Large deviation functions and fluctuation theorems in heat transport

Abhishek Dhar
Anupam Kundu (CEA, Grenoble)
Sanjib Sabhapandit (RRI)
Keiji Saito (Tokyo University)

Raman Research Institute

Statphys VII, SINP, Kolkata, India
November 2010

Outline

- Introduction
  - Biased random walks: A toy model to illustrate
    (i) large deviation functions (ldf),
    (ii) cumulant generating functions (cgf) and
    (iii) fluctuation theorems (FT).
  - Large Deviation Functions and fluctuation theorems in heat transport.
- Exact result for the cgf for heat transport in a harmonic network.
- An algorithm for computing ldf.
  Demonstration for two different models of transport.
- Summary.

Random walks

Consider the N-step random walk. Any realization is specified by the path $\mathbf{x} = \{x_1, x_2, ..., x_N\}$ where $x_l = +1, \ -1$ with probabilities $p, \ (1-p)$.
$\bar{x} = 2p - 1, \quad \sigma^2 = 4p(1-p)$.

Let $X = \sum_{l=1}^{N} x_l$. Law of large numbers implies:

$$P(X) \quad \sim \quad e^{\frac{(X-N\bar{x})^2}{2N\sigma^2}} \ .$$

This is correct for $X - N\bar{x} \sim O(N^{1/2})$, *i.e* for small deviations from the mean.

For large deviations ($X \sim O(N)$):

$$P(X) \sim e^{\,h(X/N)\ N} \qquad \text{large deviation principle (Varadhan)}$$

$$h(x) \quad = \quad \text{large deviation function (ldf)} \ .$$

Random walks

Cumulant generating function (cgf):

$$Z(\lambda) = \langle e^{\lambda X} \rangle = \int dX\, e^{\lambda X}\, P(X) \sim e^{\,\mu(\lambda)\, N}$$

$$\mu(\lambda) = \lim_{N\to\infty} \frac{1}{N} \ln Z(\lambda) = \frac{1}{N} \sum_{n=1}^{\infty} \frac{\lambda^n \, \langle X^n \rangle_c}{n!} \qquad \text{cgf}$$

Doing saddle-point integrations we see that $h(x)$ and $\mu(\lambda)$ are Legendre transforms of each other.

$$h(x) = \mu(\lambda^*) - \lambda^* x \qquad \mu'(\lambda^*) = x$$

For the biased random walk: $\langle e^{\lambda X} \rangle = [p\, e^{\lambda} + (1-p)\, e^{-\lambda}]^N$. Hence:

$$\mu(\lambda) = \ln\, [\, p\, e^{\lambda} + (1-p)\, e^{-\lambda}\,]$$

$$h(x) = \frac{1}{2}\,(1+x)\, \ln \frac{p}{1+x} + \frac{1}{2}\,(1-x)\, \ln \frac{1-p}{1-x}$$

Also follows from the binomial distribution using Sterling's approximation.

“Fluctuation theorem” for the random walk

Some properties:

$\mu'(\lambda = 0) = \langle X \rangle / N = (2p - 1) \quad \mu''(\lambda = 0) = \langle X^2 \rangle_c / N = 4p(1 - p)$

For small deviatons from the mean: $h(x) = -(x - \bar{x})^2 / 2\sigma^2$, gives the expected Gaussian distribution.

$h(x)$ non-universal.

$x = X/N$ is like a current in the system driven by the bias which we characterize by $A = \ln[p/(1-p)]$. Then we verify the following “fluctuation theorem”:

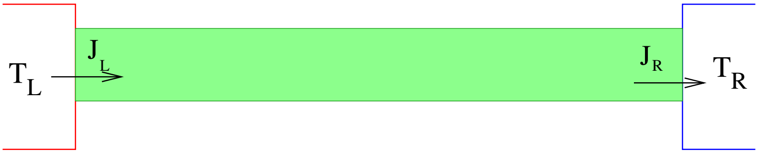
$$\frac{P(X)}{P(-X)} = e^{AX}$$

This also implies the following symmetry relations:

$$h(x) - h(-x) = Ax \; ,$$
$$\mu(\lambda) = \mu(-\lambda - A) \; .$$

The large deviation approach to statistical mechanics, H. Touchette, Phys. Rep. (2009).

Large deviation functions in heat transport



In the nonequilibrium steady state let heat transfered from left reservoir into system in time τ be $Q_L = \int_0^\tau dt\, J_L(t)\, dt = Q$. The mean current is $q = Q/\tau$.

This is a fluctuating variable with a distribution $P(Q)$.

For $\tau \to \infty$,

$$P(Q) \sim e^{\,h(q)\,\tau}\,.$$
$$Z(\lambda) = \langle\, e^{\lambda Q}\,\rangle \sim e^{\,\mu(\lambda)\,\tau}\,.$$

$h(q)$ and $\mu(\lambda)$ are the large deviation function (ldf) and cumulant generating function (cgf) for heat transfer.

$$\mu(\lambda) = \lambda q^* + h(q*) \quad \text{with} \;\; h'(q^*) = -\lambda$$

Steady state fluctuation theorem

Cohen-Gallavotti SSFT:
Let $\Delta\beta = 1/T_R - 1/T_L$. Define rate of entropy production over time τ by: $s = (\Delta\beta)\frac{Q}{\tau}$.

$$
\begin{aligned}
\frac{P(s)}{P(-s)} &= \exp[s\tau] \quad \tau \to \infty \\
\text{Equivalently :} & \quad \text{following symmetry relations hold} \\
h(q) - h(-q) &= \Delta\beta\, q \\
\mu(\lambda) &= \mu(-\Delta\beta - \lambda)\,.
\end{aligned}
$$

- Caution: There are examples where both symmetries are not valid.
  Example: When

  $$Z(\lambda) = g(\lambda)\, e^{\mu(\lambda)\tau}$$

  and $g(\lambda)$ has singularities in the region of integration. The saddle-point then fails.
  [Farago, Visco]
- $S' = Q_L/T_L - Q_R/T_R$ exactly satisfies the FT for arbitrary τ. Though $\langle S' \rangle = \langle S \rangle$, properties of $P(S)$ and $P(S')$ can be quite different.

Why are ldfs', cgfs' and the FTs interesting?

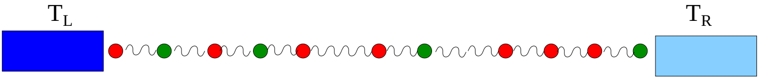
- The ldf gives the probabilites of rare events.
- The cgf gives all cumulants of the current and these are experimentally observable quantities which give information on noise properties.
- Possible candidates for nonequilibrium "free energies". [Bodineau and Derrida]
- The fluctuation theorem is a general result, proved for many systems, valid in the far from equilibrium regime.
- The symmetry of the cgf automatically implies results of linear response theory such as Green-Kubo and Onsager relations. For example it gives the conductance of a system in terms of equilibrium current auto-correlations.

  $$G = \lim_{\Delta T \to 0} \frac{\langle j \rangle_{\Delta T}}{\Delta T} = \frac{1}{k_B T^2} \int_0^\infty \langle j(0) j(t) \rangle_T \,.$$

  In addition it gives non-trivial relations between non-linear response functions.

  (Gallavotti, Lebowitz-Spohn, Andrieux-Gaspard):

Heat conduction in harmonic lattices: 1D Chain



$$H = \sum_{l=1}^{N} \left[\frac{m_l v_l^2}{2} + \frac{k_o x_l}{2} \right] + \sum_{l=1}^{N-1} \frac{k(x_l - x_{l+1})^2}{2} \; .$$

Equations of motion:

$$\begin{aligned}
m_1 \dot{v}_1 &= f_1 - \gamma_L v_1 + \eta^L \\
m_l \dot{v}_l &= f_l \qquad\qquad l = 2, 3, \ldots N-1 \\
m_N \dot{v}_N &= f_N - \gamma_R v_N + \eta^R \; . \\
f_l &= -\partial H / \partial x_l \; , \\
\langle \eta^L(t) \eta^L(t') \rangle &= 2 \gamma_L k_B T_L \delta(t - t') \; , \\
\langle \eta_R(t) \eta^R(t') \rangle &= 2 \gamma_R k_B T_R \delta(t - t') \; .
\end{aligned}$$

In matrix Form:

Hamiltonian:

$$H = \frac{\dot{X}.\mathbf{M}.\dot{X}}{2} + \frac{X.\mathbf{\Phi}.X}{2} .$$

Equations of motion:

$$\begin{aligned} \dot{X} &= V \\ \mathbf{M}\dot{V} &= -\mathbf{\Phi}X - \boldsymbol{\gamma}^{(L)}V + \eta^{(L)} - \boldsymbol{\gamma}^{(R)}V + \eta^{(R)} . \end{aligned}$$

where $\eta^{(L)} = \{\eta_L, 0, 0, ..., 0\}$, $\eta^{(R)} = \{0, 0, ..., 0, \eta_R\}$
$\boldsymbol{\gamma}^{(L)} = diag\{\gamma_L, 0, 0, ..., 0\}$,$\boldsymbol{\gamma}^{(L)} = diag\{0, 0, ..., 0, \gamma_R\}$.

Landauer-like formula for thermal conductance

Exact expression for nonequilibrium heat current ["Landauer-like" formula for phonons.]
In classical case:

$$J = \frac{k_B(T_L - T_R)}{2\pi} \int_0^\infty d\omega \mathcal{T}(\omega) ,$$

where $\mathcal{T}(\omega)$ is the phonon transmission function.

$$\begin{aligned} \mathcal{T}(\omega) &= 4\gamma_L\gamma_R\omega^2 \mathbf{G}^+_{1N}(\omega)\mathbf{G}^-_{1N}(\omega) \\ \text{where } \mathbf{G}^+(\omega) &= \frac{1}{-\omega^2\mathbf{M} + \mathbf{\Phi} - i\mathbf{\Gamma}^{(L)} - i\mathbf{\Gamma}^{(R)}} , \qquad \mathbf{G}^-(\omega) = \mathbf{G}^+(-\omega) \\ \mathbf{\Gamma}^{(L)} &= \omega\boldsymbol{\gamma}^{(L)}, \quad \mathbf{\Gamma}^{(R)} = \omega\boldsymbol{\gamma}^{(R)} . \end{aligned}$$

[Casher and Lebowitz (1971), Rubin and Greer (1971), Dhar and Roy (2006)].

Main results: cgf for a 1D harmonic chain

$$\mu(\lambda) = -\frac{1}{2\pi}\int_0^\infty d\omega \; \ln\Big[1 - \mathcal{T}(\omega) T_L T_R \, \lambda(\Delta\beta + \lambda)\Big],$$

where $\Delta\beta = T_R^{-1} - T_L^{-1}$ and

Current noise properties:

$$\frac{\langle Q\rangle_c}{\tau} = \frac{(T_L - T_R)}{2\pi}\int_0^\infty d\omega \; \mathcal{T}(\omega).$$

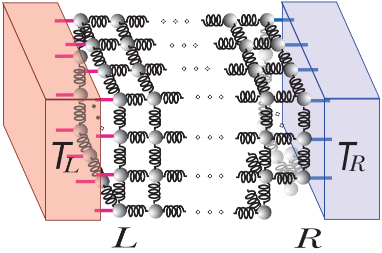
$$\frac{\langle Q^2\rangle_c}{\tau} = \frac{1}{2\pi}\int_0^\infty d\omega \, [\, \mathcal{T}^2(\omega)(T_R - T_L)^2 + 2\mathcal{T}(\omega) T_L T_R \,].$$

GC symmetry is satisfid: $\mu(\lambda) = \mu(-\lambda - \Delta\beta)$.

[A. Kundu, S. Sabhapandit, A. Dhar - to be published]

[Quantum case (using FCS): K. Saito, A. Dhar, PRL (2008)]

Main results: cgf for arbitrary harmonic network



$$\mu(\lambda) = -\frac{1}{2\pi}\int_0^\infty d\omega \,\mathrm{Tr}\, \ln\left[\mathbf{1} - \mathcal{T}(\omega) T_L T_R \lambda(\lambda + \Delta\beta)\right].$$

where $\mathcal{T} = 4[\mathbf{G}^+ \,\mathbf{\Gamma}_L\, \mathbf{G}^- \,\mathbf{\Gamma}_R]$ is now a transmission matrix.

[K. Saito, A. Dhar - to be published]

Computation of $Z(\lambda)$

Master equation for $P(X, V, t)$

$$\frac{\partial P(X, V, t)}{\partial t} = \mathcal{L}\mathcal{P}$$

Master equation for $P(Q, X, V, t)$

$$\begin{aligned}
\frac{\partial P(Q, X, V, t)}{\partial t} &= \mathcal{L}_M P \\
\frac{\partial \tilde{P}(\lambda, \mathbf{x}, \mathbf{v}, t)}{\partial t} &= \mathcal{L}_M(\lambda)\tilde{P} \\
\tilde{P}(\lambda, X, V, t) &\sim e^{\epsilon_0(\lambda)t}\, \phi(\lambda, X, V)\,, \quad Z(\lambda) = \int dX\, dV \tilde{P}(\lambda, X, V) \sim g(\lambda)\, e^{\,\mu(\lambda)\, t}.
\end{aligned}$$

$\mathcal{L}_M|\psi_0\rangle = \epsilon(\lambda)|\psi_0 >$ gives the largest eigenvalue of the evolution operator.

Thus $\mu(\lambda) = \epsilon_0(\lambda)$ but this is difficult to obtain in general.

We use a different approach which uses the linearity of our model.

Outline of proof

- The total heat flow from left reservoir into system is given by:

$$Q = \int_0^{\tau} dt \; v_1 \; (-\gamma_L v_1 + \eta_L) \; .$$

- Linear equations of motion:

$$\begin{aligned} \dot{X} &= V \\ \mathbf{M}\dot{V} &= -\mathbf{\Phi} X - \gamma^{(L)} V + \eta^{(L)} \; - \gamma^{(R)} V + \eta^{(R)} \; . \end{aligned}$$

Solve by Fourier transform:

$$\{X(t), V(t), \eta(t)\} = \sum_{n=-\infty}^{\infty} \{\tilde{X}(\omega_n), \tilde{V}(\omega_n), \tilde{\eta}(\omega_n)\} e^{-i\omega_n t} \; ,$$

$$\{\tilde{X}(\omega_n), \tilde{V}(\omega_n), \tilde{\eta}(\omega_n)\} = \frac{1}{\tau} \int_0^{\tau} \{X(t), V(t), \eta(t)\} \; e^{i\omega_n t} \; ,$$

where $\omega_n = 2\pi n/\tau$.

Outline of derivation

- Noise properties:

$$\langle \widetilde{\eta}_\alpha(\omega)\widetilde{\eta}_{\alpha'}(\omega')\rangle = 2\delta_{\alpha,\alpha'}\frac{\gamma_\alpha T_\alpha}{\tau}\,\delta[\omega+\omega'], \quad \text{with} \quad \alpha,\alpha' = \{L, R\}.$$

- Solution is:

$$\begin{aligned} \tilde{V}(\omega_n) &= -i\omega_n \mathbf{G}^+(\omega_n)\,[\tilde{\eta}^{(L)}(\omega_n) + \tilde{\eta}^{(R)}(\omega_n)] \quad + \quad \frac{1}{\tau}\mathbf{G}^+(\omega_n)\,[\,\mathbf{\Phi}\Delta X + i\omega_n \mathbf{M}\Delta V\,]\,, \\ \Delta X &= X(\tau) - X(0),\ \Delta V = V(\tau) - V(0)\,. \end{aligned}$$

- $Z(\lambda) = \langle\, e^{\lambda Q}\rangle = g(\lambda)e^{\mu(\lambda)\tau}$. (Average over NESS initial conditions and noise)
  First term $\sim O(1/\tau^{1/2})$: contributes to $\mu(\lambda)$.
  Second term $\sim O(1/\tau)$: contributes to $g(\lambda)$.
- Notice that Q is a quadratic function of the noise variables $\eta = \{\eta_L(\omega_n), \eta_R(\omega_n)\}$ and the initial conditions of $\{X, V\}$.
  Thus $Q = \eta^T.A.\eta + (X, V)^T.B.(X, V)$ and $P(\eta)$, $P(X, V, t = 0)$ are known Gaussian distrubtions.
- Perform multi-dimensional Gaussian integration to get $\mu(\lambda)$ and $g(\lambda)$. Getting explicit form for $g(\lambda)$ difficult except special cases.

For N-step unbiased random walk the event $X = N$ is a rare event. Since $P(X = N) = 2^{-N}$ obtaining this probability from a simulation would require $\sim 2^N$ realizations: difficult even for $N = 100$.

An efficient algorithm based on importance sampling:
Use a biased dynamics to generate rare-events. Use appropriate weighting factor for estimating averages.
[A. Kundu, S. Sabhapandit, A. Dhar (arXiv/1003.2106)]

- Let probability of particular trajectory be $\mathcal{P}(\mathbf{x})$. By definition:

$$P(Q,\tau) = \sum_{\mathbf{x}} \delta_{Q,Q(\mathbf{x})}\mathcal{P}(\mathbf{x}).$$

- Consider biased dynamics for which probability of the path $\mathbf{x}$ is given by $\mathcal{P}_b(\mathbf{x})$. Then:

$$P(Q,\tau) = \sum_{\mathbf{x}} \delta_{Q,Q(\mathbf{x})} e^{-W(\mathbf{x})}\mathcal{P}_b(\mathbf{x}), \qquad \text{where} \quad e^{-W(\mathbf{x})} = \frac{\mathcal{P}(\mathbf{x})}{\mathcal{P}_b(\mathbf{x})}.$$

  Note: weight factor W is a function of the path.
- In simulation we estimate $P(Q,\tau)$ by performing averages over M realizations of biased-dynamics to obtain:

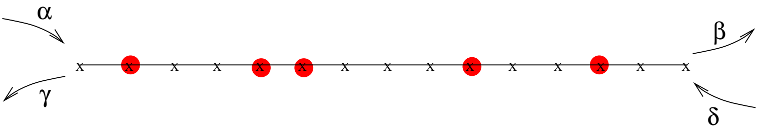
$$P_e(Q,\tau) = \frac{1}{M}\sum_r \delta_{Q,Q(\mathbf{x}_r)} e^{-W(\mathbf{x}_r)} \ . \tag{1}$$

- A necessary requirement of the biased dynamics is that the distribution of Q that it produces, i.e., $P_b(Q,\tau) = \langle \delta_{Q,Q(\mathbf{x})} \rangle_b$, is peaked around the desired values of Q for which we want an accurate measurement of $P(Q,\tau)$.

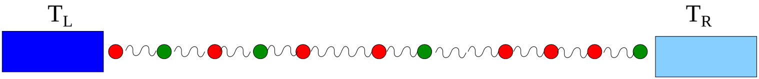
Numerical computation of large deviations

Two Examples:

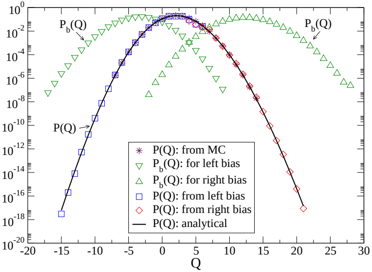
(i) Particle current in SSEP connected to particle reservoirs .



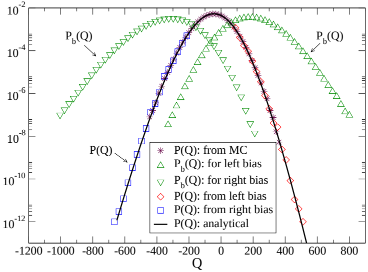
(ii) Heat current in harmonic chain connected to heat reservoirs .



Numerical computation of large deviations



Three-site SSEP with reservoirs. Bias dynamics obtained by applying bulk-field.



Harmonic chain with two particles. Biased dynamics obtained by changing temperatures.

Summary

- The ldf and cgf are important functions characterizing steady states of nonequilibrium systems.
- There are very few exact calculations of these functions for many particle systems. Their numerical computation is also very difficult.
- We have obtained the exact cgf for heat current in harmonic systems connected to Langevin reservoirs.
- We have proposed an efficient algorithm to compute ldf in transport problems.