Waiting for rare entropic fluctuations in stochastic thermodynamics

Keiji Saito (Keio University)

Abhishek Dhar (ICTS)

KS, Dhar, arXiv:1504.02187

Content

- 1. Counting statistics
- 2. From fixed time to fixed Q statistics
- 3. Basic equation
- 4. Mean residence time and integral FT
- 5. Summary and outlook

1. Counting statistics

 \Diamond Measuring charge transfer



- \diamondsuit Statistics given at the "fixed" time Probability P(Q)
 - Cumulants $\langle Q^n \rangle_c$

 \diamondsuit One expects "information" from "fixed time statistics"

Examples of experiment



♦ Distribution of transmitted charge



Information from "fixed time statistics"



◇ Finite temperature ? Fluctuation relation

Fluctuation relation at the finite temperature

♦ Robust relation derived from time reversal symmetry

- Current context

$$P(-Q) \sim e^{-Q\beta\Delta V} P(Q)$$

- Entropy context (general)

$$P(-S) = e^{-S} P(S)$$

♦ This reproduces linear response results and predicts nonlinear response

Def.
$$\langle Q^n \rangle_c / \tau := \sum_k L_{n,k} (\beta \Delta V)^k / k!$$

- FDT (Kubo formula) $L_{1,1} = L_{2,0}/2$

- Nonlinear response, e.g., $L_{1,2} = L_{2,1}$

Today's talk

2. From fixed time to fixed Q statistics

 \diamondsuit So far, statistics at the fixed time

- Questions -
- What is fixed Q statistics?

How formulated ?

Relation between fixed time and fixed Q physics?



fixed Q statistics fixed time statistics

♦ Mathematically unambiguous statistics

First passage time distribution (FPTD) to get Q

The simplest FPTD: random walk





 $\diamondsuit \text{ Distribution at large time}$ $P(x,t) = \frac{1}{\sqrt{2\pi I_2 t}} e^{-\frac{(x-I_1 t)^2}{2I_2 t}} \qquad I_n = \left\langle \left(\int_0^\tau dt \, x(t) \right)^n \right\rangle_c / \tau \Big|_{\tau \to \infty}$

$$\begin{split} & \diamondsuit \text{ First passage time distribution (FPTD) to reach X} \\ & \mathcal{F}_{rw}(X,t) = \frac{|X|e^{-\frac{(X-I_1t)^2}{2I_2t}}}{\sqrt{2\pi I_2t^3}} \longrightarrow e^{-\frac{I_1^2}{2I_2}t - \frac{3}{2}\log t} \\ & \text{ If } I_1 > 0 \quad \int_0^\infty dt \, \mathcal{F}_{rw}(X,t) = 1 \quad \text{for } X > 0 \\ & < 1 \quad \text{for } X < 0 \end{split}$$

Several models for the FPTD

(a) Driven colloidal particle Equation of motion



$$\begin{aligned} \gamma \dot{x} &= -\frac{\partial U(x)}{\partial x} + f + \eta(t) \\ \langle \eta(t)\eta(t') \rangle &= 2\gamma k_B T \delta(t - t') \\ \text{Entropy produced} &= \beta Q = \beta \int_0^{\tau} dt (\gamma \dot{x} - \eta(t)) \\ &= \beta \left[f \int_0^{\tau} dt \, \dot{x} - (U(x(\tau)) - U(x(0))) \right] \end{aligned}$$

Experiments S. Toyabe et al., Nature Physics(2010) V. Blickle et al., PRL (2007)

Target: winding number

(b) Charge transfer vi QDs

Experiments T. Fujisawa et al., Science (2006) B. Kung et al., Phys. Rev. X (2012) (c) Heat transfer J. R. Gomez-Solano, Europhys Lett. (2010) S. Ciliberto et al., PRL (2013) β_L

3. Renewal type equation for first passages

 \bigcirc Framework to reach entropic variable \mathcal{X}



$$\begin{aligned} &\diamondsuit \text{Renewal type of basic relation} \\ &T_{(\bar{j},\mathcal{X})\leftarrow(i,\mathcal{X}=0)}(t) = \sum_{\bar{j}'} \int_{0}^{t} du \, T_{(\bar{j},\mathcal{X}=0)\leftarrow(\bar{j}',\mathcal{X}=0)}(t-u) \, \mathcal{F}_{(\bar{j}',\mathcal{X})\leftarrow(i,\mathcal{X}=0)}(u) \\ &\overline{\text{transition prob}}_{.}^{\bar{j}'} \\ &(\bar{j},\mathcal{X})\leftarrow(i,\mathcal{X}=0) \end{aligned}$$

 \Diamond Laplace transformation

$$\mathcal{F}_{(\bar{j},\mathcal{X})\leftarrow(i,0)}(s) = \sum_{\bar{j}'} [\mathbf{T}^{-1}]_{(\bar{j},0)\leftarrow(\bar{j}',0)}(s) T_{(\bar{j}',\mathcal{X})\leftarrow(i,0)}(s)$$

Example with driven colloidal system

$$T_{(\overline{j},\mathcal{X})\leftarrow(i,\mathcal{X}=0)}(t) = \sum_{\overline{j}'} \int_0^t du \, T_{(\overline{j},\mathcal{X}=0)\leftarrow(\overline{j}',\mathcal{X}=0)}(t-u) \, \mathcal{F}_{(\overline{j}',\mathcal{X})\leftarrow(i,\mathcal{X}=0)}(u)$$

$$\begin{array}{c} \diamondsuit \text{ Take winding number as } \mathcal{X} \\ \mathcal{X} = \mathcal{N} \bigoplus \\ i \end{array} \begin{array}{c} \text{unique} \\ \text{entrance state} \end{array} \begin{array}{c} \overline{j} = i \\ \overline{j'} = i \end{array} \end{array}$$

 \Diamond Take bath's entropy as \mathcal{X}



The FPTD in the driven colloidal particle (model a)

Entropic variable: winding number

 $\diamondsuit \text{ Formal solution} \\ \mathcal{F}_{(i,\mathcal{N})\leftarrow(i,0)}(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \, \frac{T_{(i,\mathcal{N})\leftarrow(i,0)}(s)}{T_{(i,0)\leftarrow(i,0)}(s)} \, e^{st}$

$$\mathcal{F}(\mathcal{N},t) = \sum_{i} \mathcal{F}_{(i,\mathcal{N}\leftarrow(i,0))}(t) \, p_i^{SS}$$

$$\Diamond T_{(i,\mathcal{N})\leftarrow(i,0)}$$
 ?

- $\begin{array}{l} \cdot \text{ Master equation} \\ \dot{P}_{j}(t) = \sum_{j'=j\pm 1} W_{j\leftarrow j'} P_{j'}(t) + W_{j,j} P_{j}(t) \\ & \frac{\text{local detailed balance}}{W_{i+1\leftarrow i}} = e^{\beta(U_{i}-U_{i+1}+f)} \end{array} \end{array}$
 - · Counting the number of passing through the line: n

$$f \xrightarrow{n \to n+1}_{i \to n \to n-1}_{i \to 1}$$

ity vector 1 · L i

Define the probability vector

$$\boldsymbol{P}(n,t) = \{P_1(n,t), P_2(n,t), \cdots, P_L(n,t)\}$$
$$\frac{\partial \boldsymbol{P}(n,t)}{\partial t} = \boldsymbol{W}_{-}\boldsymbol{P}(n-1,t) + \boldsymbol{W}_{+}\boldsymbol{P}(n+1,t) + \boldsymbol{W}_{0}\boldsymbol{P}(n,t)$$

• Solution in Laplace space $\boldsymbol{T}(\mathcal{N},s) = \begin{cases} A_{+}z_{+}^{-\mathcal{N}}\boldsymbol{V}^{+} & \text{for } \mathcal{N} > 0\\ A_{-}z_{-}^{-\mathcal{N}}\boldsymbol{V}^{-} & \text{for } \mathcal{N} < 0\\ \boldsymbol{V}^{0} & \text{for } \mathcal{N} = 0 \end{cases}$

fluctuation relation

$$z_+ z_- = e^{-\beta fL}$$

1. Asymptotics

$$\mathcal{F}_{(i,\mathcal{N})\leftarrow(i,0)}(t) \sim \int ds \, e^t \, \left[(\mathcal{N}/t) - \ln z_+(s) \right]$$
$$s - \mu(\log z_+(s)) = 0$$

→ General expression in terms of cumulants

2. Mean residence time and integral FT in model (a)

1. Asymptotics

$$\begin{split} \mathcal{F}_{\mathrm{asym}}(\mathcal{X},t) &= A(\mathcal{X}) \exp\left(-\Gamma t - (3/2)\log t\right) \\ \Gamma &= \frac{I_1^2}{2I_2} + \frac{I_3I_1^3}{6I_2^3} + \frac{(3I_3^2 - I_2I_4)I_1^4}{24I_2^5} + \cdots \qquad I_k = \langle \mathcal{X}^k \rangle_c / \tau \Big|_{\tau \to \infty} \\ \text{More precisely} \\ \Gamma &= \sum_{n=0}^{\infty} \frac{(-I_1)^{n+2}}{(n+2)!} q_n(\xi)|_{\xi=0} \qquad q_n(\xi) = \left((\frac{d^2\mu(\xi)}{d\xi^2})^{-1} \frac{d}{d\xi} \right)^n (\frac{d^2\mu(\xi)}{d\xi^2})^{-1} \\ \mu(\xi) \text{ the cumulant generating function} \\ \langle \mathcal{X}^n \rangle_c &= \partial^n \mu(\xi) / \partial \xi^n \Big|_{\xi=0} \end{split}$$

- Asymptotic behavior does not depend on the target values (even negative entropy follows the same form)
- 2. Relaxation rate is written with cumulants
- 3. First order reproduces random walk picture valid for linear response (small I_1)
- 4. (3/2)log t correction

Numerical demonstration



Normalized FPTD for winding number Random walk fitting (fails to fit)



Numerical demonstration

2. Mean residence time expression and integral FT

Statement:

Model (a): colloidal particle in the ring geometry

$$\diamondsuit$$
 Exact expression of mean residence time
$$\int_{0}^{\infty} dt \, T_{(i,S=0)\leftarrow (i,S=0)}(t) = \frac{p_{i}^{SS}}{J}$$

 \diamondsuit Integral FT in terms of first passage

$$\langle e^{-S_{\text{tot}}} \rangle_{\text{FP}:S} = 1$$

All first passage trajectories to get S (S<0)

Usual definition

Total entropy $S_{\rm tot}$ = system's entropy + bath's entropy $S_{\rm sys}$ S

Formula on mean residence time

Remark on this formula

- 1) In equiibrium case, it diverges, as we know.
- 2) The formula includes equilibrium result.
- 3) Residence time is connected to the steady state as well as steady state current.

Integral FT in terms of first passages

 Mean residence formula + basic equation leads to integral FT in terms of first passages

$$T_{(\bar{j},S)\leftarrow(i,S=0)}(t) = \sum_{\bar{j}'=\bar{j}_{\pm}} \int_0^t du \, T_{(\bar{j},0)\leftarrow(\bar{j}',0)}(t-u) \, \mathcal{F}_{(\bar{j}',S)\leftarrow(i,0)}(u)$$

$$S_{j\leftarrow i}^{\text{tot}} = \ln(p_i^{SS}/p_j^{SS}) + S$$

$$\langle e^{-S^{tot}} \rangle_{\text{FP:S}} = \int_0^\infty dt \sum_{\overline{j}} e^{-S^{\text{tot}}_{\overline{j}\leftarrow i}} \mathcal{F}_{(j,S)\leftarrow(i,S=0)}(t) p_i^{SS} = 1$$

All first passage trajectories to get S (S<0)

Numerical demonstration

Summary

- \diamond We considered fixed target value statistics
- The first passage time distribution was studied (FPTD)
- \diamondsuit Basic equation on first passages are considered
- \diamondsuit Asymptotic behaviour has universal expression
- \diamondsuit Exact mean residence time expression was derived
- Integral FT in terms of first passage exists for the model (a).
 Validity for the other models is open problem

Thank you for attention !

