Current fluctuations in heat transport

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Outline

- Introduction to large deviation functions (LDF) and cumulant generating functions (CGF).
- Exact results for the cumulant generating function $\mu(\lambda)$ and the leading correction term $g(\lambda)$ for heat transport in a harmonic network with Langevin dynamics.
- Applications of the formula for $\mu(\lambda)$.

  (i) $3D$ harmonic crystal – test of additivity principle.

  (ii) Small system : a single harmonic oscillator -
  experiments on micro-cantilevers and optically trapped particles.
- Discussion of fluctuation theorems.

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:

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

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

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

$$P(X) \quad \sim \quad e^{\,h(X/N)\ N} \quad - \text{large deviation principle}$$
$$h(x) \quad = \quad \text{large deviation function (LDF)} \ .$$

Random walks

Cumulant generating function (CGF):

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

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

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

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

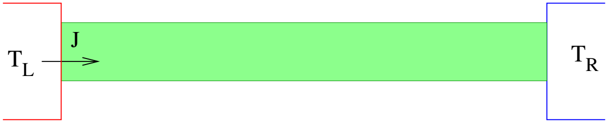
For the biased random walk: $\langle e^{\lambda X} \rangle = [p\, e^{\lambda} + (1-p)\, e^{-\lambda}]^N$. Hence:

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

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

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

Large deviation functions in heat transport



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

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

$$\text{For } \tau \to \infty , \quad P(Q) \sim e^{\,h(q)\,\tau} .$$
$$Z(\lambda) = \langle\, e^{-\lambda Q}\,\rangle \sim e^{\,\mu(\lambda)\,\tau}\, g(\lambda).$$

$h(q)$ — large deviation function (LDF).
$\mu(\lambda) = \frac{1}{\tau}\sum_{n=1}^{\infty} \lambda^n \frac{<Q^n>_c}{n!}$ — cumulant generating function (CGF).

Usually (but not always) related by:

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

Why are the LDF, CGF and the FTs interesting?

- Fluctuation theorem symmetries:

$$h(q) - h(-q) = \Delta\beta q \qquad \text{OR} \qquad \frac{P(q)}{P(-q)} = e^{\Delta\beta q\tau}$$

$$\mu(\lambda) = \mu(\Delta\beta - \lambda)$$

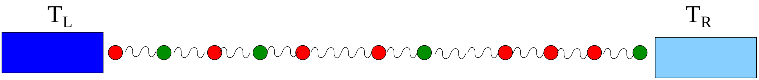
This is a general result, proved for many systems, and valid in the far from equilibrium regime.

- The symmetry of the CGF automatically implies results of linear response theory such as Green-Kubo and Onsager relations.
  In addition it gives non-trivial relations between non-linear response functions and correlation functions.

  (Gallavotti, Lebowitz-Spohn, Kurchan):

- 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".

Heat conduction in harmonic lattices: 1D Chain



$$H = \sum_{\ell=1}^{N} \left[\frac{m_\ell v_\ell^2}{2} + \frac{k_o x_\ell^2}{2} \right] + \sum_{\ell=1}^{N-1} \frac{k(x_\ell - x_{\ell+1})^2}{2} \ .$$

Equations of motion:

$$\begin{aligned} m_1 \dot{v}_1 &= f_1 - \gamma_L v_1 + \eta_L \\ m_\ell \dot{v}_\ell &= f_\ell \qquad\qquad \ell = 2, 3, ...N-1 \\ m_N \dot{v}_N &= f_N - \gamma_R v_N + \eta_R \ . \\ f_\ell &= -\partial H / \partial x_\ell \ , \end{aligned}$$

$$\begin{aligned} \langle \eta_L(t) \eta_L(t') \rangle &= 2\gamma_L k_B T_L \delta(t-t') \ , \\ \langle \eta_R(t) \eta_R(t') \rangle &= 2\gamma_R k_B T_R \delta(t-t') \ . \end{aligned}$$

Matrix form of equations of motion:

Hamiltonian:

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

Equations of motion:

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

where:

$$\begin{aligned} \eta^{(L)} &= \{\eta_L, 0, 0, ..., 0\}, \quad \eta^{(R)} = \{0, 0, ..., 0, \eta_R\} , \\ \gamma^{(L)} &= diag\{\gamma_L, 0, 0, ..., 0\}, \quad \gamma^{(L)} = diag\{0, 0, ..., 0, \gamma_R\} . \end{aligned}$$

Steady state current

Gaussian steady state measure. Let $U = (X, V)$. Then

$$P_{SS}(U) \sim e^{-U\mathbf{C}^{-1}U/2} ,$$

where $\mathbf{C}$ is the correlation matrix with elements $\langle X_i X_j \rangle$, $\langle X_i V_j \rangle$ and $\langle V_i V_j \rangle$.

Two ways to obtain the correlation matrix **C**.

Method 1– Write the Fokker-Planck equation:

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

$$\text{Solve } \mathcal{L}P_{SS} = 0 .$$

Linear equation for **C** which can be explicitly solved for ordered chain (Rieder,Lebowitz, Lieb, 1967).

Steady state current in the harmonic chain

Method 2– Solve linear Langevin equations by Fourier transforms.

$$\mathbf{M}\ddot{X} = -\mathbf{\Phi}X - \boldsymbol{\gamma_L}\dot{X} - \boldsymbol{\gamma_R}\dot{X} + \eta_L + \eta_R$$

$$X(t) = \int d\omega \, \widetilde{X}(\omega) \, e^{-i\omega t}, \quad \eta(t) = \int d\omega \, \tilde{\eta}(\omega) \, e^{-i\omega t}.$$

Steady state current in the harmonic chain

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$$X(t) = \int d\omega\, \widetilde{X}(\omega)\, e^{-i\omega t}, \quad \eta(t) = \int d\omega\, \tilde{\eta}(\omega)\, e^{-i\omega t}.$$

$$\text{This gives :} \quad \widetilde{X}(\omega) = \mathbf{G}^{+}(\omega)\,[\,\tilde{\eta}_L(\omega) + \tilde{\eta}_R(\omega)\,]$$

$$\text{where } \mathbf{G}^{+}(\omega) = [-\boldsymbol{M}\omega^2 + \boldsymbol{\Phi} - i\omega\gamma_L - i\omega\gamma_R]^{-1}$$

$$\langle \tilde{\eta}_L(\omega)\tilde{\eta}_L(\omega')\rangle = T_L\,\gamma_L\,\delta(\omega+\omega')\,, \langle \tilde{\eta}_R(\omega)\tilde{\eta}_R(\omega')\rangle = T_R\,\gamma_R\,\delta(\omega+\omega')\,.$$

$$\textit{Find}\ \ \langle X_i V_j\rangle = \int d\omega \langle \widetilde{X}_i(\omega)\widetilde{V}_j(-\omega)\rangle\ , etc.$$

Landauer-like formula for heat current

In particular the steady state heat current is given by

$$J = k\langle X_\ell V_{\ell+1}\rangle$$

and using the "second method", one gets:

$$\begin{aligned} J &= \frac{k_B(T_L - T_R)}{2\pi}\int_0^\infty d\omega \mathcal{T}(\omega)\,, \\ \text{where } \mathcal{T}(\omega) &= 4\gamma_L\gamma_R\omega^2|\mathbf{G}^+_{1N}(\omega)|^2 \text{ is the phonon transmission function.} \end{aligned}$$

["Landauer-like" formula for phonons.]
[Casher and Lebowitz (1971), Rubin and Greer (1971), Dhar and Roy (2006)].

Second approach more useful because:
(1) Has simple physical interpretation.
(2) For disordered systems this is easier to evaluate numerically, as well as study analytically.
(3) Quantum generalization is straightforward
— [A. Dhar and D. Roy, J. Stat. Phys. (2006), A. Dhar and D. Sen, PRB (2006)].
(4) Higher-dimensional generalization is straightforward.

Current fluctuations in the steady state

We look at the heat current flowing from heat reservoir into system:

$$Q = \int_0^\tau dt[\,-\gamma_L v_1(t) + \eta_L(t)\,]\, v_1(t)\ .$$

We want to calculate the expectation $\langle e^{-\lambda Q} \rangle$ in the NESS.

Let us define:

$$Z(\lambda, U, \tau | U_0) = \langle\, e^{-\lambda Q}\, \delta(U_\tau - U)\, \rangle_{U_0}\ . \qquad U = (X, V)$$

Our final interest is in:

$$Z(\lambda) = \int dU_0\, P_{SS}(U_0) \int dU\, Z(\lambda, U, \tau | U_0)\ .$$

As before, here also two approaches are possible.

Method 1

Master equation for $Z(\lambda, U, \tau | U_0)$:

$$\frac{\partial Z(\lambda, U, \tau)}{\partial \tau} = \mathcal{L}_\lambda Z$$

Solve for initial conditions : $Z(\lambda, U, 0) = \delta(U - U_0)$:

$$Z(\lambda, U, \tau) \sim e^{\epsilon_0(\lambda)\tau} \chi_0(\lambda, U_0) \Psi_0(\lambda, U),$$

where $\mathcal{L}_\lambda \Psi_0(\lambda, U) = \epsilon_0(\lambda)\Psi_0(\lambda, U)$ −largest eigenvalue of $\mathcal{L}_\lambda$.

Hence :

$$Z(\lambda) \sim e^{\mu(\lambda)t} g(\lambda)$$

$$\text{where } \mu(\lambda) = \epsilon_0(\lambda) \text{ and}$$

$$g(\lambda) = \int dU \, \Psi(\lambda, U) \int dU_0 \, \Psi(0, U_0)\chi(\lambda, U_0).$$

Thus we need to find the smallest eigenvalue and corresponding eigenfunction of $\mathcal{L}(\lambda)$ – usually very difficult.

We instead use the Fourier transform solution.

Outline of our derivation–Method 2

Linear equations of motion:

$$\mathbf{M}\ddot{X} = -\mathbf{\Phi}X - \gamma^{(L)}\dot{X} + \eta^{(L)} - \gamma^{(R)}\dot{X} + \eta^{(R)} .$$

Solve by <u>discrete</u> Fourier transform:

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

where $\omega_n = 2\pi n/\tau$.
Noise properties:

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

Outline of our derivation–Method 2

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Solution is:

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

First term $\sim O(1/\tau^{1/2})$: contributes to $\mu(\lambda)$.
Second term $\sim O(1/\tau)$: contributes to $g(\lambda)$.

Outline of derivation

- Q is a quadratic function of the noise variables $\tilde{\eta}$ and the coordinates U, U_0.
- Perform Gaussian integrations over noise to get:

  $\mu(\lambda)$, $\Psi_0(\lambda, U)$ and $\chi_0(\lambda, U_0)$.

  Recall: $Z(\lambda, U|U_0) \sim e^{\mu(\lambda)\tau}\, \chi_0(\lambda, U_0)\, \Psi_0(\lambda, U)$
- Final result:

  (1) Expression for $\mu(\lambda)$ in terms of $\mathcal{T}(\omega)$.

  (2) Wavefunctions and $g(\lambda)$ are expressed in terms of $\mathbf{G}^+(\omega)$.

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

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

Current noise properties:

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

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

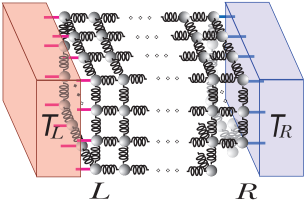
GC symmetry is satisfid: $\mu(\lambda) = \mu(-\lambda - \Delta\beta)$.

[A. Kundu, S. Sabhapandit, A. Dhar - J. Stat. Mech. (2011)]

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

$g(\lambda) = ...$

Results for arbitrary harmonic networks



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

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

It is non-trivial to arrive at this expression in terms of the transmission matrix $\mathcal{T}$.
Use of a number of non-trivial matrix identities.
[K. Saito, A. Dhar - PRE (2011)]
J.S. Wang, B. K. Agarwalla, and H. Li (2012)

Fogedby and Imparato (2012) - reproduce results for harmonic chain, find symmetry relation satisfied by $\mathcal{L}_\lambda$ which implies fluctuation symmetry.

Application to test of additivity principle

We now use the formula for the cumulant generating function of the $3D$ harmonic crystal to test the validity of the additivity principle in this system.

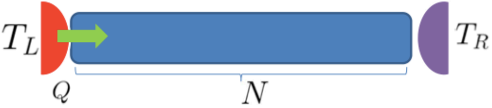
The additivity principle is a conjecture, originally stated for one-dimensional diffusive systems, which allows one to determine the LDF and CGF for current from a variational approach.

K. Saito and A. Dhar, PRL **107**, 250601 (2011)

Additivity Principle

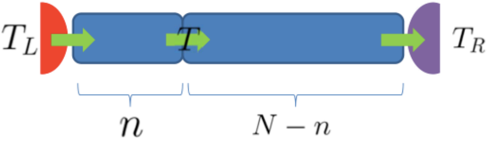
Additivity principle conjecture

◆ Probability of transmitted heat during time τ



$$P_N(q, T_L, T_R) \sim e^{\tau h_N(q, T_L, T_R)} \qquad (q = Q/\tau)$$

◆ Additivity principle: Variational principle for divided two pieces



$$h_N(q, T_L, T_R) = \max_T \left[h_n(q, T_L, T) + h_{N-n}(q, T, T_R) \right]$$

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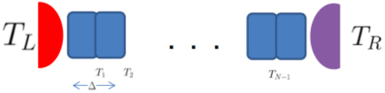
Additivity Principle

Use this for many pieces in the system



$$h_N(q, T_L, T_R) = \max_{T_1, T_2, \cdots} \sum_i h_1(q, T_i, T_{i+1})$$

- **One piece (Local equilibrium)**

$$h_1(q, T_i, T_{i+1}) \sim -\frac{[q - \kappa(T_i)(T_i - T_{i+1})/\Delta]^2}{2\sigma(T_i)/\Delta}$$

$\kappa(T)$ Thermal conductivity

$\sigma(T)$ Current Fluctuation

- **Variational Problem for in continuous limit**

$$h_N(q, T_L, T_R) = -\min_{T(x)}\left[\int_0^1 \frac{[q + \kappa(T)\partial T/\partial x]^2}{2\sigma(T)} dx\right]$$

- **Solution**

$$h_N(q, T_L, T_R) = q \int_{T_L}^{T_R} \left[\frac{1 + K\kappa(T)}{1 + 2K\kappa(T)^{1/2}} - 1\right] \frac{\sigma(T)}{\kappa(T)} dT$$

$$Nq = \int_{T_L}^{T_R} \frac{\sigma(T)}{[1 + 2K\kappa(T)]^{1/2}} dT$$

◆ Cumulant generating function from Additivity Principle

$$\mu_N(\lambda, T_L, T_R) = \frac{1}{\tau}\ln\langle e^{\lambda Q}\rangle$$

$$\mu_N(\lambda, T_L, T_R) = -\frac{K}{N}\Big[\int_{T_L}^{T_R} dT\, \frac{\kappa(T)}{\sqrt{1+2K\sigma(T)}}\Big]^2,$$

$$\lambda = \int_{T_L}^{T_R} dT\, \frac{\kappa(T)}{\sigma(T)}\Big[\frac{1}{\sqrt{1+2K\sigma(T)}} - 1\Big],$$

$\kappa(T)$ Thermal conductivity
$\sigma(T)$ Current Fluctuation

T. Bodineau and B. Derrida 2004

Remarkably, all higher current cumulants are obtained with only two parameters i.e.,
thermal conductivity $\kappa(T)$ and current fluctuation $\sigma(T)$

Verification of the AP conjecture

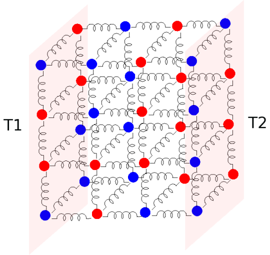
- It has been shown to reproduce exactly, known current cumulants upto several orders, of the symmetric exclusion process (Bodineau and Derrida, 2007).
- Has been verified for heat conduction in the Kipnis–Marchioro–Presutti model which has stochastic dynamics (Hurtado and Garrido, 2009).
- So far no verification in any Hamiltonian system or in higher dimensions. Difficult because one needs to do simulations with large system sizes and in that case it is hard to compute LDF or CGF accurtely.
- We test the AP in the $3D$ mass-disordered harmonic crystal using our exact formula for CGF, which can be numerically evaluated accurately.

Heat conduction in mass disordered harmonic crystal

A. Kundu, A. Chaudhuri, D. Roy, A. Dhar, J.L. Lebowitz, H. Spohn
PRB (2010), EPL (2010)

$$H = \sum_{\mathbf{x}} \frac{m_{\mathbf{x}}}{2} \dot{q}_{\mathbf{x}}^2 + \sum_{\mathbf{x},\hat{\mathbf{e}}} \frac{k}{2} (q_{\mathbf{x}} - q_{\mathbf{x}+\hat{\mathbf{e}}})^2 + \sum_{\mathbf{x}} \frac{k_o}{2} q_{\mathbf{x}}^2$$

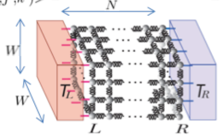
$q_{\mathbf{x}}$: scalar displacement, masses $m_{\mathbf{x}}$ random.
$k_o = 0$: Unpinned. $k_o > 0$: Pinned.



Disordered pinned crystal: $J \sim 1/N$
($\kappa \sim N^0$ - Diffusive transport - Fourier's law).

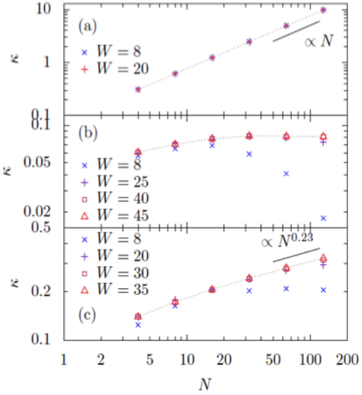
Disordered unpinned crystal: $J \sim 1/N^{0.75}$
($\kappa \sim N^{0.25}$ - Anomalous transport).

$$\mathcal{H} = \sum_{i,j,k} \frac{p_{i,j,k}^2}{2m_{i,j,k}} + \sum_{<(i,j,k)(i',j',k')>} \frac{k}{2}(x_{i,j,k} - x_{i',j',k'})^2 + \frac{k_0}{2} x_{i,j,k}^2$$



–Thermal Conductivity –

$$\kappa = \frac{J}{(T_L - T_R)/N}$$



(a) Uniform Mass

=> Ballistic Transport

(b) Random Mass with onsite potential $k_0 \neq 0$

=> Fourier's law for sufficiently large W

(c) Random Mass without onsite potential $k_0 = 0$

=> Anomalous Transport

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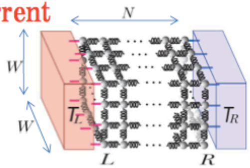
Testing the additivity Principle

- For a harmonic crystal, κ is independent of temperature. $\sigma = 2\kappa T^2$. Hence the prediction of CGF from the additivity principle $\mu_{AP}(\lambda)$ can be expressed in terms of a single parameter κ. Closed form expression for μ_{AP}.
- We evaluate both κ and $\mu(\lambda)$ numerically using the exact formula in terms of $\mathcal{T}(\omega)$.
- Use this κ to evaluate $\mu_{AP}(\lambda)$.
- Compare $\mu(\lambda)$ and $\mu_{AP}(\lambda)$.
- Do the above for different system parameters.

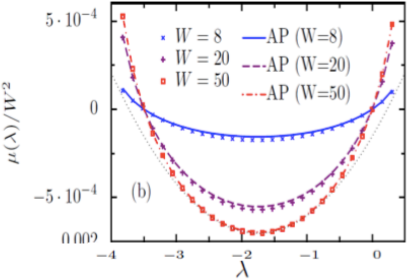
(b) Random Mass with onsite potential $k_0 \neq 0$

: Fourier's law for large W in average current

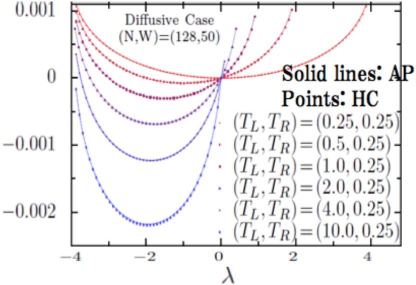
$$\mathcal{H} = \sum_{i,j,k} \frac{p_{i,j,k}^2}{2m_{i,j,k}} + \sum_{<(i,j,k)(i',j',k')>} \frac{k}{2}(x_{i,j,k} - x_{i',j',k'})^2 + \frac{k_0}{2} x_{i,j,k}^2$$



$(T_L, T_R) = (2.0, 0.25)$ $N = 128$



Different temperature sets



Clear agreement with the Additivity Principle (AP) prediction for large W

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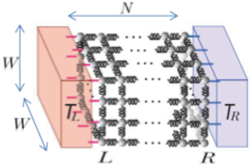
(c) Random Mass without onsite potential $k_0 = 0$

: Anomalous Transport in average current

$$\mathcal{H} = \sum_{i,j,k} \frac{p_{i,j,k}^2}{2m_{i,j,k}} + \sum_{<(i,j,k)(i',j',k')>} \frac{k}{2}(x_{i,j,k} - x_{i',j',k'})^2 + \frac{k_0}{2} x_{i,j,k}^2$$



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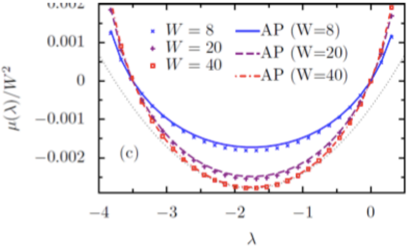
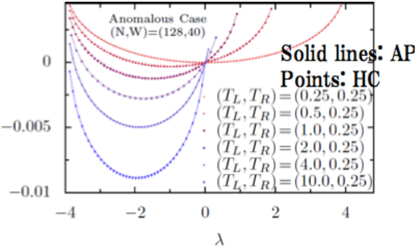


Different temperature sets



Conclusions

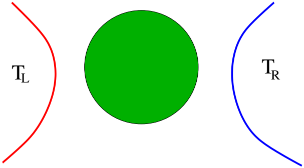
- The additivity principle seems to be be very accurate for the disordered $3D$ harmonic crystal both for the diffusive (pinned) and anomalous (unpinned) cases.
- This implies that for systems with anomalous transport, all order cumulants have the same scaling with system size as the average current.
- We have also verified that the additivity principle does not work in disordered harmonic crystals in lower dimensions where the effect of Anderson localization is very strong.

Model of P. Visco (JSM, 2006)

Single Brownian particle interacting with two heat baths.

$$m\frac{dv}{dt} = -\gamma_L v + \eta_L - \gamma_R v + \eta_R$$

Look at $Q = \int_0^\tau dt(-\gamma_L v + \eta_L)v$.



In this case $\mathcal{L}$ can be transformed to the Schroedinger equation for particle in a harmonic well. Exact closed form-solution for $Z(\lambda, U, \tau)$.

Some interesting observations of the paper:

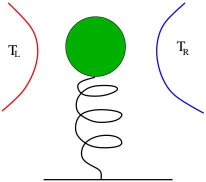
1) $\mu(\lambda) = \mu(\Delta\beta - \lambda)$ – Always true.

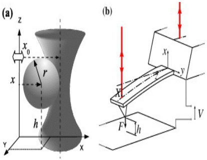
2) However $h(q) - h(-q) = \Delta\beta q$ – Not always true. The Legendre transformation is sometimes not valid for some range of values of q. This happens when $g(\lambda)$ has singularities.

3) Question: Does this happen quite generically or is this a very special case ?

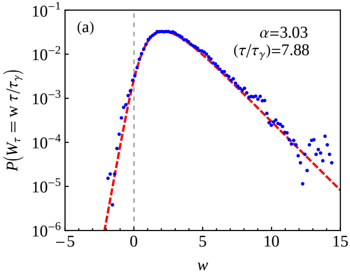
Single particle in a harmonic trap coupled to two heat baths

Sanjib Sabhapandit (EPL,2011).





Using our solution, both $\mu(\lambda)$, $g(\lambda)$ and $h(q)$ can be explicitly computed. Direct comparisions can be made with the experiments of Ciliberto et al on micro-cantilevers (EPL, 2010).



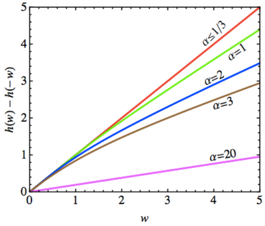


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Fig. 2: (Color online). Asymmetry function for various α.

Fluctuation theorems

Let Q_L be the heat flow from left reservoir into system in time τ and Q_R the heat flow from right reservoir into system.

Then, for systems with Markovian dynamics

$$S = -Q_L/T_L - Q_R/T_R + \ln[P_{SS}(U_f)] - \ln[P_{SS}(U_i)]$$

satisfies an exact FT relation, valid *for any finite time interval* τ.

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

Here we have looked at $S' = Q_L\,(1/T_R - 1/T_L)$ which seems physically more relevant than S. This differs from S by a boundary term. For systems with a bounded phase-space the transient SSFT relation for S implies the large τ SSFT for S'. For systems with unbounded phase space it seems to be difficult to make any general FT statment for S', even for large τ.

Our work shows that a FT relation for S' is not always valid. However the FT symmetry relation for the corresponding CGF $\mu(\lambda)$ seems to be more robust and probably follows from a symmetry property of the relevant Fokker-Planck operator.

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, $\mu(\lambda)$, for heat current in harmonic systems connected to Langevin reservoirs. The leading order correction to $\mu(\lambda)$ is also obtained.
- Applications: Test of additivity principle. Understanding the reasons as to why the AP works remains an open problem.
- Applications: Explicit calculation of LDF for single harmonic oscillator and comparision with experimental data.

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 (PRE, 2011)]

This algorithm is complimentary to the algorithm proposed by Giardina, Kurchan, Peliti (PRL, 2006) which computes $\mu(\lambda)$. We directly obtain $P(Q)$.

- 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.

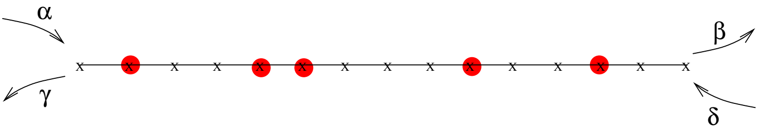
- In simulation we estimate $P(Q,\tau)$ by performing averages over M realizations of biased-dynamics to obtain:

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

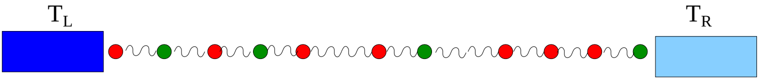
- A necessary requirement of the biased dynamics is that the distribution of Q that it produces, i.e., $P_b(Q,\tau) = \langle \delta_{Q,Q(\mathbf{x})} \rangle_b$, is peaked around the desired values of Q for which we want an accurate measurement of $P(Q,\tau)$.
- Also choose biased dynamics such that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

Numerical computation of large deviations

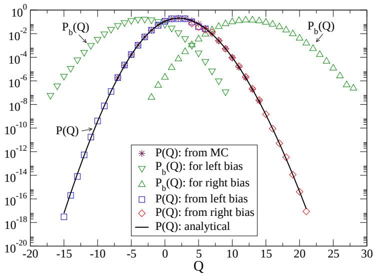
Two Examples:
(i) Particle current in SSEP connected to particle reservoirs .



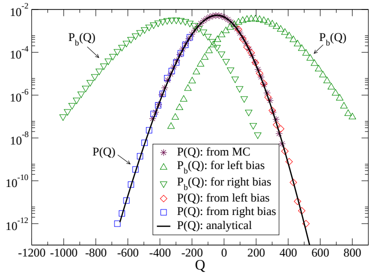
(ii) Heat current in harmonic chain connected to heat reservoirs .



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.

Simulations

- This works very well for small systems but gets difficult for large systems.
- Open problem: $\langle A \rangle = \langle e^{-W} A \rangle_B$.
  How to choose the biased dynamics in an optimum way, so that the weight factor remains small?