Bangalore 2020

Statistical physics of rare events & large deviations

- Mathematical question + trick
- Motivations
- Weak small noise $\nearrow$ Lagrangian
  $\searrow$ Hamiltonian

  detailed balance vs. without.
- Large deviation in diffusive systems
- Active particles.

The mathematical question

N coin tosses outcome $0, 1$

$P(\mathbb{A} = A)$ where $\mathbb{A} = \frac{1}{N} \sum_{i=1}^{N} s_i$ intensive.
$s_i \rightsquigarrow 0, 1$

1) Central limit theorem

$$\langle s \rangle_c = \frac{1}{2} \quad ; \quad \langle s^2 \rangle_c = \frac{1}{2} - \frac{1}{4} = \frac{1}{4}$$

$$\lim_{N \to \infty} p\left(y = \frac{NA - N\langle s \rangle_c}{\sqrt{N}}\right) = \frac{1}{\sqrt{2\pi \langle s^2 \rangle_c}} e^{-y^2/2\langle s^2 \rangle_c}$$

when $NA - N\langle s \rangle_c$ does <u>not</u> scale like $\sqrt{N}$ CLT predicts a zero probability $\quad A - \langle s \rangle_c \sim \frac{1}{\sqrt{N}}$

2) Exact solution

$$P(\mathbb{A} = A) = \frac{1}{2^N} \frac{N!}{[NA]!\,[N(1-A)]!}$$

$$n! \sim n^n e^{-n} \sqrt{2\pi n}$$

$$P(\mathcal{A}=A) = \frac{1}{\sqrt{2\pi}\sqrt{N}\sqrt{A(1-A)}} e^{-N[\ln 2 + A\ln A + (1-A)\ln(1-A)]}$$

$$\equiv e^{-NI(A) + o(N)}$$

with $\boxed{I(A) = \ln 2 + A\ln A + (1-A)\ln(1-A)}$

In large N limit clearly the probability of $\mathcal{A}=A$ is give to leading order by

$$\boxed{P(\mathcal{A}=A) \sim e^{-NI(A)}}$$

$I(A)$ - Rate function / large deviation function

Comment:

* N extensive, A - intensive
* Formally $I(A) = -\lim_{N\to\infty} \frac{1}{N} \ln P(\mathcal{A}=A)$
* $I(A)$ describes fluctutions much beyond CLT
* If we look close to ave value of $1/2$ we can expand $A = \frac{1}{2} + \varepsilon$

$$I(A) \approx 2(A - 1/2)^2 \Rightarrow \text{CLT}$$

Taking a scaling for of $\varepsilon = \alpha/\sqrt{N}$ and then $N\to\infty$ brings back the CLT.

Trick

Equilibrium – want to calculate the entropy → to simplify go to the canonical ensemble

$$Z(\beta) = \sum_{\varepsilon} \Omega(\varepsilon) e^{-\beta\varepsilon}$$

Ω ↘ density of states

$\varepsilon = \frac{E}{N}$

$\delta\varepsilon \sim \frac{1}{\sqrt{N}}$

$$Z(\beta) \sim \Omega(\varepsilon^*) e^{-\beta\varepsilon^*}$$

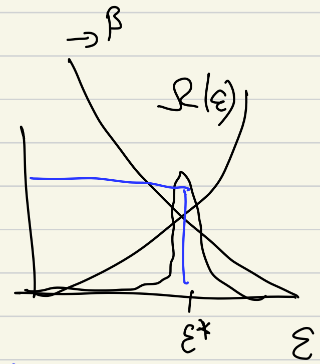
$$= e^{-\beta(\varepsilon^* - \frac{1}{\beta}\ln\Omega(\varepsilon^*))} = e^{-\beta F(\varepsilon^*)}$$

where ε^* is a solution of $\beta = \frac{\partial \ln\Omega}{\partial\varepsilon}$

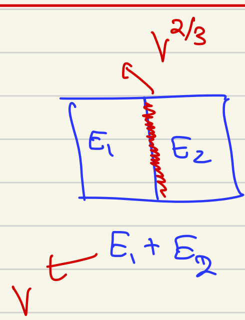
⇒ can obtain the entropy from $F(\varepsilon^*)$

– Calculate $E(\beta) = \varepsilon^*$ $\quad \left(E(\beta) = -\frac{\partial \ln Z}{\partial\beta}\right)$

⇒ $\boxed{S(\varepsilon^*) = (\varepsilon^* - F(\varepsilon^*))\beta}$



$N \sim N\varepsilon$



$\ln\Omega \sim N\phi\left(\frac{E}{N}\right)$

Use same idea for coin problem

$$\langle e^{NkA}\rangle = e^{\ln\langle e^{NkA}\rangle} = \sum_A p(A)\, e^{NkA} \sim p(A^*) e^{NkA^*}$$

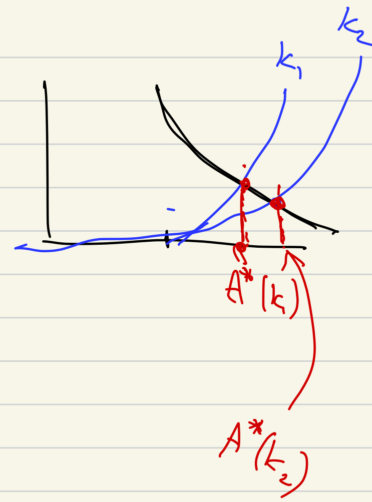
$p(A) = e^{\ln p(A)}$

saddle point

$$\sim e^{NkA^* + \ln p(A^*)}$$

get $N\left[k + \frac{p'(A)}{Np(A)}\right] = 0$

Look at coin toss problem



$$\langle e^{NkA} \rangle = \langle e^{k\sum_{i=1}^{N} s_i} \rangle = \left(\frac{1}{2}\right)^N (1+e^k)^N$$

$$A^*(k) = \frac{1}{N}\frac{\partial \ln \langle e^{NkA} \rangle}{\partial k} = \frac{e^k}{1+e^k}$$

$$\Rightarrow \quad k = \ln \frac{A}{1-A} \quad ; \quad e^k = \frac{A}{1-A}$$

$$\ln p(A^*) = \ln \langle e^{NkA} \rangle - NkA^*$$

$$\ln p(A) = -N\ln 2 + N\ln(1+e^k) - NA \overbrace{\ln\left(\frac{A}{1-A}\right)}^{k}$$

$$= -N \underbrace{[\ln 2 + (1-A)\ln(1-A) + A\ln A]}_{I(A)}$$

Homework – Blackbody – probability of observing N photons in the system?

Have introduce generating function which is related to the number of photons

$$\langle e^{\beta\mu N} \rangle \qquad \beta\mu \to k$$

Motivation

Outside physics

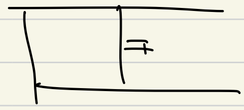
1) Risk managment – probability to go bust.
2) Population dynamics – covid-19 $\Rightarrow$ probability to go extinct?
3) Climate problems –

Physics

1) Reaction rates

2) Fluctuation theorems

$$\langle e^{-\Delta S} \rangle = 1$$



probability of violating the 2nd law

3) Fluctuation in macroscopic system

Consider a macroscopic system with N deg of freedom

In eq. we can ask → given that the system is connected to a bath what is the prob. of observing an energy E.

$$p(E) = \frac{\Omega(E)\, e^{-\beta E}}{Z} = \frac{e^{-\beta(E-TS)}}{Z} = \frac{e^{-\beta F(E)}}{Z}$$

$$Z = \sum_{E} e^{-\beta F(E)} \sim e^{-\beta F(E^*)}$$

$$p(E) \sim e^{-\beta(F(E) - F(E^*))}$$

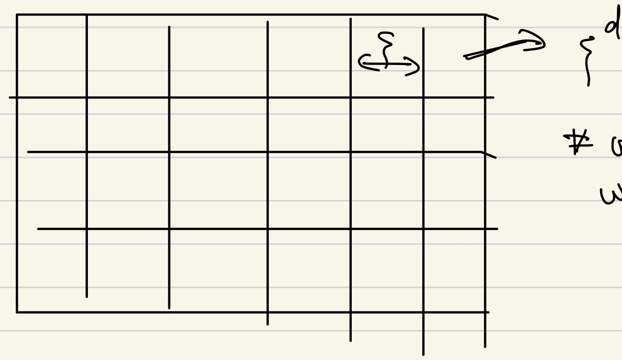
→ prob. of observing a rare energy

F(E) is extensive $\quad F(E) = N f(\varepsilon)$

ε → $\frac{E}{N}$

$$p(\varepsilon) \sim e^{-N \underbrace{[\beta(f(\varepsilon) - f(\varepsilon^*))]}_{\text{rate function/ large deviation function}}}$$

Dynamical picture



\# of segments scales with N

Eq. for fluctuations in E

$$\frac{dE}{dt} = N \begin{pmatrix} \text{deterministic} \\ \text{part pulls} \\ \text{to } E^* \end{pmatrix} + \underbrace{[\text{Noise}]}_{\sqrt{N}\,[\text{Noise}]}$$

In fact, write eq. for $\varepsilon = \frac{E}{N}$

$$\frac{d\varepsilon}{dt} = \begin{pmatrix} \text{det} \\ \text{part} \end{pmatrix} + \frac{1}{\sqrt{N}} [\text{Noise}]$$

$\rightarrow$ weak noise

In eq. this small noise leads to

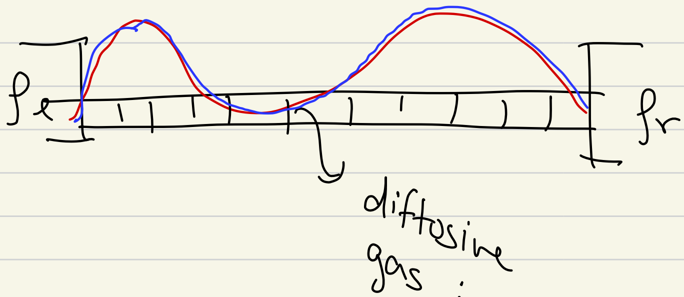
$$p(\varepsilon) \sim e^{-N[\beta(f(\varepsilon) - f(\varepsilon^*))]}$$

Can ask $\Rightarrow$ look at system out of equilibrium and ask probability for some event. X

$$p(x) \sim e^{-N \underbrace{I(x)}}$$

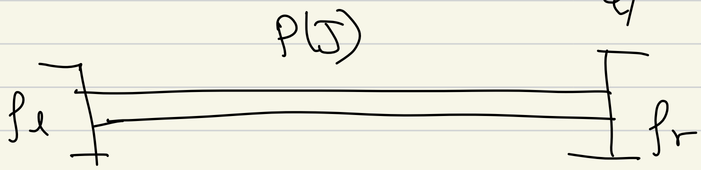
$\rightarrow$ rate function

$\rightarrow$ replaces free-energy.



$\rho_l > \rho_r$

non-local



singular

Yesterday

- Large deviation $\Rightarrow$ rate / large deviation function

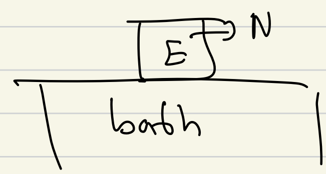
$$I(A) = -\lim_{N\to\infty} \frac{1}{N} \ln P(\mathcal{A}=A)$$

or

$$P(\mathcal{A}=A) \sim e^{-N I(A)}$$

Coins $\quad I(A) = \ln 2 + A \ln A + (1-A)\ln(1-A)$

- Method evaluating LDF $\Rightarrow$ similar to changing ens. in eq.
- Motivation - macroscopic system

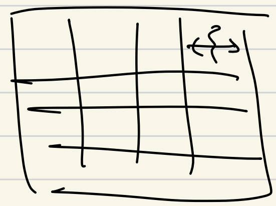


$$P(\varepsilon) \sim e^{-N \big[\underbrace{\beta(f(\varepsilon) - f(\varepsilon^*))}_{I(\varepsilon)}\big]}$$

$\varepsilon = \frac{E}{N}$

ext. $\quad$ int.

Dynamical: $\quad \dfrac{d\varepsilon}{dt} = \underset{\searrow\, \varepsilon^*}{(\text{det})} + \underbrace{\frac{1}{\sqrt{N}}\,\text{noise}}$



$\varepsilon = \dfrac{E}{N} \qquad \sqrt{N}$

$A \sim \dfrac{1}{\sqrt{N}} \qquad A \sim 1.$

$A = \frac{1}{2} + \varepsilon \rightarrow \frac{1}{\sqrt{N}}$

Ref

Varadhan, Frieidlin Wentzell, Ellis

$\Rightarrow$ A. Dembo U. Zeitouni

Physics: 80's R. Graham & T. Tel FP weak noise

2000's B. Derrida, Rome group

Bertini Lasinio

B. Derrida JSM P07023 (07)

L. Bertini et. al. PMP **87** 593 (15)

Y. Baek + YK JSM P08026 (15)

H. Touchette Physics Reports **478** 1 (09)

Weak noise

N independent harmonic oscillator

1 osc $$\partial_t P = -\partial_x \left[-\mu \partial_x V \, P(x,t) - \partial_x (\gamma P(x,t)) \right]$$

$$\frac{kx^2}{2}$$

$$P^s(x) \propto e^{-\frac{\mu k x^2}{2\gamma}} \qquad \gamma = \mu T$$

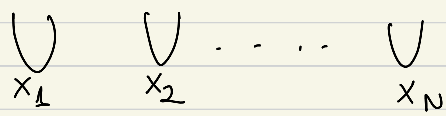
$$= e^{-\beta V(x)}$$

Same physics $$\dot{x} = -\mu \partial_x V + \sqrt{2\gamma}\, \eta(t)$$

$$\langle \eta(t) \rangle = 0$$

$$\langle \eta(t') \eta(t) \rangle = \delta(t-t')$$

N <u>independent</u> oscillators



$$\dot{x}_i = -\mu k x_i + \sqrt{2\gamma}\, \eta_i(t)$$

$$\langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \delta(t-t')$$

Intensive quantity $$X = \frac{1}{N} \sum_{i=1}^{N} x_i$$

$$\dot{X} = \frac{1}{N} \sum_{i=1}^{N} \dot{x}_i = \frac{1}{N} \sum_{i=1}^{N} \left(-\mu k x_i + \sqrt{2\gamma}\, \eta_i(t) \right)$$

$$\dot{X} = -\mu k X + \frac{1}{N} \sqrt{2\gamma} \sum_{i=1}^{N} \eta_i(t)$$

Define $$\bar{\eta} = \sum_{i=1}^{N} \eta_i(t) \Rightarrow \langle \bar{\eta}(t) \bar{\eta}(t') \rangle = \sum_{i=1}^{N} \delta(t-t')$$

$$= N \delta(t-t')$$

Amplitude of $\bar{\eta}$ is $\sqrt{N} \Rightarrow$ define $\eta(t) = \sqrt{N}\,\bar{\eta}(t)$

$$\boxed{\dot{x} = -\mu k x + \sqrt{\frac{2\gamma}{N}}\,\eta(t)}$$

$\delta(t-t') = \langle \eta(t)\eta(t') \rangle$

Exact solution $\partial_t P = -\partial_x \left(-\mu k x P - \frac{\gamma}{N}\partial_x P\right)$

$$P^s(x) \propto e^{-N\frac{\mu k x^2}{2\gamma}}$$

$$= e^{-N I(x)}$$

$$I(x) = \frac{\mu k x^2}{2\gamma}$$

Path integral methods $\rightarrow$ Langrangian

$\rightarrow$ Hamiltonian

$$\dot{x} = v(x) + \sqrt{2\gamma(x)}\,\eta(t)$$

$$P_{TR}(x_f, t_f) = \int_{(0,0)}^{(x_f,t_f)} \mathcal{D}x(t)\, e^{-\int_0^{t_f} dt' \frac{(\dot{x}-v(x))^2}{4\gamma(x)}}$$

$(0,0)$

$\rightarrow \gamma/N$

$$= \int_{(0,0)}^{(x_f,t_f)} \mathcal{D}x(t)\, e^{-N S(x_f, t_f; 0, 0)}$$

$\rightarrow$ large

$\left(\equiv \frac{1}{\hbar}\right)$

$$S = \int_0^{t_f} dt' \frac{(\dot{x}+\mu k x)^2}{4\gamma}$$

ACTION

$$L(\dot{x}, x) = \frac{(\dot{x}+\mu k x)^2}{4\gamma}$$

LAGRANGIAN

Since N is large can get leading order behavior in N using a saddle point approximation

To do: - find most probable trajectory $X(t) \Rightarrow$ most probable history

- plug solution into action $\Rightarrow$ get the probability

LDF

$$S(x_f, t_f ; 0, 0) = \min_{x(t)} \int_0^{t_f} L(\dot{x}, x) dt$$

To minimize Euler-Largrange

$$-\frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{x}} + \frac{\partial L}{\partial x} = 0$$

In the large N limit given that a fluctuation which leads to x_f at t_f occured $\Rightarrow$ it is dominated by a single history

After Euler-Lagrange

$$\ddot{x} = (\mu k)^2 x \quad \Rightarrow \quad \text{uphill}$$

Use this to obtain steady-state distribution

$$0, t_f \to \infty \qquad (-\infty, 0)$$

$$\swarrow 0 \qquad \searrow x_f$$

$$\boxed{x(t) = x_f e^{-\mu k (t_f - t)}}$$

$$\underline{(\dot{x} + \mu k x)} = 2\mu k x_f e^{-\mu k (t_f - t)}$$

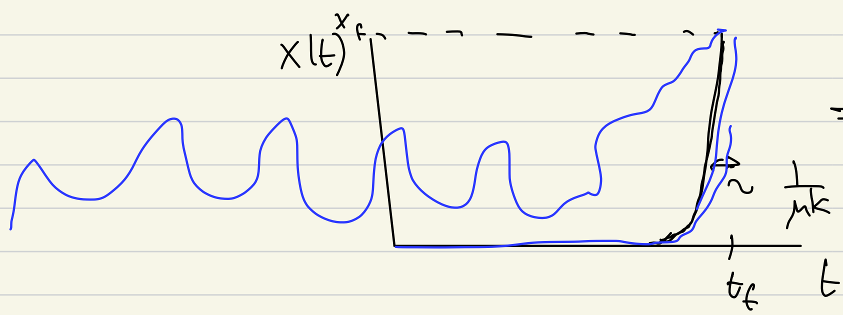
$$S = \lim_{t_f \to \infty} \int_0^{t_f} dt \frac{x_f^2 (\mu k)^2}{\gamma} e^{-2\mu k (t_f - t)} = \frac{x_f^2 \mu k}{2\gamma}$$

In the steady-state $(x_f \to x)$

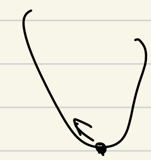
$$P(x) \sim e^{-\frac{N x^2 \mu k}{2\gamma}} \quad \text{as before}$$

Note: solution is 0 except for a period of time $\frac{1}{\mu k}$

$\Rightarrow$ a short time interval



$\Rightarrow$ instantons



Interesting $\Rightarrow$ what is the most probable path for relaxing to the most probable configuration $(x=0)$

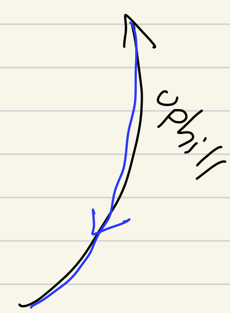
$$\ddot{x} = (\mu k)^2 x$$

Equation is symmetric under time reversal !

$\Rightarrow$ relaxation is time reversed trajectory

$\Rightarrow$ direct consequence of fact that the system

$\Rightarrow$ equilibrium



Going downhill $\Rightarrow$ no cost in action

$$\dot{x} = -\mu k x$$

$$\ddot{x} = -\mu k \dot{x} = (\mu k)^2 x$$

Hamiltonian method

$$\dot{x} = v(x) + \sqrt{\frac{2\gamma}{N}}\,\eta(t)$$

Martin–Siggia–Rose

$$P_{TR}(x_f, t_f; 0, 0) = \left\langle \int_{x(0)=0}^{x(t_f)=x_f} \mathcal{D}x\, \delta\!\left(\dot{x} - v(x) - \sqrt{\frac{2\gamma}{N}}\,\eta(t)\right) \right\rangle_{\eta} \to \text{histories of } \eta$$

$$\tilde{\hat{x}} = N\hat{x}$$

$$\delta\!\left(\dot{x} - v(x) - \sqrt{\frac{2\gamma}{N}}\,\eta(t)\right) = \int_{-i\infty}^{i\infty} \mathcal{D}\hat{x}\; e^{-N\int_0^{t_f} dt\, \hat{x}\left(\dot{x} - v(x) - \sqrt{\frac{2\gamma}{N}}\,\eta(t)\right)}$$

$$P_{TR} = \left\langle \int \mathcal{D}x \int \mathcal{D}\hat{x}\; e^{-N\int_0^{t_f} dt\left(\hat{x}\left(\dot{x} - v(x) - \sqrt{\frac{2\gamma}{N}}\,\eta(t)\right)\right)} \right\rangle_{\eta}$$

$$e^{-\int_0^{t_f} \frac{\eta^2(t)}{2}\,dt}$$

HW

$$\boxed{P_{TR}(x_f, t_f) = \int_{x(0)=0}^{x(t_f)=x_f} \mathcal{D}x\,\mathcal{D}\hat{x}\; e^{-N\int_0^{t_f} dt\,\left[\hat{x}\dot{x} - H[x,\hat{x}]\right]}}$$

momentum

$$H(x,\hat{x}) = \hat{x}\,v(x) + \gamma\hat{x}^2 = -\mu k\hat{x}x + \gamma\hat{x}$$

$$\dot{\hat{x}} = -\frac{\partial H}{\partial x} \quad \Longrightarrow \text{solve}$$

$$\dot{x} = \frac{\partial H}{\partial \hat{x}}$$

$$e^{-N\Phi}$$

Yesterday

Weak noise $\frac{1}{\sqrt{N}} \Rightarrow P(x) \sim e^{-NI(x)}$

Steady-state distribute

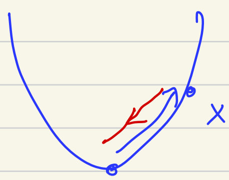
$$\dot{x} = v(x) + \sqrt{\frac{2\gamma(x)}{N}}\,\eta(t) \qquad v(x) = -\mu k x \qquad \gamma(x) = \gamma$$

Path integral

$$P_{TR} \sim \int_{(0,0)}^{(x_f,t_f)} \mathcal{D}x \, e^{-N\int_0^{t_f} dt' \underbrace{\frac{(\dot{x}+\mu k x)^2}{2\gamma}}_{L}}$$

Lagrangian

$t_f \Rightarrow \infty$ $(-\infty, 0) \Rightarrow$ min action $\Rightarrow$ plug solution in $\Rightarrow$ cost of reaching x



$$\dot{x} = -\mu k x$$

MSR method

$$P_{TR} = \int_{x(0)=0}^{x(t_f)=x_f} \mathcal{D}x\,\mathcal{D}\hat{x}\; e^{-N\int_0^{t_f} dt\,[\hat{x}\dot{x} - H(x,\hat{x})]}$$

$$H(x,\hat{x}) = \hat{x}\,v(x) + \gamma\hat{x}^2 = -\mu k x\hat{x} + \gamma\hat{x}^2$$

Could also use

$$\hat{x} = \frac{\partial L}{\partial \dot{x}}$$

$$\dot{\hat{x}} = -\frac{\partial H}{\partial x}$$

$$\dot{x} = \frac{\partial H}{\partial \hat{x}}$$

$$\hat{x} = \frac{1}{2\gamma}(\dot{x} + \mu k x) = (\dot{x} - v(x))/2\gamma$$

Recall that

$$\dot{x} = v(x) + \sqrt{\frac{2\gamma}{N}}\,\eta(t)$$

$$\eta(t) = (\dot{x} - v(x))\sqrt{\frac{N}{2\gamma}}$$

up to prefactor $\hat{x}$ describes the most probable history of the noise.

$$\frac{1}{\sqrt{2\gamma N}}\eta = \frac{(\dot{x} - v(x))}{2\gamma}$$

Look at eqs.

$$H(x,\hat{x}) = \hat{x}\,v(x) + \gamma\hat{x}^2 = -\mu k x\hat{x} + \gamma\hat{x}^2$$

$$\dot{\hat{x}} = -\hat{x}\frac{\partial v(x)}{\partial x} = \mu k\hat{x}$$

$$\dot{x} = v(x) + 2\gamma\hat{x} = -\mu k x + 2\gamma\hat{x}$$

Solving for $\hat{x}(t) = \frac{\mu k}{\gamma}\underset{\text{final position}}{x_f}\, e^{-\mu k(t_f - t)}$

Look at downhill trajectory $\hat{x} = 0$

$$H(\hat{x},x) = -\mu k x\hat{x} + \gamma\hat{x}^2 = 0$$

Since H does not depend explicitly on time $H(x,\hat{x})$ is conserved along a trajectory $\Rightarrow$ Here $H=0$.

Uphill $\Rightarrow$ what is the value of $H(x,\hat{x})$

$$\hat{x} = \frac{\mu k}{\gamma} x_f \, e^{-\mu k (t_f - t)}$$

$$x = x_f \, e^{-\mu k (t_f - t)}$$

$$H(\hat{x}, x) = -\frac{(\mu k)^2}{\gamma} x_f^2 \, e^{-2\mu k (t_f - t)} + \frac{(\mu k)^2}{\gamma} x_f^2 \, e^{-2\mu k (t_f - t)}$$

$$= 0 .$$

$H(\hat{x}, x)$ for $t_f \to \infty$ has to be zero.

Trajectories that are used to calculate steady-state distribution have zero H.

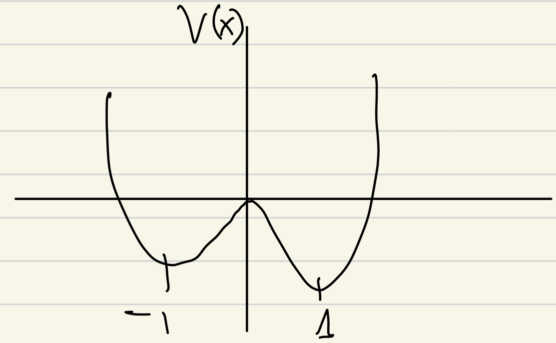
Recap: Lagrangian

Hamiltonian

$$P_{TR}(x_f, t_f) = \int_{x(0)=0}^{x(t_f)=x_f} \mathcal{D}x \, \mathcal{D}\hat{x} \; e^{-N \int_0^{t_f} dt \left[\hat{x}\dot{x} - \cancel{H[x, \hat{x}]} \right]}$$

Consequences of the Hamiltonian structure

$$V(x) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}x^4 \qquad \text{set } \gamma = 1/2$$



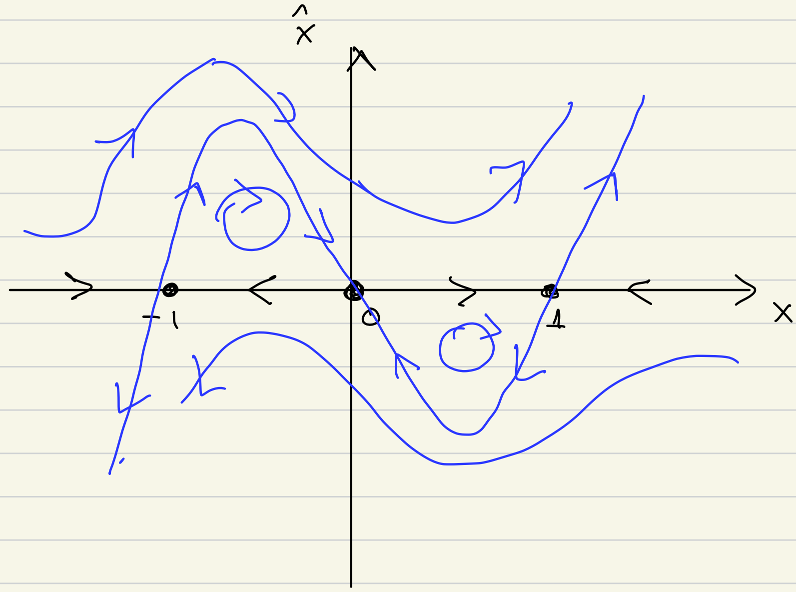
$$v(x) = -\partial_x V(x) = x - x^3$$

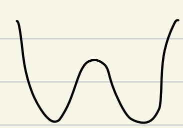
$$H(x,\hat{x}) = \hat{x}(x - x^3) + \hat{x}^2/2$$

$$\dot{x} = x - x^3 + \hat{x} = \frac{\partial H}{\partial \hat{x}}$$

$$\dot{\hat{x}} = \hat{x}(3x^2 - 1) = -\frac{\partial H}{\partial x}$$

(i) The extrema of the potential $(x = -1, 0, 1)$ are fixed points of the dynamics with $\hat{x} = 0$





(ii) Liouvilles $\Rightarrow$ area is preserved $\Rightarrow$ no purely attractive
in unstable fixed point.

(iii) If we want to start at a fixed and end at another point it take an infinite amount of time to the point.

(iv) We can formally draw a graph between fixed points & look at transition probabilities between them

$$
\begin{aligned}
(\hat{x}, x) = \; & 0, -1 \quad \mathrm{I} \\
& 0, \; 0 \quad \mathrm{II} \\
& 0, \; 1 \quad \mathrm{III}
\end{aligned}
$$

$$
\begin{tikzcd}
\mathrm{I} \arrow[r, bend left] & \mathrm{II} \arrow[l, bend left] \arrow[r, bend left] & \mathrm{III} \arrow[l, bend left] \\
(0,-1) & (0,0) & (0,1)
\end{tikzcd}
$$

(v) Trajectories which cross $\hat{x}=0$ have zero energy

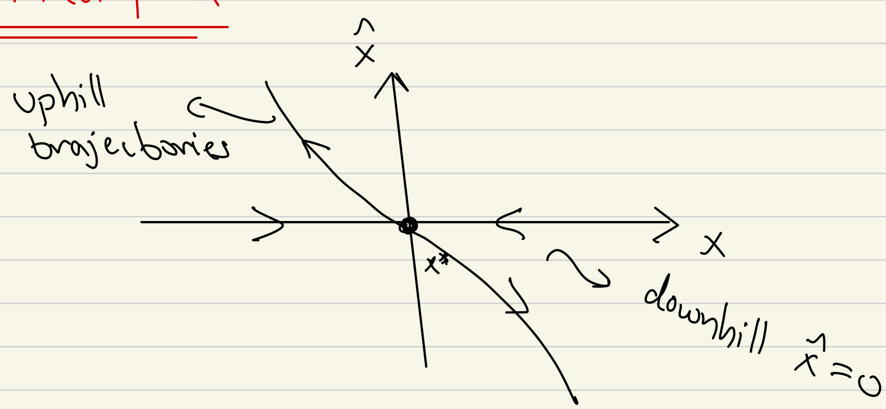
(vi) Dynamics with $H(\hat{x}, x)=0$ minimize the action & should used for steady-state calculations

$$\hat{x}(x - x^3) + \frac{\hat{x}^2}{2} = 0$$

$$\hat{x} = 2(x^3 - x)$$

Now have tools to evaluate $P(x) \sim e^{-N\phi(x)}$ using Lagrangian on Hamiltonian structure.

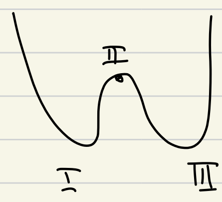
Single fixed point



To find prob. to be at x calc eqs. of motion with solution such that $x(0)=x^*$ and $x(t_f)=x$ with $t_f \to \infty$

$$\Phi = \int_{0}^{\infty} \hat{x}\dot{x}\, dt \qquad (H=0)$$

Several fixed points



$e^{-N\Phi(x_{I})}$

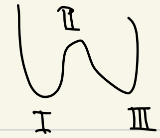
Need to to evaluate

$\Phi(x_{I})$, $\Phi(x_{II})$, $\Phi(x_{III})$

Imagine someone gives you $\Phi(x_{I})$ ....

To evaluate the prob. of being at x

$$\Phi(x) = \min_{\alpha} \Big[\Phi(x_{\alpha}) + \underbrace{S(x, t_f = \infty \mid x_{\alpha}, 0)}_{\text{const of going from fixed point to } x} \Big]$$



Problem ⇒ we don't know $\Phi(x_I)$, $\Phi(x_{II})$, $\Phi(x_{III})$

To do this ⇒ balance fluxed. Example: flux into and out of flux II.

$$e^{-N[\phi(x_I) + S(x_{II}, t_f \to \infty | x_I, 0)]} + e^{-N[\Phi(x_{III}) + S(x_{II}, t_f \to \infty | x_{III}, 0)]}$$

$$= e^{-N[\Phi(x_{II}) + S(x_{II} \to x_I)]} + e^{-N[\Phi(x_{II}) + S(x_{II} \to x_{III})]}$$

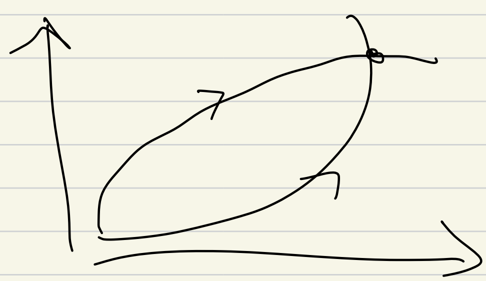
$$\min_{\alpha = I, III} [\phi(x_\alpha) + S(x_{II}, \infty | x_\alpha, 0)] = \Phi(x_{II}) + \min_{\alpha = I, III} S(x_\alpha, \infty | x_{II}, 0)$$

A closed equation for the prob to be at fixed points.

$$\partial_t P = -\frac{\partial}{\partial x}[v(x) P] + \frac{1}{N}\frac{\partial^2}{\partial x^2}[\gamma(x) P] = 0$$

$$P[x) \sim e^{-N\Phi(\vec{x})}$$

$$H[x, \hat{x}] = \hat{x}\, v(x) + \hat{x}^2 \gamma = 0$$



Up to now

$\frac{1}{\sqrt{N}}$ small noise

Model can be in or out of eq.

1d $\qquad \dot{x} = v(x) + \sqrt{\frac{2\gamma(x)}{N}}\,\eta(t)$ $\rightsquigarrow$ gaussian

d $\qquad \dot{\vec{x}} = \vec{V}(\vec{x}) + \mathbb{G}(\vec{x})\,\vec{\eta}(t)$

$$\langle \eta_i(t)\,\eta_j(t')\rangle \propto \delta(t-t')$$

$$P \sim e^{-N\phi(x)}$$

Langrangian form

Bray McKane 90s

1d $\qquad N\int_0^t dt' \frac{(\dot{x}-v(x))^2}{4\gamma(x)}$

d $\qquad N\int_0^t dt' \frac{1}{4}\left(\dot{\vec{x}}-\vec{V}(\vec{x})\right)\cdot \mathbb{\Gamma}^{-1}(\vec{x})\left(\dot{\vec{x}}-\vec{V}(\vec{x})\right)$

$$\mathbb{\Gamma} = \frac{1}{2}\mathbb{G}\mathbb{G}^T$$

Hamiltoian

1d $\qquad N\int_0^t dt' \left[\hat{x}\dot{x} - H[x,\hat{x}]\right]$

$$H[x,\hat{x}] = \hat{x}\,v(x) + \gamma(x)\,\hat{x}^2$$

d $\qquad N\int_0^t dt' \left[\hat{\vec{x}}\cdot\dot{\vec{x}} - H[\vec{x},\hat{\vec{x}}]\right]$

$$H(\vec{x},\hat{\vec{x}}) = \hat{\vec{x}}\cdot\vec{V}(\vec{x}) + \hat{\vec{x}}\cdot\mathbb{\Gamma}\,\hat{\vec{x}}$$

Steady-state $\rightarrow$ minimize action $\rightarrow$ most probable history

$\rightarrow$ plug in action $\rightarrow$ LDF function

find trajectory $\quad x(t)$ Lagrangian

$x(t), \hat{x}(t)$ Hamiltonian

Steady-state $\quad H[x, \hat{x}] = 0$

$t = -\infty \Rightarrow t = 0$

- Because the trajectory takes an infinite amount of time $\rightarrow$ only solution are ones which start at fixed points of dynamics $\Rightarrow$ no noise $\hat{x} = 0$

$$H = \hat{x} (\quad) \Rightarrow H = 0$$

steady-state

$$0 = \partial_t P = -\partial_x (v(x) P) + \frac{1}{N} \partial_x^2 (\gamma P) \Rightarrow P(x) \sim e^{-N\phi(x)}$$

$$0 = v \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial x} \gamma \frac{\partial \phi}{\partial x}$$

Recall

$$H = \hat{x} v(x) + \hat{x} \gamma \hat{x}$$

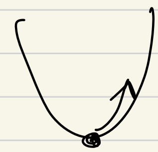
$$H[x, \frac{\partial \phi}{\partial x}] = 0$$

momenta at the end of the path

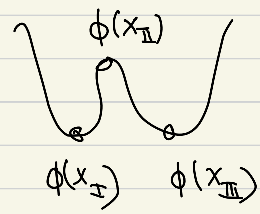
$$S = \int_0^{t_f} dt \, (\dot{x} - v(x)) \frac{1}{4\gamma} \underbrace{(\dot{x} - v(x))}_{\eta \Rightarrow \hat{x}} = \int_0^{t_f} dt \, \hat{x} \gamma \hat{x}$$

$$\Phi(x) = \int_{-\infty}^{0} dt' \, \hat{x} \, \dot{x}$$

Ended : Single fixed point



Metastable

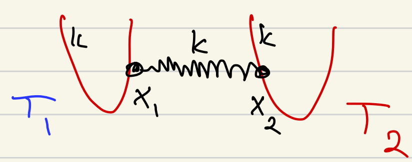


In equilibrium - trajectory uphill time reversed version of the downhill trajectory

$\dot{x} = -v(x) \rightarrow$ down

$\dot{x} = v(x) \rightarrow$ uphill

Homework

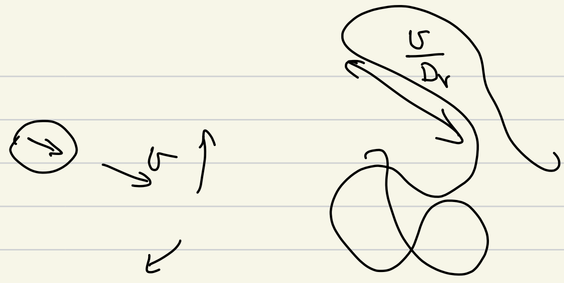


$$\dot{x}_1 = -\mu k x_1 + \mu k (x_2 - x_1) + \sqrt{\frac{\sigma_{11}}{N}} \, \eta_1(t)$$

$$\dot{x}_2 = -\mu k x_2 + \mu k (x_1 - x_2) + \sqrt{\frac{\sigma_{22}}{N}} \, \eta_2(t)$$

$$\langle \eta_i(t) \rangle = 0 \qquad \langle \eta_i(t) \, \eta_j(t') \rangle = \delta_{ij} \, \delta(t - t')$$

Active escape problems



Active Ornstein-Uhlenbeck particle

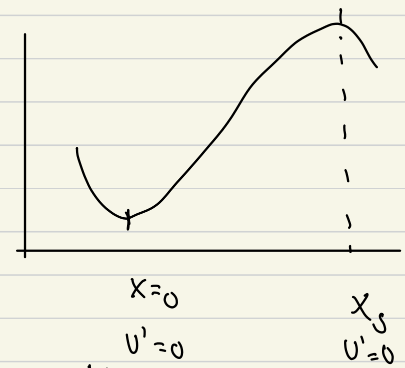
$$\xi = \frac{\tau\dot v + v}{\sqrt{2D}}$$

$$e^{-\int dt\, \xi^2/2}$$

$$\dot x = v - U'(x)$$

$$\tau \dot v = -v + \sqrt{2D}\,\xi(t)$$

$$\langle v(t)\, v(t')\rangle = \frac{D}{\tau} e^{-|t-t'|/\tau}$$



Note $\tau = 0$ $\quad v = \sqrt{2D}\,\xi(t) \Rightarrow$ equilibrium problem

$\tau = 0$ $\quad \dot x = -U'(x) + \sqrt{2D}\,\xi(t)$

Evaluate prob to cross brarrier $\quad e^{-\Phi(x_s)/D}$

$$P_{TR} \sim \int \mathcal{D}x\, \mathcal{D}v\, e^{-\frac{1}{D} S(x,v)}$$

$$S(x,v) = \int_{-\infty}^{0} L(x, v, \dot x, \dot v)\, dt$$

$$L(x, v, \dot x, \dot v) = \begin{cases} \frac{1}{4}(\tau\dot v + v)^2 & \text{if} \quad v = \dot x + U'(x) \\ +\infty & \text{otherwise} \end{cases}$$

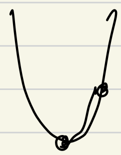
If wanted could enforce δ function on $v = \dot x \cdots$)

$$L(x, \dot x, \ddot x) = \frac{1}{4}\Big(\underbrace{\dot x + U'(x)}_{v} + \tau\underbrace{(\ddot x + \dot x U''(x))}_{\dot v}\Big)^2$$

$$P_{TR} = \left\langle \int \mathcal{D}x\, \mathcal{D}v\, \delta(\dot{x} - v + U'(x))\, \delta(\tau\dot{v} + v - \sqrt{2D}\,\xi(t)) \right\rangle_{\xi}$$

$$= \left\langle \int \mathcal{D}x\, \mathcal{D}v\, \mathcal{D}P_x\, \mathcal{D}P_v\; e^{-\frac{1}{D}\int_{-\infty}^{0}\{P_x(\dot{x} - v + U') + P_v(\tau\dot{v} + v - \sqrt{2D}\,\xi(t))\}} \right\rangle_{\xi(t)}$$

$$= \int \mathcal{D}x\, \mathcal{D}v\, \mathcal{D}P_x\, \mathcal{D}P_v\; e^{-\frac{1}{D}\int_{-\infty}^{0}\{P_x\dot{x} + P_v\dot{v} - H\}}$$



$$H(x, v, P_x, P_v) = (v - U'(x))P_x - \frac{vP_v}{\tau} + \frac{P_v^2}{\tau^2}$$

$\hat{x} = 0$

$x = 0$

Boundary conditions

$x(t) = 0$ $\qquad v(t),\ P_x(t),\ P_v(t) \xrightarrow[t \to -\infty]{} 0$

$t = -\infty$

$x(0) = x_s$

To select velocity at end have to choose the velocity that minizes the action

$\partial_v S = 0 = P_v \rightarrow$ momentum at the end of the process is zero

Note $H = 0$ at $t = 0$

$\dot{x} = v - U'$

$\dot{p}_x = U'' p_x$

$\dot{v} = -\frac{v}{\tau} + 2\frac{P_x}{\tau}$

$\dot{p}_v = \frac{p_v}{\tau} - P_x$

$$H = (v - U')P_x - \cancel{\frac{vP_v}{\tau}} + \cancel{\frac{P_v^2}{\tau^2}} \Rightarrow v = U' \text{ at } t=0$$

$$\dot{x} = v - U'$$

$$\dot{x}(0) = 0$$

For general $\tau \Rightarrow$ hard problem

$\Rightarrow$ perturbative solution in small τ

$$S(x, v) = \frac{1}{4}\int_{-\infty}^{0} (\tau\dot{v} + v)^2 dt \quad \text{s.t.} \quad v = \dot{x} + U'(x)$$

$$= S_0 + \tau S_1 + \tau^2 S_2$$

$$\frac{1}{4}\int_{-\infty}^{0} v^2 dt \qquad \cancel{\frac{1}{2}\int_{-\infty}^{0} v\dot{v}\, dt = \frac{1}{4}v(0)^2} \qquad \frac{1}{4}\int_{-\infty}^{0} \dot{v}^2 dt$$

$$v(0) = U' = 0$$

No terms prop τ

$$\tilde{x}(t) = \tilde{x}_0(t) + \tau^2 \tilde{x}_2(t) + \dots$$

$$\underline{\Phi}_\tau(x_s) = \underline{\Phi}_0(x_s) + \tau^2 \underline{\Phi}_2(x_s)$$

Zeroth order $\tau = 0 \Rightarrow$ eq.

$$\text{downhill} \qquad \dot{\tilde{x}}_0 = -U'(\tilde{x}_0(t))$$

$$\text{uphill} \qquad \dot{\tilde{x}}_0 = U'(\tilde{x}_0(t))$$

Plug into S_0

$$S_0 = \frac{1}{4}\int_{-\infty}^{0} v^2 dt = \frac{1}{4}\int_{-\infty}^{0} (\dot{\tilde{x}}_0 + U'(\tilde{x}_0(t)))^2 dt$$

$$= \frac{1}{4}\int_{-\infty}^{0} \left(2U'(\tilde{x}_0(t))\right)^2 dt$$

$$dt = \frac{d\tilde{x}_0}{|U'|} \qquad = \int_0^{x_s} U'(y)\,dy = U(x_s) - U(0)$$

$$P_{TR} \sim e^{-\frac{1}{D}\left(U(x_s) - U(0)\right)}$$

Next order $\Phi_2(x_s)$

$$\Phi(x_s) = \int \underbrace{\frac{\delta S_0}{\delta x}[\tilde{x}_0(t)]}_{0} \tilde{x}_2(t)\,dt + S_2[\tilde{x}_0(t)]$$

$$\Phi_2(x_s) = S_2(\tilde{x}_0(t)) = \frac{1}{4}\int_{-\infty}^{0} \dot{v}_0^2\,dt$$

recall

$$v_0 = \dot{x}_0 + U'(x_0) = 2U'(x_0)$$

$$\dot{v}_0 = 2U''(x_0)\dot{x} = 2U''(x_0)U'(x_0)$$

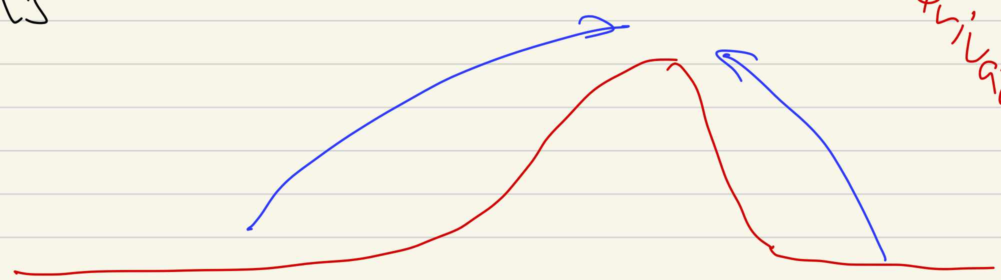
$$\Phi_2 = \int_{-\infty}^{0} \left(U''(x_0)\,U'(x_0)\right)^2 dt = \int_0^{x_s} (U''(y))^2\, U'(y)\,dy$$

$$dt = \frac{dx}{|U'|}$$

$$\boxed{\Phi_2 = \int_0^{x_s} (U''(y))^2\, U'(y)\,dy}$$

Non-local because not a full derivative.

Ratchets



Harmonic potential → solved exactly (any τ)

$T(k)$

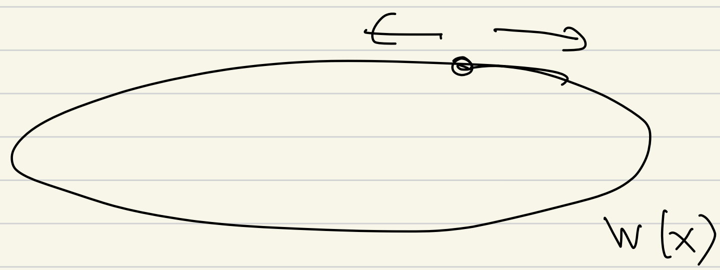
$\tau \to \infty$ limit can do calculation

E. Woillez, YK, V. Lecomte 2020

Bray & McKane 80s

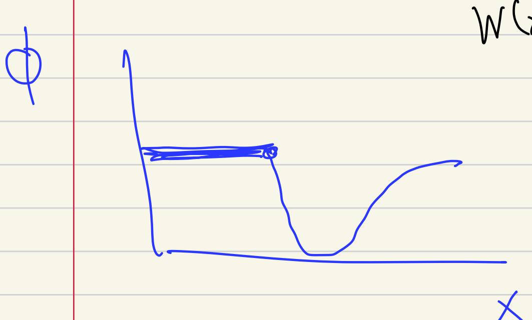
Q: how different are prob. dist out of eq. vs in eq.

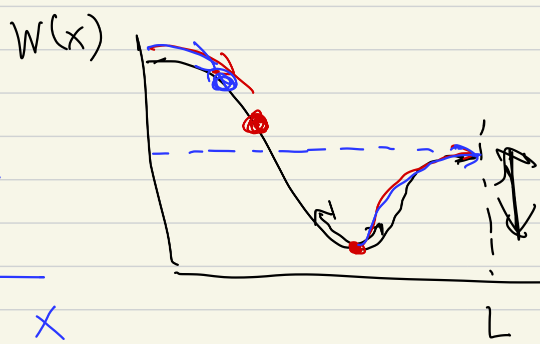
- Non-local (potential)
- Even if eqs of motion are smooth
  $\rightarrow$ LDF can be singular



$$\dot{x} = \mu f - \mu \partial_x W(x) + \sqrt{\frac{2\gamma}{N}}\,\eta(t)$$

Effective potentiam $W(x) - f x$



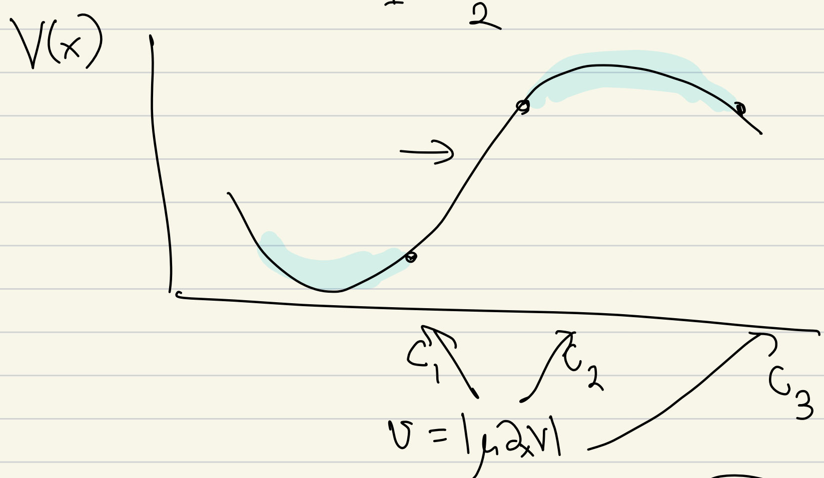


$$e^{-N\phi}$$

Escape Run and Tumble

$$\dot{x} = -\mu \partial_x V + v \hat{u} + \sqrt{2D}\,\xi(t)$$

$\pm 1 \quad \frac{\alpha}{2}$



$$L = \frac{1}{4}\left(\dot{x} + \mu \partial_x V - v \hat{u}\right)^2$$

add randomness in u

$$P_{TR} = \int \mathcal{D}x\, \mathcal{D}\hat{u}\; e^{-\frac{1}{D}\int_{-\infty}^{0} L\, dt}\; P(u)$$

$$\Rightarrow L = \frac{1}{4}\Big(\dot{x} \underbrace{-\mu \partial_x V - v}_{V(x) - v/\mu\, x}\Big)^2$$

$$\boxed{\Phi = \mu\left[V(c_2) - V(c_1)\right] - v\,(c_2 - c_1)}$$

function of v

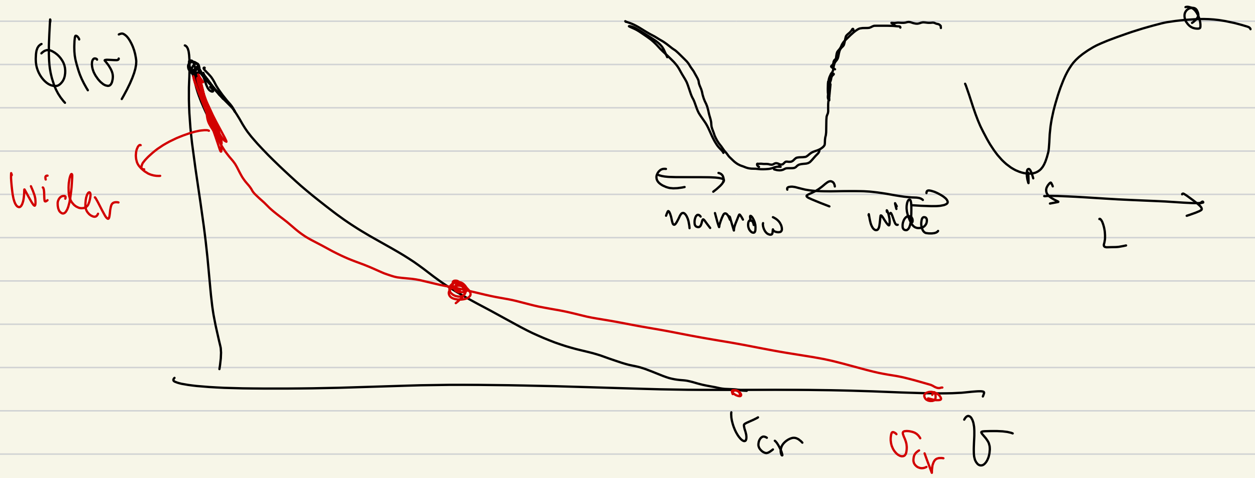
$$\phi(v) = \mu\left[V(c_2(v)) - V(c_1(v))\right] - v\left(c_2(v) - c_1(v)\right)$$

$v=0$ Kramers $\mu\left(V(c_2) - V(c_1)\right)$

→ top → bottom

$$\phi'(v) = -(c_2 - c_1)$$ → monotonically decreasing function

$v > v_{cr} = \max\{\mu |V'(x)|\}$ where beyond point $\Phi = 0$



$$e^{-\frac{\alpha}{2} T_{int}}$$

$$(\;\;)\, e^{-\frac{1}{D}\Phi}$$

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G. Woillez ⇒ PRL (19)