Fluctuation Theorem and Quantum Measurements

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1 Fluctuation Theorem in Classical Systems •Experiment by Wang, Sevick, Mittag, Evans, Searles (02)



1 Fluctuation Theorem in Classical Systems

Langevin analysis of experiment by Wang, Sevick, Mittag, Evans, Searles (02)



Experiment by Wang et al.

FT-prediction

$$\frac{\Pr(\Sigma_t < 0)}{\Pr(\Sigma_t > 0)} = \left\langle e^{-\Sigma_t} \right\rangle_{\Sigma_t > 0}$$



Fluctuating $\langle f(t)f(t')\rangle = 2k_BT\zeta\delta(t-t')$ Initial position distribution $\propto e^{-kx_0^2/(2k_BT)}$

Mazonka, Jarzynski (99): FT
Tasaki, Terasaki, Monnai (02), van Zon, Cohen (03)

Initial state distr. for t<0

t=0.01(s)

:0.5 (s)

t=1.5(s)

k xo/ ζ vo





1 Fluctuation Theorem in Classical Systems

Example (detailed FT by Jarzynski):

- equilibrium to different equilibrium
 <Process>
 - 1. A system is prepared to be in equilibrium.
 - 2. Interaction V(t) is turned on at t=0 and is kept to be V_f after t=T.

<Probability Distribution for Forward Process:

Backward Process: $'_0$ $'_1 >$

$$P_F(\Gamma_0 \to \Gamma_1) \equiv \delta \left(\gamma(T, 0 : \Gamma_0) - \Gamma_1 \right) \frac{e^{-\beta H_0(\Gamma_0)}}{Z_0}$$
$$P_B(\Gamma'_0 \to \Gamma'_1) \equiv \delta \left(\widetilde{\gamma}(T, 0 : \Gamma'_1) - \Gamma'_0 \right) \frac{e^{-\beta H_1(\Gamma'_1)}}{Z_1}$$

': time reversal of , (t,0): sol. of eq. of motion, (t,0): sol. for V(T-t)

Detailed FT>

If V(t)' = V(t) (time reversal symmetric) then

$$\frac{P_F(\Gamma_0 \to \Gamma_1)}{P_B(\Gamma_1' \to \Gamma_0')} = e^{\Delta S(\Gamma_0)}$$

 $\Delta S(\Gamma_0) = \beta \{F_1 - H_1(\gamma(T, 0:\Gamma_0)) - F_0 + H_0(\Gamma_0)\}$ ^{Entropy change for each initial condition}

<Proof>

Forward evolution and Backward evolution:

$$\widetilde{\gamma}(t:\Gamma') = \gamma(T-t:\Gamma)'$$

$$e^{-\beta W(\Gamma_0)} P_F(\Gamma_0 \to \Gamma_1) = \delta \left(\gamma(T, 0 : \Gamma_0) - \Gamma_1 \right) \frac{e^{-\beta H_1(\Gamma_1)}}{Z_0}$$
$$= \delta \left(\Gamma_0 - \gamma^{-1}(T, 0 : \Gamma_1) \right) \frac{e^{-\beta H_1(\Gamma_1)}}{Z_0} = \delta \left(\Gamma'_0 - \widetilde{\gamma}(T, 0 : \Gamma'_1) \right) \frac{e^{-\beta H_1(\Gamma'_1)}}{Z_0}$$
$$= \frac{Z_1}{Z_0} P_B(\Gamma'_1 \to \Gamma'_0) = e^{-\beta \Delta F} P_B(\Gamma'_1 \to \Gamma'_0)$$

where $W(\Gamma_0) = H_1(\gamma(T, 0:\Gamma_0)) - H_0(\Gamma_0)$ is work done externally

<Corr>

Jarzynski equality: work measurement free energy difference $\langle e^{-\beta W} \rangle_{\beta,H_0} = \int d\Gamma_0 d\Gamma_1 e^{-\beta W(\Gamma_0)} P_F(\Gamma_0 \to \Gamma_1)$ $= e^{-\beta \Delta F} \int d\Gamma'_0 d\Gamma'_1 P_B(\Gamma'_1 \to \Gamma'_0) = e^{-\beta \Delta F}$ valid even far from eq., includes (higher order) Onsager relations etc

Fluctuation Theorem

Prob(): probability of observing an average entropy production rate/work externally done during time interval

$$\left(\lim_{\tau \to +\infty}\right) \frac{1}{\tau} \log \frac{\operatorname{Prob}(\sigma)}{\operatorname{Prob}(-\sigma)} = \sigma$$

Classical Systems:

:SSFT (Evans-Cohen-Morriss, Gallavotti-Cohen) Stocahstic systems (Spohn-Lebowitz,Kurchan) Chemical reaction (Gaspard) Finite :TFT (Evans-Searles), Detailed FT (Jarzynski) etc

Jarzynski equality

Classical systems (Jarzynski), Quantum systems (Yukawa) Relation with Fluctuation Theorem (Crooks), Quantum version (Monnai)

Quantum Systems: Finite system, finite (Kurchan), Generalization (Maes-Netocny) C*-version (Matsui-ST)

2 Fluctuation Theorem in Quantum Systems

Prob(): probability of observing an average entropy production rate/work externally done during time interval

$$\left(\lim_{\tau \to +\infty}\right) \frac{1}{\tau} \log \frac{\operatorname{Prob}(\sigma)}{\operatorname{Prob}(-\sigma)} = \sigma$$

To measure entropy change or work done externally,

[A] Measure energy, particle numbers etc. twice and evaluate the entropy change or work done as the difference of the two observed values. (Kurchan's protocol)

[B] Measure flows of energy, particle numbers etc. and evaluate the entropy change or work done as accumulated values of the flows.

Classical Mechanically: [A] = [B]

Quantum Mechanically: [A] [B] <- noncommutativity of observables

2 Fluctuation Theorem in Quantum Systems

examples based on Kurchan's view:

(a) equilibrium to different equilibrium (single system) <Process>

1. A systems is prepared to be in equilibrium. $ho^{(i)}=e^{-eta(H-\mu N-\Phi^{(i)})}$

2. Interaction V(t) is turned on at t=0.

<'Entropy' measurement>

- 1. Measure energy, particle #, etc at t=0. $\epsilon_{\lambda}, n_{\lambda}$
- 2. Measure energy, particle #, etc at t₀. $\bar{\epsilon}_{\mu}$, \bar{n}_{μ}

<Probability Distribution for Forward Process>

Distribution of $\eta_{\lambda\mu} \equiv \beta \left(\bar{\epsilon}_{\mu} - \mu \bar{n}_{\mu} - \Phi^{(f)} - \epsilon_{\lambda} + \mu n_{\lambda} + \Phi^{(i)} \right)$

$$P_F(\eta) \equiv \operatorname{Prob.}(\eta_{\lambda\mu} = \eta)$$

where
$$\begin{cases} \Phi^{(f)} = -\beta^{-1} \log \operatorname{Tr} e^{-\beta(H+V(t_0)-\mu N)} \\ \Phi^{(i)} = -\beta^{-1} \log \operatorname{Tr} e^{-\beta(H-\mu N)} \end{cases}$$

<Backward Process>

Evolution generated by the interaction V(t₀-t) Initially in $\rho^{(f)} = e^{-\beta(H+V(t_0)-\mu N-\Phi^{(f)})}$ P_B(): corresponding distribution of for backward process If $\iota V(t)\iota = V(t)$ (ι : time reversal operation) then $\frac{P_F(\eta)}{P_P(-n)} = e^{\eta}$ 2 Fluctuation Theorem in Quantum Systems

examples based on Kurchan's view:

(b) nonequilibrium transient states

<Process>

1. Two independent systems are prepared to be in different equilibria.

2. Interaction V is turned on at t=0.

<'Entropy' measurement>

1. Measure energy, particle #, etc at t=0. $\epsilon_{j\lambda}$, $n_{j\lambda}$

2. Measure energy, particle #, etc at t. $\bar{\epsilon}_{j\mu}$, $\bar{n}_{j\mu}$ <Probability Distribution>

Distribution of $\eta_{\lambda\mu} \equiv \sum_{j} \beta_j \left(\bar{\epsilon}_{j\mu} - \mu_j \bar{n}_{j\mu} - \epsilon_{j\lambda} + \mu_j n_{j\lambda} \right)$

$$P_F(\eta) \equiv \text{Prob.}(\eta_{\lambda\mu} = \eta)$$

If $\iota V \iota = V$ (ι : time reversal operation)

then
$$\label{eq:prod} \frac{P_F(\eta)}{P_F(-\eta)} = e^\eta$$

-system version (Matsui, ST)

FT In Infinitely extended quantum systems



SETTING: infinitely extended systems coupled by a bdd interaction

QUESTIONS: what would be the quantum analog of TFT?

Theorem : Relative Entropy (0jima et al. (88,89), Jaksic Pillet (01,02)) The relative entropy $S(\omega|\omega_t)$ between the initial and present states is given by

$$S(\omega|\omega_t) = \sum_{j=1}^N \beta_j \int_0^t \omega_s(J_j^q) ds - \omega_t(D_S) + \omega(D_S)$$

where $\omega_s \equiv \omega \circ \tau_s$ and J_j^q corresponds to the heat flow to the *j*th reservoir:

$$J_j^q \equiv -\tilde{\delta}_j(V) + \sum_{\lambda=1}^L \mu_\lambda^{(j)} \tilde{g}_\lambda^{(j)}(V) \left(\sim \frac{d}{dt} \tau_t \left(H_j \right) - \sum_{\lambda=1}^L \mu_\lambda^{(j)} \frac{d}{dt} \tau_t \left(N_j^{(\lambda)} \right) \right)$$

Moreover if τ_t is asymptotically abelian, (i) $Ep(\omega_t) \equiv \frac{d}{dt}S(\omega|\omega_t) \to Ep(\omega_{\pm\infty}) = \sum_j \beta_j \omega_{\pm\infty}(J_j^q)$ for $t \to \pm\infty$, (ii) $Ep(\omega_{\pm\infty})$ does not depend on e^{-D_S} , (iii) $Ep(\omega_{\pm\infty}) \ge 0$ and $Ep(\omega_{-\infty}) \le 0$.

NB1:Araki's Relative Entropy: C*-extension of
 S(2 | 1) = Tr { (log 1 - log 2) }
NB2:NESS Entropy Production is independent of system division.

GNS representation and Relative modular operator

GNS representation

conventional view

GNS view (Hilbert space)

- NB. Similarity with Thermofield dynamics of Umezawa et al.(Ojima)conventional viewGNS view (Hilbert space)

Relative modular (super)operator: $\Delta_{\Omega_t\Omega} |\Omega'\rangle \Leftrightarrow \rho_t \rho'^{1/2} \rho^{-1}$ $\log \Delta_{\Omega_t\Omega} |\Omega'\rangle \Leftrightarrow \log \rho_t \rho'^{1/2} - \rho'^{1/2} \log \rho$ $\langle \Omega_t | \log \Delta_{\Omega_t\Omega} |\Omega_t\rangle \Leftrightarrow \operatorname{Tr} \{\rho_t (\log \rho_t - \log \rho)\} = S(\rho|\rho_t)$

Theorem : Transient Fluctuation Theorem (T.Matsui, ST 03)

Let Ω be a vector representation of the initial state ω in the GNS representation, where ω_t corresponds to the vector Ω_t , and $\Delta_{\Omega_t,\Omega}$ be the relative modular operator of the two states. Then, Araki's relative entropy is given by $S(\omega|\omega_t) = (\Omega_t, \ln \Delta_{\Omega_t,\Omega}\Omega_t).$

Define the probability of finding the values of the mean relative entropy production within the interval [a, b] as

$$\Pr([a,b];\omega_t) = (\Omega_t, \{P_t(b) - P_t(a-0)\} \Omega_t) \qquad (t > 0)$$

where $P_t(b)$ is the spectral family satisfying

$$\frac{1}{t}\ln\Delta_{\Omega_t,\Omega} = \int_{-\infty}^{+\infty} \lambda dP_t(\lambda)$$

Then, if the initial state ω is time reversal symmetric, for $0 \leq a \leq b$, the probability satisfies

$$a \le \frac{1}{t} \log \frac{\Pr\left([a, b]; \omega_t\right)}{\Pr\left([-b, -a]; \omega_t\right)} \le b$$

NB: Natural extension of Evans-Searles transient fluctuation Theorem
 NB: Relative entropy is not a usual observable, but can acquire meaning in connection with twice measurements.

4 Fluctuation Theorem and Measurements

Example with the effect of noncommutativity

Quantum version of Externally dragged Langevin equation

$$\zeta \frac{dx}{dt} + k(x - v_0 t) = f(t)$$

Fluctuating $\langle f(t)f(t')\rangle = 2k_BT\zeta\delta(t-t')$ Initial position $\propto e^{-kx_0^2/(2k_BT)}$

Mazonka, Jarzynski (99): FT
Tasaki, Terasaki, Monnai (02), van Zon, E.G.D. Cohen (03) Analysis of experiment by Wang, Sevick, Mittag, Evans, Searles (02)

4 Fluctuation Theorem and Measurements

Example with the effect of noncommutativity

Quantum version of Externally dragged Langevin equation (ST, Monnai)

Model:

$$H(t) = H_0 + \frac{k}{2}f(t)\left(-2q + f(t)\right) , \qquad (f(t) \equiv 0 \qquad (t < 0))$$

$$H_0 = \frac{p^2}{2m} + \frac{k}{2}q^2 + \frac{1}{2} : \int d\lambda((p_\lambda - \kappa_\lambda q)^2 + \omega_\lambda^2 q_\lambda^2) :$$

$$\rho_i \propto e^{-\beta H_0}$$



Example with the effect of noncommutativity

Quantum version of Externally dragged Langevin equation

quantity of interest = work externally done/temperature

[A] Twice measurement case

·Backward evolution is identical to the forward evolution.

·Fluctuation theorem holds:

$$\int e^{i(-\xi+i)\eta} P_F(\eta) d\eta = \int e^{i\xi\eta} P_F(\eta) d\eta$$

Distribution is not simple. Particularly, it is not Gaussian.
In classical limit, it becomes Gaussian.

[B] Flow measurement case

·Distribution is Gaussian.

•Mean value and variance are Identical to those in case [A].

·It does not satisfy Fluctuation Theorem.

·In the classical limit, it agrees with that of case [A].

$$\log \frac{P(\Sigma_{\tau} = A)}{P(\Sigma_{\tau} = -A)} = \left(1 + \hbar^2 \epsilon_2 + \mathcal{O}(\hbar^4)\right) A$$
$$\epsilon_2 = -\frac{\beta^3 k^2}{48m} \int d\lambda \frac{\omega_{\lambda} v_{\lambda}^2}{|\eta_+(\omega_{\lambda})|^2} \left|\int_0^{t_0} ds e^{i\omega_{\lambda} t} \dot{f}(s)\right|^2$$

- The distribution of entropy production or work externally done obeys a simple symmetry relations. Fluctuation Theorem (FT)
- In Classical case, FT holds for a wide range of systems such as the stochastic dynamics, Hamiltonian dynamics, etc.
- In Quantum case, the measurement procedures do influence the final results.
 Problem of selecting appropriate method is an open problem.
- Entropy production and fluctuation theorem for infinite systems

Entropy production = time derivative of Araki's relative entropy Fluctuation theorem for this entropy production holds. Modular operator Observable via twice measurements