Macroscopic Fluctuation Theory (MFT)

"A set of techniques developed recently to study non-equilibrium system"

* Addressing the following big problem:

To study thermodynamic properties of system in equilibrium we have a systematic theoretical framework given by Equilibrium statistical mechanics

Equi:	Microscopic	$\longrightarrow$	Macroscopic.
Non-eq:		X no such general framework.	

* Over the past few decades: new direction started which was a concept called Large deviation borrowed probability theory [S.R.S Varadhan Courant Inst]

> A generalization of free energy to non-equilibrium.

Large-deviation function

* Non-equilibrium fluctuations are characterized in terms of Large-D.F.
* Typically very hard to compute

> * MFT provides a systematic framework to calculate and analyze Large-deviation function in Non-equilibrium system of many degrees of freedom

* $\boxed{\text{Starts at}}$

Coarse-grained description $\longrightarrow$ [redacted] field theory

(fluctuating hydrodynamics) (effective action)

min Action $\equiv$ Large deviation function.

version I will talk

References: ① Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim
Rev. Mod. Phys 87, 593 (2015)

② Derrida: J. Stat. Mech, P07023 (2007)
Many in discussion with him.

~~③ Yariv Kafri Beg-rohu summer school lecture~~ (2016)

Out-line: ① Fluctuations in equilibrium, Large-deviation.

② Non-equilibrium fluctuation

* Master eqn, FP, Langevin, [redacted] trajectory
on configuration
their time reversibility.

③ MFT in Langevine equation (single-degree of freedom)

④ Systems with many-degrees of freedom.

[redacted]

Equilibrium fluctuations :

" If a system is very weakly coupled to a heat bath at a given "temperature", ~~if the coupling is indefinite or not known precisely~~, if the coupling has been on for a long time, and if all the "fast" things happened and all the "slow" things not, the system is said to be in thermal equilibrium"

Rechard Feynman : Stat mech a set of lectures.

* Equilibrium defined on a time and length scal'

Equilibrium.

Principles of thermodynamics :

Many micro degrees of freedom $\longrightarrow$ few macroscopic state variables

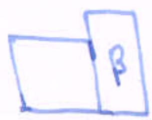
V, E, N : Extensive variables

P, T, μ : Intensive variable.

S, F, G : Thermodynamic potentials.

Statistical Mechanics :

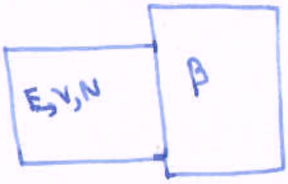
Microcan : $\boxed{E,V,N}$ $\quad S(E,V,N) = k_B \log \Omega(E,V,N)$ $\uparrow 1$

Canonical :  $\quad F(\beta,V,N) = -\log Z_n(\beta,V,N)$

Ensemble equivalence : $\quad F(\beta) = \beta E - S(E)$; $\beta = S'(E)$

Legendre transform

Statistical properties calculated from thermodynamic potential.



- Average: $\langle E \rangle = \frac{d}{d\beta} \mathcal{F}(\beta)$

- <u>Variance</u>: $\langle E^2 \rangle_c = \langle E^2 \rangle - \langle E \rangle^2 = -\frac{d^2 \mathcal{F}(\beta)}{d\beta^2}$

$$= T^2 C_V$$

<u>How about higher moments ; Full distribution ?</u> write in terms of $\mathcal{F}$?

$$P_{V,N}(E) = \frac{\Omega(E,V,N)\, e^{-\beta E}}{\mathcal{Z}(\beta,V,N)} = e^{S(E,V,N) - \beta E + \mathcal{F}(\beta,V,N)}$$

$$\left[\ S(E) = \beta E - \mathcal{F}(\beta) \text{ with } \frac{\partial \mathcal{F}}{\partial \beta} = E = \langle E \rangle \equiv E^* \qquad \left.\frac{\partial S}{\partial E}\right|_{E^*} = \beta\ \right]$$

$$\Rightarrow P_{V,N}(E) = e^{S(E,V,N) - \beta E + \beta E^* - S(E^*)}$$

$$* \quad S(E,V,N) \simeq V\, s(e,\rho) \Rightarrow P_{V,N}(E) \asymp e^{V[s(e,\rho) - s(e^*,\rho) - s'(e^*)(e-e^*)]}$$

$$\Rightarrow \boxed{P(E = V\cdot e) \asymp e^{-V\phi(e,\rho)}}$$

what this means?

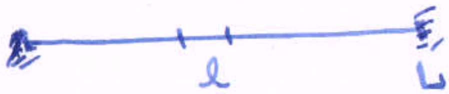
$$\text{where } \boxed{\phi(e,\rho) = s(e^*) - s(e) + s'(e^*)(e-e^*)}$$

⊛ Large-deviation form

Large-deviation function.

$\boxed{\text{Fluctuations of order } V}$

Ex1:



one-dim;
Isolated system

$$P\left[\frac{E_1}{l}=e_1\right] \asymp e^{-l\,\phi(e_1)}$$

$$\boxed{\phi(e_1) = s(\underbrace{e^*}_{\to E/L}) - s(e_1) + s'(e^*)(e_1-e^*)}$$

Ex2:

$$\boxed{\frac{\xi}{a} \ll l \ll L}$$

$x=\frac{il}{L}$; $\frac{E_i}{l} \approx e(x)$ [fluctuations beyond scale l]

$$P(e(x)) \asymp e^{-L\,\phi[e(x)]}$$

$$\boxed{\phi[e(x)] = \int dx \left\{ s(e^*) - s(e(x)) + s'(e^*)\underbrace{(e(x)-e^*)}_{\text{vanish}} \right\}}$$

Ex3:

$$P[\rho(x)] \asymp e^{-L\,\phi[\rho(x)]}$$

$$\boxed{\phi[\rho(x)] = \int dx \left\{ f(\rho(x)) - f(\rho^*) - f'(\rho^*)(\rho(x)-\rho^*) \right\}}$$

$$f(\rho) = -\frac{1}{L}\ln Z_n(\beta, L\rho, L)$$

$$f''(\rho) = \frac{1}{\rho^2 K}$$

Exercise 5:

β, N

Marginal

$$P[\rho(\vec{s})] \asymp e^{-V\phi[\rho(s)]}$$

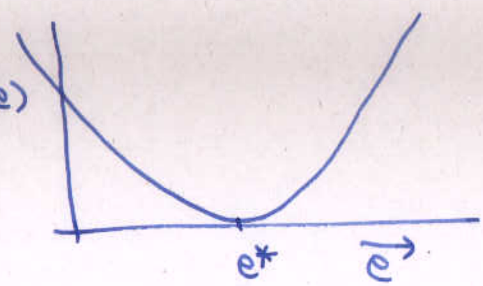
$$\boxed{\phi[\rho(s)] = \int ds \left\{ f(\rho(s)) - f(\rho^*) - f'(\rho^*)(\rho(s)-\rho^*) \right\}}$$

$$\boxed{f = \frac{1}{V}\ln Z(\beta,N,V)}$$

will be used later

$$\boxed{f'' = \frac{1}{\rho^2 \chi}}$$

Properties of ϕ



- $\phi(e^*) = 0$
- Minimum:

$$\left.\frac{\partial\phi}{\partial e}\right|_{e^*} = -s'(e) + s'(e^*)\Big|_{e^*}$$
$$= 0$$

$$\frac{\partial^2\phi}{\partial e^2} = -s''(e^*) = \frac{1}{T^2 (c_V)} \geq 0$$

specific heat per unit volume

- Fluctuations are Gaussian:

$$\phi(e) = \frac{1}{2}\cdot \phi''(e)\Big|_{e^*} (e-e^*)^2 + \cdots O(e^3)$$

$$= \frac{1}{2}\cdot\frac{1}{T^2 c_V}\cdot\frac{(E-E^*)^2}{V^2} + O\left(\frac{1}{V^3}\right)$$

$$\Rightarrow P(E) \asymp e^{-V\phi(e)} \equiv e^{-\frac{(E-E^*)^2}{2T^2 c_V \cdot V} + O\left(\frac{1}{V^2}\right)}$$

Gaussian

with $\boxed{\langle E^2\rangle_c = \langle E^2\rangle - \langle E\rangle^2 = T^2 c_V \cdot V}$

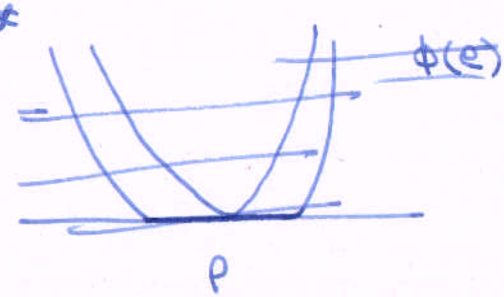
- Near phase transition: C_v diverge

$\equiv$ Non-Gaussian fluctuations ~~be~~

Large fluctuations become important

~~$* \ \phi(e) \sim (e-e^*)^2$~~

~~Ex: in coexistence phase~~



* Any ~~moment~~ is derived from $\phi(e)$:

cumulant generating function:

$$\log \langle e^{\lambda E} \rangle = \lambda \langle E \rangle_c + \frac{\lambda^2}{2!} \langle E^2 \rangle_c + \frac{\lambda^3}{3!} \langle E^3 \rangle_c + \cdots$$

- $\langle E \rangle_c = \langle E \rangle$
- $\langle E^2 \rangle_c = \langle E^2 \rangle - \langle E \rangle^2$
- $\langle E^3 \rangle_c = \langle E^3 \rangle - 3\langle E^2 \rangle \langle E \rangle + 2\langle E \rangle^3$

$\Rightarrow \langle E^n \rangle_c = G^{(n)}(\lambda)$

~~How is $G(\lambda)$ related to $\phi(e)$~~?

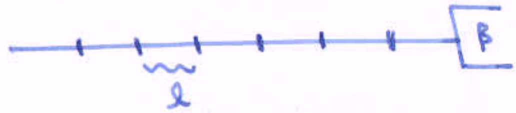
$$\log \int dE \, e^{\lambda E} P(E) \asymp \log \int de \, e^{V[\lambda e - \phi(e)]}$$

$$= V \underbrace{\max_e \{\lambda e - \phi(e)\}}_{G(\lambda)}$$

$$\Rightarrow \boxed{G(\lambda) = \max_e (\lambda e - \phi(e))}$$

$$\Rightarrow \boxed{\langle E^n \rangle_c \approx V \cdot G^{(n)}(\lambda)}$$

Spatial correlation



One-dim

What are correlations $\langle E_i E_j \rangle_c$?

$\boxed{\xi \ll \ell \ll L}$

Ans: $\frac{E_i}{\ell} \simeq e(x)$ where $x = \frac{i\ell}{L}$

Then
$$\boxed{\begin{aligned} \langle E_i \rangle &= \ell \langle e(x) \rangle \\ \langle E_i E_j \rangle_c &= \ell^2 \langle e(x) e(y) \rangle \end{aligned}}$$

Cumulant generating function:

$$\log \left\langle e^{\sum_i \lambda_i E_i} \right\rangle \xrightarrow[\lambda_i \to \lambda(x)]{} \log \left\langle e^{L \int dx\, \lambda(x) e(x)} \right\rangle$$

$\downarrow \quad P(e(x)) \asymp e^{-L \Phi[e(x)]}$

$$\cdot\ L \cdot \underbrace{\max_{e(x)} \left\{ \int dx\, \lambda(x) e(x) - \phi[e] \right\}}_{G[\lambda(x)]}$$

By definition

$$L\, G[\lambda(x)] = L \int dx\, \lambda(x) \langle e(x) \rangle + \frac{L^2}{2!} \int dx\, dy\, \lambda(x) \lambda(y) \langle e(x) e(y) \rangle$$

$$L\, G[\lambda] = L \cdot \int dx\, \lambda(x) \frac{\delta G}{\delta \lambda} + \frac{L}{2!} \int dx\, dy\, \lambda(x) \lambda(y) \frac{\delta^2 G}{\delta \lambda \delta \lambda} + \cdots$$

$$\Rightarrow \boxed{\begin{aligned} \langle e(x) \rangle &= \frac{\delta G}{\delta \lambda(x)} \\ \langle e(x) e(y) \rangle_c &= \frac{1}{L} \frac{\delta^2 G}{\delta \lambda(x) \delta \lambda(y)} \end{aligned}}$$

⊛ ~~leading~~ correlation of fluctuation of order of $\langle E_1 \cdots E_k \rangle \sim \frac{\ell^k}{L^{k-1}}$

⊛ In equilibrium: Short-range correlation

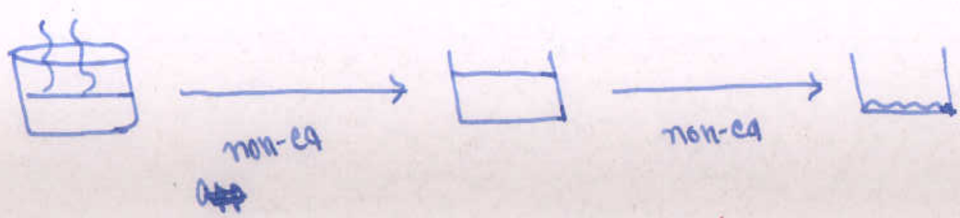
⊛ $\Phi(c(x)) = \int dx\,[f(x)]$ local function

⇒ Correlations are short ranged.

⊛ Differen in non-equilibrium ⊛

$\boxed{\text{How much of these can be extended to non-equilibrium system?}}$

What is non-equilibrium: any thing not in equilibrium.



⊛ Approach to equilibrium:

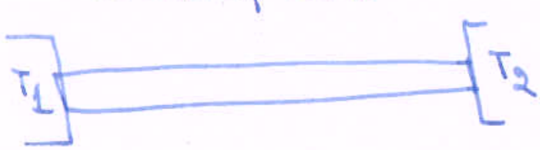
① 

② 

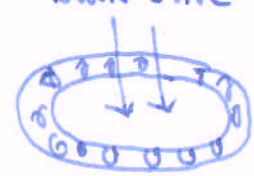
quench, coarsening in Ising model.

⊛ <u>Non-equilibrium stationary state</u>

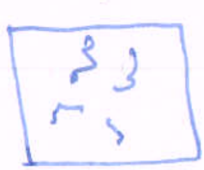
Boundary drive



Bulk drive



Self-propelled particle: active matter



Bacteria colony | collective behavior
Fish school
Flock of Birds

Granular matter | Epidemic spread | Trafic

Sand box

No-thermal mixing

~~Q? Is there a general framework to describe macroscopic properties starting from microscopic dynamics~~

~~micro~~ $\xrightarrow{\text{bridge}}$ macro

Some ~~characteristics~~ comments on non-equilibrium (relevant to us)

Equilibrium	Non-equilibrium
① Zero average current	① non-zero.
② Statistical properties (one-time) do not depend on specific details of the dynamics	② Dynamics is important
③ Relevant state variables • Equation of state Thermodynamic potential	③ ?
④ Universal distribution $P(c) \propto e^{-\beta E(c)}$	④ None
⑤ linear respons	⑤ Recent-progress.
⑥ Universal properties $\Delta S \geq 0$	⑥ Fluctuation theorem: Gallavotti-cohen Jarzynski equality
⑦ ~~Critical~~ phenomena	⑦ ~~Non-equilibrium phase transition~~.

Non equilibrium studies:

* Structural properties: Fluctuation theorem

  Stochastic thermodynamics

  [Van den Broeck, Esposito

  Physica A, 418 (2015)]

* Method of exact solution: Microscopic models

  Domb-Green Vol 18

  ASEP, Katz-Spohn Lebowitz model [Zia] Smittmann

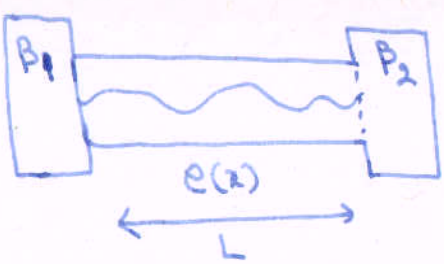
  Adv. in physics. 57(2008), 457 ← Models of heat conduction : [A. Dhar] Adv. Phys.

  Matrix ansatz, Bethe ansatz : [B. Derrida]

  Aci

* Hydrodynamic approach: Coarse-grain scale

~~Recall~~. Large-deviation out-side equilibrium



$$P[e(x)] \asymp e^{-L\phi[e(x)]}$$

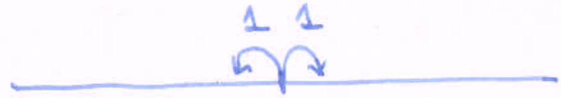
$\boxed{\text{A formal } \cancel{\text{definiti..}} \text{ introduction to LDF}}$

~~What is large~~

$\boxed{\text{Ref on large-deviation : H. Touchette 2009}}$

Phys. Reports. 478, 1−69

Typical example of large deviation:



Discrete time Random walk

$$X_T = \epsilon_1 + \epsilon_2 + \cdots + \epsilon_T$$

- Law of large number: $\frac{X_T}{T} \to 0$ for T large
- Central limit theorem: $\langle X_T^2 \rangle \propto T$ Typical displacement $\sim \sqrt{T}$

$$P\left(\frac{X_T}{\sqrt{T}} = x\right) \sim e^{-x^2}$$

- What about a-typical displacement

$$P\left(\frac{X_T}{T} = r\right) \asymp e^{-T\phi(r)}$$

Exercise 1: Starting from Binomial distribution, show using sterling approximation

$$\boxed{\phi(r) = \frac{1+r}{2}\ln(1+r) + \frac{1-r}{2}\ln(1-r)}$$

Ex 2: ~~↑↑↓↑~~ $p_\uparrow = e^{-h}/(e^{h}+e^{-h}) \mid p_\downarrow = \frac{e^{h}}{e^{h}+e^{-h}} \Rightarrow P\left(\frac{M}{L} = m\right) \sim e^{-L\phi(m)}$

Example: single-file diffusion

$$P\left(\frac{X_T}{\sqrt{T}} = r\right) \asymp e^{-\sqrt{T}\phi(r)}$$

extreme value statistics $e^{e^{-x}}$

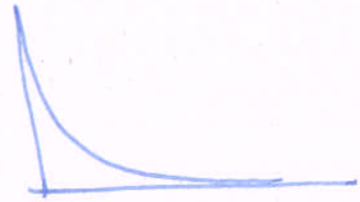
Example:

Net Energy flow $Q_t \simeq t \cdot j$

$$P\left(\frac{Q_t}{t} = j\right) \asymp e^{-t\phi(j)}$$

Example:

Activity $A(t)$



$$P\left(\frac{A_t}{t}=a\right) \asymp e^{-\sqrt{t}\,\phi(a)}$$

* when can one have large-deviation form?

Gärtner-Ellis theorem [H. Touchette (2009)]

Characteristic of large-deviation out-side equilibrium:

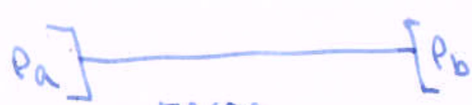
density, current.

①  + All moments can be derived from derivative.

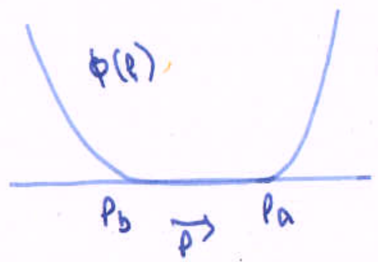
② non-local: $\phi[\rho(x)] = \int dx \int dy\, f(x,y)$

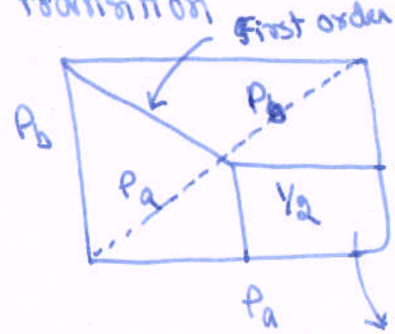
$\Rightarrow$ long-range correlations at generic parameter value.

③ Non-analyticity near phase transition



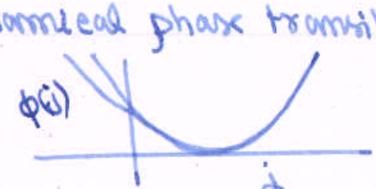
TASEP





non-gaussian.

Dynamical phase transition: where ϕ is non-analytic.



* Symmetries in Large-deviation

$$P\left(\frac{Q_t}{t}=j\right) \simeq e^{-t\,\phi(j)}$$

$$\boxed{\phi(-j)-\phi(j) = j\left(\frac{1}{T_2}-\frac{1}{T_1}\right)}$$

(Gallavotti-Cohen ~~symmetry relation~~ fluctuation theorem)

$$\Rightarrow \quad \frac{P(-j)}{P(j)} \simeq e^{-t\left[\phi(-j)-\phi(j)\right]} = e^{-t\cdot j\left(\frac{1}{T_2}-\frac{1}{T_1}\right)}$$

(* Generalization of Kubo linear response theory)

at eq^n: both equally probable

no-eq^n: are not

(*) ~~[illegible]~~

<u>Broad goal:</u> characterize non-equilibrium fluctuation in terms of Large-deviation.

$\boxed{\text{MFT}}$ <u>gives a tool</u>.

* $\boxed{\text{Why Large deviation important}}$!

① Plays the role of thermodynamic potential (Free energy) in non-equilibrium system:

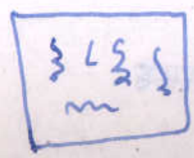
Correlations,

non-analyticity ⟺ Phase transition.

Long-goal "Landau-type" theory for non-equilibrium and its critical phenomena.

(build them from symmetry ground, RG and so on.

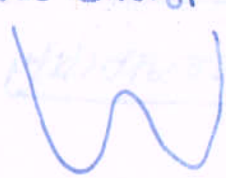
Example: Active matter



Active Brownian particle

(liquid-gas phase coexistence)

can one understand from a free energy-like function



② Contains ^structural properties ~~information~~ of the non-equilibrium: a

$$\Phi(-\delta) - \Phi(\delta) = \delta \cdot \left(\frac{1}{T_2} - \frac{1}{T_1} \right)$$

③ Large [illegible] does not mean not measurable.

Macroscopic observable

as in standard thermodynamics.

• Total Energy; Fluctuation of "measurable" macroscopic density.