Macroscopic Fluctuations in Statistical Physics

- Large Deviations -

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Warm up: Coin tossing

A simple probabilistic model: tossing a fair coin

$$\boldsymbol{P}\{X = 1\} = \boldsymbol{P}\{X = -1\} = \frac{1}{2}$$

$\{X_i\}$ - identically independently distributed random variables

- paradigm of physical systems consisting of many microscopic components
- self-averaging property $\leftrightarrow$ law of large numbers

$$\lim_{N} \boldsymbol{P}\{|\frac{1}{N}\sum_{i=1}^{N} X_i| > \epsilon\} = 0$$

What can we say about fluctuations?

Structure of normal fluctuations

Typical fluctuations of the sum $S_N = X_1 + \cdots + X_N$

- take place on the scale $\sqrt{N}$
- have a universal form - central limit theorem

$$\lim_N \boldsymbol{P}\{a < \frac{S_N}{\sqrt{N}} < b\} = \frac{1}{\sqrt{2\pi}} \int_a^b e^{-\frac{x^2}{2}} \, \mathrm{d}x$$

The fluctuation on other scales are rare:

$$\lim_N \boldsymbol{P}\{a < \frac{S_N}{N^\alpha} < b\} = 0 \qquad 0 \le \alpha \le 1, \quad \alpha \neq \frac{1}{2}$$

Structure of rare fluctuations

- Microscopic fluctuations ($\alpha = 0$)
  - Local central limit theorem:

$$\boldsymbol{P}\{a < S_N < b\} \simeq \frac{1}{\sqrt{2\pi N}} \int_a^b e^{-\frac{x^2}{2}}\,\mathrm{d}x$$

- Macroscopic fluctuations ($\alpha = 1$)
  - Large deviation behavior:

$$\boldsymbol{P}\{0 \leq a < \frac{S_N}{N} < b\} \simeq \frac{1}{\sqrt{2\pi N}} e^{-N\mathcal{I}(a)}$$

with the rate function coinciding with the entropy

$$\mathcal{I}(a) = -\frac{1+a}{2}\log\frac{1+a}{2} - \frac{1-a}{2}\log\frac{1-a}{2} = \frac{a^2}{2} + \mathcal{O}(a^4)$$

General features of macroscopic fluctuations

The exponential law of large deviations

- describes in detail the speed of the macrovariable $\frac{S_N}{N}$ self-averaging
- is a generic law for the probabilities of large fluctuations
- occurs with the rate function $\mathcal{I}$ which has the meaning of "entropy"

$$\mathcal{I}(a) = \sup_t (ta - \log\langle e^{tX} \rangle)$$

- gives an extension of the central limit theorem

$$\mathcal{I}(\frac{a}{\sqrt{N}}) = \frac{a^2}{2N} + o(\frac{1}{N})$$

Thermodynamic theory of fluctuations

- Boltzmann: Thermodynamic entropy has a microscopic interpretation: $S = k \log W$
- Einstein: Read the formula as $\boldsymbol{P}\{M\} = e^{\frac{S(M)}{k}}$!
  - starting point of the fluctuation theory
  - since the entropy S is extensive, $S(M) = Vs(M)$, the entropy density $s(M)$ is a large deviation rate function
  - a usual application: analysis of normal fluctuations

Statistical approach: Cramer's trick

In order to compute the large deviation probability

$$\boldsymbol{P}_V\{M_V = Vm\} = \frac{1}{\mathcal{Z}_V} \int \mathrm{d}\sigma\, e^{-\beta H_V(\sigma)} \delta(M_V(\sigma) = Vm)$$

change $H_V \longrightarrow H_V + hM_V$ so that

$$\langle M_V \rangle^h = Vm$$

Actually, then $M_V \simeq Vm$ typically!

$$\begin{aligned} \boldsymbol{P}_V\{M_V = Vm\} &= \boldsymbol{P}_V^h\{M_V = Vm\} e^{-\beta hmV} \frac{Z_V^h}{Z_V} \\ &\simeq e^{\beta V(-hm + f^h - f)} \\ &\sim e^{\beta V g(m)} \end{aligned}$$

General mathematical results

- Gartner-Ellis theory: if a sequence of variables X_V has a differentiable thermodynamic limit

$$\phi(t) = \lim_V \frac{1}{V} \log\langle e^{tX_V} \rangle_V$$

then

$$\boldsymbol{P}\{X_V = Va\} \sim e^{-V\mathcal{I}(a)} \qquad \mathcal{I}(a) = \sup_t \left(ta - \phi(t)\right)$$

- Bryc's theory: analytical generating function $\phi(t) \Longrightarrow$ normal fluctuations by expanding $\mathcal{I}$ to the quadratic order
- Olla's extension: Still true in the regime of phase transitions, where $\mathcal{I}(a) = 0$

- For a collection of macrovariables

$$\phi(t_1,\ldots,t_n) = \lim_V \frac{1}{V} \log \langle e^{\sum_i t_i X_i} \rangle_V$$

- Large deviations for empirical distributions (=types)

$$\begin{aligned}
\boldsymbol{P}\{L_V^X = \nu\} &\sim e^{-V\mathcal{I}(\nu)} \\
\mathcal{I}(\nu) &= S(\nu \,|\, \mu_{\text{eq}}) = -\beta(f^X(\nu) - f^X) \\
f^X(\nu) &= \lim_V \frac{1}{V} \log[\int (H_V + X_V)\,\mathrm{d}\nu - \frac{1}{\beta} S(\nu)]
\end{aligned}$$

- Variational principle:

$$\inf_\nu f^X(\nu) = f$$

To Remember:

- Large deviation rate function is generically a thermodynamical potential.
- Not true for quantum systems!

Macroscopic fluctuations in quantum systems

(1) K. Netočný and F. Redig, J. Stat. Phys., 117:521-547 (2004)

(2) M. Lenci, L. Rey-Bellet, math-ph/0406065 (2004)

Macroscopic fluctuations for a single observable:

$$\boldsymbol{P}_V\{M_V = Vm\} = \frac{1}{\mathcal{Z}_V}\int \mathrm{d}\sigma\, e^{-\beta \hat{H}_V(\sigma)}\delta(\hat{M}_V(\sigma) = Vm)$$

Observe:

- Cramer's idea does not work because $[H, M] \neq 0$
- By the Gartner-Ellis theory we need to know the analytical properties of the generating function

$$\phi(t) = \lim_V \frac{1}{V}\log\langle e^{tM_V}\rangle_V$$

- Since $\phi(t)$ is not a "free energy", usual methods to prove the thermodynamic limit fail!
- We resort to perturbative regimes and develop convergent perturbation expansions for $\phi(t)$

High-temperature regime

- Spin-lattice model: the Hilbert space $\mathcal{H}^{\otimes \mathbb{Z}^d}$ and the Hamiltonian
$$H_V = \sum_{A \subset V} \Phi_A$$
- For $M_V = \sum_i M_i$ where M_i is a one-site observable, compute this:
$$\langle e^{tM_V} \rangle_\beta = \frac{1}{\mathcal{Z}_V} \mathrm{Tr}[e^{-\beta H_V} e^{tM_V}] = \frac{\mathrm{Tr}[e^{tM_0}]^V}{\mathcal{Z}_V} \langle e^{-\beta H_V} \rangle_t$$
where $\langle \cdot \rangle_t$ is an infinite-temperature (product) distribution with density matrix e^{tM_V}

- A trick:

$$\langle e^{-\beta H_\Lambda}\rangle_t = \langle \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{A_1,\dots,A_n \subset \Lambda} \Phi(A_1)\dots\Phi(A_n)\rangle_t$$

  is the partition function of a hard-core lattice gas

- Use the cluster expansion,

$$\log\langle e^{-\beta H_\Lambda}\rangle_t = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{\gamma_1,\dots,\gamma_n \sqsubset \Lambda} a_T(\gamma_1,\dots,\gamma_n) \prod_{i=1}^{n} \rho^{t,\beta}(\gamma_i)$$

  where γ is a cluster of interaction sets and

$$\rho^{t,\beta}(\gamma = A_1,\dots,A_k) = \frac{(-\beta)^k}{k!} g_C(A_1,\dots,A_k)\, \langle \Phi(A_1)\dots\Phi(A_i)\rangle_t$$

  is a correlation function

Results

- For $\beta \ll 1$ the (limit) generating function $\phi(t)$ is analytic in a strip $\Im t < \delta$
- This implies the exponential decay of macroscopic fluctuations of M_V and gives a perturbation expansion for the rate function
- A consequence: central limit theorem for normal fluctuations
- A similar approach can be used for semiclassical systems in low-temperature regime
- Open problems
  - The nature of macroscopic fluctuations in the criticality?
  - Large deviation theory for correlated macroscopic fluctuations of non-commuting observables?

Transport in chain of coupled oscillators

- Model Hamiltonian

$$H(p,q) = \sum_{i=1}^{N} \frac{p_i^2}{2} + U(q) \qquad U(q) = \sum_{i=1}^{N} U_i(q_i) + \sum_{i=1}^{N-1} \lambda_i \Phi(q_{i+1} - q_i)$$

- Heat baths modelled via Langevin forces $\longrightarrow$ total stochastic dynamics:

$$\begin{aligned} dq_i &= p_i dt, \quad i = 1, \dots, N \\ dp_i &= -\frac{\partial U}{\partial q_i}(q) dt, \quad i = 2, \dots, N-1 \\ dp_i &= -\frac{\partial U}{\partial q_i}(q) dt - \gamma p_i dt + \sqrt{\frac{2\gamma}{\beta_i}} dW_i(t), \quad i = 1, N \end{aligned}$$

- Fokker-Planck equation:

$$\frac{\partial\rho}{\partial t} = (p\cdot\nabla_q - \nabla_q U\cdot\nabla_p + \gamma\sum_{i=1,N} p_i\frac{\partial}{\partial p_i} + \sum_{i=1,N}\frac{\gamma}{\beta_i}\frac{\partial^2}{\partial p_i^2})\rho$$

Detailed balance regime

A consistency check that the model is physically meaningful:
For $\beta_1 = \beta_N$, the canonical distribution

$$\rho^\beta(p,q) = \frac{1}{\mathcal{Z}} e^{-\beta H(p,q)}$$

is

- stationary: $\frac{\partial \rho^\beta}{\partial t} = 0$
- reversible:

$$\rho(q,p)\boldsymbol{P}\{(q,p) \xrightarrow{t} (q',p')\}$$
$$= \rho(q',p')\boldsymbol{P}\{(q',-p') \xrightarrow{t} (q,-p)\}$$

Breaking the detailed balance

- Time-integrated heat current into the i-heat bath, $i = 1, N$:

$$J_i^\tau(\omega) \equiv \int_{-\tau}^{\tau} [\gamma p_i^2(t) dt - \sqrt{\frac{2\gamma}{\beta_i}} p_i(t) \circ dW_i(t)] \qquad \omega = [(p_t, q_t), -\tau \leq t \leq \tau]$$

- Conservation of energy:

$$H(\omega_\tau) - H(\omega_{-\tau}) = -\sum_{i=1,2} J_i^\tau(\omega)$$

- Fluctuating entropy production:

$$R_\rho^\tau(\omega) = \sum_{i=1,2} \beta_i J_i^\tau(\omega) + \ln \rho(\omega_{-\tau}) - \ln \rho(\omega_\tau)$$

- Mean entropy production:

$$\langle R_\rho^\tau \rangle = \sum_{i=1,N} \beta_i \langle J_i^\tau(\omega) \rangle + S(\rho_\tau) - S(\rho_{-\tau}) \qquad S(\rho) := -\langle \ln \rho \rangle$$

Mean entropy production explicitly

The mean entropy production is

$$\langle R_\rho^\tau \rangle = \int_{-\tau}^{\tau} \dot{R}(\rho_t)\,\mathrm{d}t$$

where the mean entropy production rate has the form

$$\dot{R}(\rho) \equiv \sum_{i=1,N} \frac{\gamma}{\beta_i} \int \mathrm{d}p\mathrm{d}q \left[\frac{e^{-\beta_i p_i^2/2}}{\sqrt{\rho}} \frac{\partial}{\partial p_i} (e^{\beta_i p_i^2/2} \rho) \right]^2$$

Consequences:

- Second law: $\dot{R}(\rho) \geq 0$
- Stationary transport:
  $\beta_1 < \beta_N \Longrightarrow \dot{R}(\rho_s) > 0 \Longrightarrow \langle J_N \rangle_s = -\langle J_1 \rangle_s > 0$

Fluctuation symmetry

Basic observation:

Fluctuating entropy production quantifies
the breaking of the detailed balance symmetry

$$R_\rho^\tau(\omega) = \log \frac{\boldsymbol{P}_\rho^\tau\{\omega = (q_t, p_t)\}}{\boldsymbol{P}_{\rho_\tau}^\tau\{\Theta\omega = (q_{-t}, -p_{-t})\}}$$

Time reversal of trajectories in detail:

$$(\Theta\omega)(t) := \pi\omega(-t) \qquad \pi(q,p) = (q,-p)$$

The fluctuation symmetry in a standard form:

$$\frac{\boldsymbol{P}\{R\}}{\boldsymbol{P}\{-R\}} = e^R$$

Steady state fluctuation symmetry for dissipated heat

For the entropy production in the reservoirs

$$Q^\tau(\omega) = \sum_{i=1,N} \beta_i J_i^\tau(\omega)$$

the fluctuation symmetry holds true in the sense of large deviations, i.e. asymptotically for large spans τ:

$$\lim_\tau \frac{1}{\tau} \log \frac{\boldsymbol{P}\{Q^\tau = q\tau\}}{\boldsymbol{P}\{Q^\tau = -q\tau\}} = q$$

Equivalently, the generating functional

$$\phi(z) = \lim_\tau \frac{1}{\tau} \langle e^{-\sum_{i=1,N} z_i J_i^\tau} \rangle$$

has the symmetry

$$\phi(z) = \phi(\beta - z)$$

Miscellaneous consequences of fluctuation symmetry

- Second law in mean: $\langle R_\rho^\tau \rangle \geq 0$, respectively $\langle Q \rangle \geq 0$.
- In general, $\langle e^{-R} \rangle = 1$
- A bound on the probability of the "violation" of the second law:

$$\boldsymbol{P}\{R_\rho^\tau \leq -\Delta\} \leq e^{-\Delta}$$

- The symmetry of the generating functional implies the (Green-)Kubo formula

$$\chi_{ik} \equiv \frac{\partial \langle J_i^\tau \rangle}{\partial \beta_k}(\beta_i = \beta) = \frac{1}{2}\langle J_i^\tau(\omega) J_k^\tau(\omega)\rangle_\beta$$

- Onsager relations follow: $\chi_{ik} = \chi_{ki}$
- Note that the fluctuation symmetry is not restricted to the linear-response regime!

Jarzynski identity

- Add an external driving to the dynamics:

$$dp_i = -\frac{\partial(U + U_t^{\text{ext}})}{\partial q_i}\,dt$$

- Modified energy conservation:

$$H(\omega_\tau) - H(\omega_{-\tau}) = -J^\tau(\omega) + W^\tau(\omega) \qquad W^\tau(\omega) = \int_{-\tau}^{\tau} \frac{\partial U_t^{\text{ext}}}{\partial t}(q_t)\,dt$$

- Assume both the initial and final states to be in equilibrium

$$\rho_{-\tau} = \frac{1}{\mathcal{Z}_{-\tau}} e^{-\beta H_{-\tau}} \qquad \rho_\tau = \frac{1}{\mathcal{Z}_\tau} e^{-\beta H_\tau}$$

- The total entropy production:

$$R = \beta J + S(\rho_\tau) - S(\rho_{-\tau}) = \beta[W - \mathcal{F}(\rho_\tau) + \mathcal{F}(\rho_{-\tau})]$$

Fluctuation symmetry in the form

$$\langle e^{-R} \rangle = 1$$

implies

Jarzynski identity

$$\langle e^{-W} \rangle = e^{-\Delta\mathcal{F}} \quad \longrightarrow \quad \langle W \rangle \geq \Delta\mathcal{F}$$

Microscopic origin of the fluctuation symmetry

- Gallavotti, Cohen: The first rigorous derivation in the framework of dynamical systems
- Crooks, Jarzynski, Spohn: Derivation for stochastic systems
- Jarzynski: Derivation for (classical) Hamiltonian systems
- Fluctuation symmetry is intimately related to the microscopic reversibility of the underlying dynamics

A hint (from Maes-N.[2003]):
For a closed Hamiltonian system, write the detailed balance condition in the form

$$\log \frac{\boldsymbol{P}\{M \longrightarrow N\}}{\boldsymbol{P}\{\pi N \longrightarrow \pi M\}} = \log \rho(N) - \log \rho(M) = S_B(N) - S_B(M)$$

Summary and open problems

- Large deviations formalism is a natural framework for the classical equilibrium statistical mechanics but finds non-trivial applications in the dynamical problems too
- Macroscopic fluctuations in the quantum models also have a large deviation behavior but the rate functions do not allow for a direct thermodynamic interpretation
- It reminds to understand the structure of correlated macroscopic fluctuations for non-commuting observables
- Steady state fluctuation symmetry for the dissipated heat only holds true in the large deviation regime, in contrast to the Jarzynski identity for transient processes
- A precise formulation and meaning of the fluctuation symmetry for quantum systems remains to be cleared up