be a new invariant density $\exp(-\varphi(x))$

but it doesn't satisfy neither the **detailed balance**, nor a **modified detailled balance**.

Steady-state out of equilibrium.

What relation can repace the **MDB**, two way of generalization :

We can compare the process with another process called the **backward process :**

Chernyak …(2006)

$$\exp(-\varphi(X))P^{T}(X \to Y) = \exp(-\varphi(Y))P^{T,r}(Y \to X)$$

transition probability of a new system obtained by **current reversal**

We can restrict our space of path such that a functionnal of path take a special value :

$$\exp(-\beta H(q_1, p_1))P^{T}(q_1, p_1 \to q_2, p_2, \mathrm{W})\exp(\text{-}\mathrm{W}) = \exp(-\beta H(q_2, p_2))P^{T}(q_2, -p_2 \to q_1, -p_1, \text{-}\mathrm{W})$$

Here, the fonctionnal is :

$$W^{T} = \int_0^T dt[\beta G^{i}(x_t)\partial_i H(x_t) - \nabla G]$$

One dimensional Langevin equation with flux solution (IV) :

$$\frac{dx}{dt} = -\frac{dH}{dx} + \eta_t$$

$$\langle \eta_t \eta_{t'} \rangle = \frac{2}{\beta} \delta(t - t')$$

With : $H(x) \propto ax^{2k+1}$

Then , the Gibbs density $\exp(-\beta H)$ is not normalisable , and there is an unique invariant probability measure , the state breaking **Witten's QM SUSY** :

$$\mu(dx) = \frac{dx \exp(-\beta H(x)) \int_{-\infty}^{x} \exp(\beta H(x'))dx'}{N} = \exp(-\varphi(x))dx$$

Exemple : one dimensionnal Anderson localisation

Stationary Schrodinger equation : $$-\frac{d^2}{dt^2}w + U(t)w = Ew$$

In the random gaussian potential with correlation : $$\langle U(t)U(t')\rangle = 2D\delta(t-t')$$

Halperin(1965) introduces the real variable : $$X = \frac{d}{dt}(\ln|w|)$$

Satisfying the Langevin equation of type IV : $$\frac{dX}{dt} = -(X^2 + E) + U(t)$$

General result

For a general diffusive system, the **detailled balance** may be replaced by the **Detailed fluctuation relation (DFR)** **:**

$$\mu_0(dx)P^T(x \to y, W)\exp(\text{-W})\text{dy} = \mu^r{}_0(dy^*)P^{T,r}(y^* \to x^*, \text{-W})\text{dx}^*$$

Where :

⇨ $\mu_0(dx) = \exp(-\varphi_0(x))dx$ is the initial distribution of the forward process.

⇨ $\mu_0^r(dy) = \exp(-\varphi_0^r(y))dy$ is the initial distribution of the backward process.

Time inversion leading to the backward process **:**

Involution : $(t, x) \rightarrow (T - t, x^{*})$

Splitting : $u_t(x) = u_{t,+}(x) + u_{t,-}(x)$

Transfo as a vector field

Tranfo as a pseudo-vector field

The **backward process** satisfies the SDE :

$$\frac{dx^{r}}{dt} = R[u_{+,T-t}(x) - u_{-,T-t}(x) - v_{T-t}(x)]$$

With : $$R^{i}_{j}(x) = \frac{\partial x^{*i}}{\partial x^{j}}(x)$$

The time inversion is the choice of the spatial involution and of a split.

Examples of time reversal

Reversed protocol : it's the choice :

$$x^* \equiv x\,, \qquad u_{t,+} = u_t\,, \qquad u_{t,-} = 0$$

First written by Lebowitz-Spohn

Current reversal :

it's the choice which permits that the **current** of the density $\varphi_t^r = \varphi_{T-t}$ for the backward process is the **opposite** of the current of the direct process : $J_t^r = -J_{T-t}$

$$x^* \equiv x\,, \qquad \hat{u}^i_{t,+} = -\tfrac{1}{2} d_t^{ij} \partial_i \varphi_t\,, \qquad u^i_{t,-} = \hat{u}^i_t + \tfrac{1}{2} d_t^{ij} \partial_i \varphi_t$$

First written by Chernyak,Chertkov and Jarzynski

$\exp(-\varphi_t(x))\,dx$ That would be an invariant measure if the time-dependance were frozen

Time reversal in Langevin-Kramers dynamics :

We want that the backward process be also of the Langevin type , the canonical choice is :

$$(q,p)^* = (q,-p)$$

First written by Kurchan

And :

$$u_{t,-} = \Pi \nabla H_t + G_t\,, \qquad u_{t,+}(x) = -\Gamma \nabla H_t$$

The backward process verifies a Langevin equation with :

$$\begin{cases} H_t^r(x) = H_{T-t}(x^*) \\ G_t^r(x) = -RG_{T-t}(x^*) \end{cases}$$

Functional W :

(Considered in special cases by many authors)

$$W_T = \Delta_T \varphi + \int_0^T J_t dt$$

Where $\Delta_T \varphi = \varphi_T(x_T) - \varphi_0(x_0)$ With $\exp(-\varphi_T(x))dx = \exp(-\varphi_0^r(x^*))dx^*$

And the functionnal J depends on the system and on the inversion :

$$J_t = 2\hat{u}_{t,+}(x_t)d^{-1}{}_t(x_t)(\dot{x}_t - u_{t,-}(x_t)) - \nabla . u_{t,-}(x_t)$$

The proofs use a combination of the Girsanov and Feymann-Kac formulae :

Kac Marc (1914-1984)

Feymann Richard (1918-1988)

Reformulation of DFR : generalization Crooks relation

For any functional F on the space of trajectories , we note F' the functional defined by :

$$F'[X] = F[\tilde{X}] \qquad \text{with :} \quad \tilde{X}_t = X^*_{T-t}$$

The fluctuation relation : DFR'

$$\langle F[X]\exp(-W_T[X])\rangle = \langle F'[X^r]\rangle^r$$

We define the measures on the space of trajectories on [O,T] :

$$\langle F[X]\rangle = \int dx \exp(-\varphi_0(x)) E_x[F[X]] = \int M[dX] F[X]$$

$$\langle F[X^r]\rangle^r = \int dx \exp(-\varphi_0^r(x)) E_x^r[F[X]] = \int M^r[dX] F[X]$$

So , we get :

$$\tilde{M}^r[dX] = \exp(-W[X]) M[dX]$$

Entropic interpretation of W

Recall that the relative entropy of the measure $\nu = \exp(-w)\mu$ w.r.t μ

is defined as $S(\mu/\nu) = \int w(x)\mu(dx)$ and is non-negative.

We have then : $\langle W_T \rangle = S(M / \tilde{M}^r) \geq 0$

$\langle W_T \rangle$ is the entropy creation if $\mu_T = \mu_0 P_{O,T}$ ⇒ Second law for diffusion process

Other Fluctuations relations

DFR' with F=1 : **Jarzynski relation**

$$\langle \exp(-W_T[X]) \rangle = 1$$

Weakly out equilibrium limit ⇒

- Fluctuation dissipation theorem
- Green-Kubo relations
- Onsager relations

First obtained by Jarzynski in 1997 for time-dependant hamiltonian dynamical system.

Generalised Gallavotti-Cohen relation :

For a time-independent dynamics, one may expect , and sometimes prove the convergence at long time to a non-equilibrium stationnary state and the emergence of the large deviation regime :

$$P^T(x \to y, W = Tw) \propto \exp(-TZ(w))$$

Then **DFR** imply the **generalised Gallavotti-cohen relation (GC)** :

$$Z(w) + w = Z^r(w)$$

First proven by Gallavotti-Cohen in 1995 for chaotic deterministic dynamical systems and extended by Kurchan and Lebowitz-Spohn to (some) diffusion processes.

Langevin case IV :

$$\frac{dx}{dt} = -\frac{dH_t}{dx} + \eta_t$$

$$\langle \eta_t \eta_{t'} \rangle = \frac{2}{\beta}\delta(t-t')$$

With $H_t(x) \propto a x^{2k+1}$

The ''generalized invariant density" is :

$$\mu_t(dx) = \frac{\exp(-\beta H_t(x)\int_{-\infty}^{x}\exp(\beta H_t(x')dx'}{N} = \exp(-\varphi_t(x))dx$$

So, by the **current reversal** :

$$W_T = \int_0^T (\partial_t \varphi_t)(x_t)dt = \beta\int_0^T (\partial_t H_t)(x_t) - \beta\frac{\int_{-\infty}^{x_t}(\partial_t H_t)(y)\exp(\beta H(y))dy}{\int_{-\infty}^{x_t}\exp(\beta H(y))dy}$$

Weakely time-dependent hamiltonian $H_t(x) = H(x) - h^i(t)O^i(x)$

$$\langle \exp(-W_T) \rangle = 1$$

⇓

Fluctuation-Dissipation theorem has an additional term prop to flux (Falkovich-Gawedzki).

Multiplicative fluctuation relations

One way to generate new fluctuations relation is to apply them to different systems obtained from the original one. An example is provided by the **tangent process** satisfying the SDE :

$$\begin{cases} \dot{x} = u_t(x) + v_t(x) \\ \dot{W}^i_{\ j} = \left(\partial_k u^i_t(x_t) + \partial_k v^i_t(x_t)\right) W^k_{\ j} \end{cases}$$

Where the matrix W propages small separations of solutions of the original SDE :

$$\delta x_t = W_t(x)\delta x_0$$

We can cast the matrix W in the form :

$$W = ODiag(\exp(\rho_1),.....,\exp(\rho_d))O'$$

With O and O' orthogonal matrix and the **streching exponents** ρ_i are ordered.

LYAPUNOV (1857 – 1918)

One can hopes to have in general the **multiplicative large deviation** form :

$$P^T(x \to y, \vec{\rho})dy \propto \exp(-TZ(\frac{\vec{\rho}}{T}))dy$$

Z is accesible analytically in the **Kraichnan model** via relation to integrable quantum models :

Isotropic : Calogero-Sutherland model

With symetry of the square : Lamé-Hermite elliptic hamiltonian.

The function Z verifies a generalized **GC** relation : $Z(\frac{\vec{\rho}}{T}) - \sum \frac{\rho_i}{T} = Z(-\frac{\overleftarrow{\rho}}{T})$

Chetrite-Dellanoy-Gawedzki, J.Stat.Phys 2006

We use here the ''natural'' time inversion , we take : $(x,W)^* = (x,W)$

and the split with vanishing plus part (the drift is a pseudo-vector under time inversion)

The **backward tangent process** is then :

$$\begin{cases} \dot{x} = -u_{T-t}(x) + v_{T-t}(x) \\ \dot{W}_j^i = (-\partial_k u_{T-t}{}^i + \partial_k v_{T-t}{}^i) W_j^k \end{cases}$$

For the Kraichnan case : the backward process is identical to the forward process.

We apply our formalism and we obtain the **DFR** :

$$dxP^{T}(x, Id \to dy, dW)\det(W) = dydWP^{T,r}(y, Id \to dx, d(W^{-1}))$$

The **generalized Gallavotti-Cohen** relation :

$$Z(\frac{\vec{\rho}}{T}) - \sum \frac{\rho_i}{T} = Z^{r}(-\frac{\overleftarrow{\rho}}{T})$$

Kraichnan case :

$$Z(\frac{\vec{\rho}}{T}) - \sum \frac{\rho_i}{T} = Z(-\frac{\overleftarrow{\rho}}{T})$$

→ Generalises **GC** relation because it's for a random dynamics, and it's large deviation of the streching rates vector and not just of the phase space contraction.

→ It may also be worth to study a hierarchy of new fluctuations relations obtained for N-particle processes.

Conclusion

For diffusive system, all the known fluctuations relations may be deduced from the **DFR** that employs different time inversions.

The **DFR** may be viewed as a constraint version ot the detailled balance, with the constraint related to the **entropy production**.

New fluctuation relations may be obtained applying the same scheme to diffusive systems induced from the original one
(as the tangent or N-particle flows)

POUR QUESTIONS

Feyman-Kac-Martin-Girsanov formulae :

$$\overrightarrow{\exp}[\int_0^T (L_t + f_t^i \partial_i + g_t{}^i)dt](X,Y) =$$

$$E_X[\delta(x_T - Y)\exp(\int_0^T f_t^i (d_t^{-1})^{ij} dx_t^j + dt(-f_t^i (d_t^{-1})^{ij} u_t^j - \frac{1}{2} f_t^i (d_t^{-1})^{ij} f_t{}^j + g_t{}^i)]$$

Langevin case

With the canonical choice and $\varphi_t(x) = \beta H_t(x) + \ln(Z_t)$

Then : $$W_T = \ln(Z_T) - \ln(Z_0) + \int_0^T [\beta\partial_t H_t + \beta(\nabla H_t)G_t - \nabla G_t]dt$$

For the particular case G=0, we have the so called **dissipative Jarzynski-work** $W_T = \ln(Z_T) - \ln(Z_0) + \beta\int_0^T (\partial_t H_t)(x_t) = W_{DISS}$

For system with no explicit time-dependance (**Langevin Kramers III**) : $$W_T = \int_0^T (\beta G\nabla H - \nabla G)dt$$

So : $$dx \exp(-\beta H(x)) P^T(x \to y, W)\exp(W)dy = dy \exp(-\beta H(y)) P^{T,r}(y^* \to x^*, -W)dx^*$$

And for Kramers $P^r = P$ Because $H^r = H, G^r = G$

and with **current reversal**, W=0 and :

$$\exp(-\varphi(x))P^T(x \to y)dy = \exp(-\varphi(y))P^{T,CR}(y \to x)dx$$

If G=0 and no time-dependence **(Langevin-Kramers II) :**

$$dx \exp(-\beta H(x)) P^T(x \to dy) = dy \exp(-\beta H(y)) P^T(y^* \to dx^*)$$

Reversed protocol :

$$W_T = \Delta_T \varphi + 2\int_0^T \hat{u}_t(x_t) d_t^{-1}(x_t) \dot{x}_t \, dt$$

Current reversal :

$$W_T = \int_0^T (\partial_t \varphi_t)(x_t) \, dt$$

Convention ITO-STRATONOVICH

- ITO :

$$\int_a^b X(t)dW(t) = \lim_{n\to\infty}\sum_{k=1}^{k=n} X(t_k)(W(t_{k+1}) - W(t_k))$$

- STRATONOVICH :

$$\int_a^b X(t)dW(t) = \lim_{n\to\infty}\sum_{k=1}^{k=n} \left(\frac{X(t_k) + X(t_{k+1})}{2}\right)(W(t_{k+1}) - W(t_k))$$

Transport passif d'un scalaire

KOLMOGOROV (1903 − 1987)

$$\partial_t \theta + (\vec{v}.\vec{\nabla})\theta = \kappa \Delta \theta + f$$

- Avec v un champs aleatoire synthetique.
- f terme de forcage, κ diffusivité thermique.
- Equation LINEAIRE, LOCALE (différence avec la turbulence de Navier-Stokes).

MAIS : L'étude de tel model simplifié de turbulence peut nous permettre de comprendre et de mieux definir quels sont les concepts clé de la turbulence develloppé.

DE PLUS : interêt intrinséque pour la physique des particules polluantes dans l'atmosphére,pour le phenomene d'initiation de pluie, pour le melange turbulent dans un moteur…

- FLOT ISOTROPE :
- Les exposants de Lyapunovs ont été trouvés par les mathematiciens Badenxale et Le Jan en 1984, la fonction de grandes deviations par Falkovich et al en 1999.
- Du fait de l'isotropie,le generateur markovien L du procesus isotrope sur W se réduit à un hamiltonien quantique de CALOGERO-SUTHERLAND hyperbolique.

$$H_{CSH} = -\frac{(\beta+\gamma)}{2}\left(\sum \frac{\partial^2}{\partial \sigma_i^2} + \frac{1}{4}\sum_{i\neq j} \frac{1}{\sinh^2(\sigma_i - \sigma_j)}\right)$$

$$-\frac{\beta}{2}\left(\sum \frac{\partial}{\partial \sigma_i}\right)^2 + cst$$

La densité de probabilité exacte a temps fini de σ est accessible est donné par le noyau de la chaleur de H_{CSH} .

L'approximation du point col sur cette densité donne la fonction de grandes deviations qui est une gaussienne et des exposants de Lyapunovs equiespacés.

On pensait jusqu'à présent par des arguments qualitatifs(Balkovsky-Fouxon 1999) que la fonction de grande deviation était toujours gaussienne pour le modele de Kraichnan.

- Flots bidimensionnel avec symmetrie du carré(Gawedzki et Chetrite 2006):
- Apres manipulation, le generateur L du procesus markovien devient equivalent a un hamiltonien quantique integrable de Calogero Sutherland elliptique ou a un opérateur de Lamé.

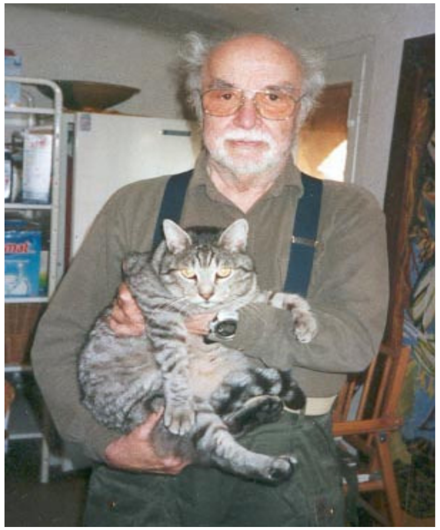
$$L \propto -\frac{d^2}{du^2} + \upsilon(\nu+1)(-k^2 + k^2 sn^2(u,k)) \text{ avec } k = \sqrt{\frac{\alpha}{\alpha+\gamma}}$$

- On obtient alors la fonction de large deviation pour la difference des taux d'expansions qui est NON GAUSSIENNE :

$$H\left(\frac{\sigma_1}{t},\frac{\sigma_2}{t}\right) = \frac{\left(\frac{\sigma_1+\sigma_2}{t} + 2\alpha + 3\beta + \gamma\right)^2}{4(2\alpha+3\beta+\gamma)} + \max_{\mu}\left(\mu\left(\frac{\sigma_1+\sigma_2}{t}\right) - (\beta-\gamma)\mu(\mu+1) + 2E_{\mu}\right)$$

ou E_{μ} est l'etat fondamental du hamiltonien de Lamé.

- L'apparition de ces systemes se
- comprend en mecanique hamiltonnienne
- avec la notion de reduction symplectique
- introduit par J.M Souriau, A.Mardsen...
- Par exemple, dans le cas isotrope,
- le systeme classique equivalent est



$$\mathrm{g} \in \mathrm{GL(d)}, \mathrm{p} \in \mathrm{gl(d)}$$

$$2\,\text{Forme symplectic}: \omega = d(tr(p.dg.g^{-1}))$$

$$\text{Hamiltonien}:$$

$$H = \frac{1}{2}(\gamma tr(pp^t) + \beta tr(p^2) + \beta(tr(p))^2 + (\gamma + (d+1)\beta)tr(p)$$

$$\text{Systemes symetrique sous } SO(d) \times SO(d),$$

Apres réduction, on tombe sur Calogero Sutherland hyperbolique classique.

Holder Regime

- Si on se place a une distance plus grande que l’echelle de viscosité, alors v est non differentiable.

$$v(t,r) - v(t,r') \propto |r - r'|^h \text{ avec } h \leq \frac{1}{3}$$

- On a alors un systeme dynamique aleatoire non différentiable, un domaine mathematique embryonnaire. Les theoremes d’existence et unicité a la Cauchy ne sont plus valables, les ’’trajectoires’’ lagrangiennes ont des comportements nouveaux, separation explosive, coalescence...