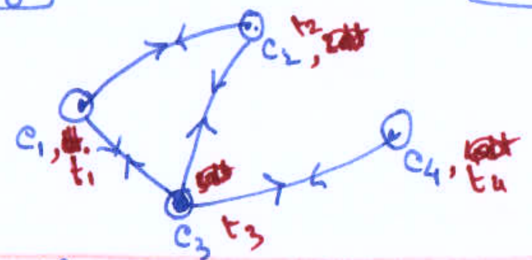
• Introductory concepts: Master equation, Langevin, Fokker-Plank, Path-integral, Path measure.

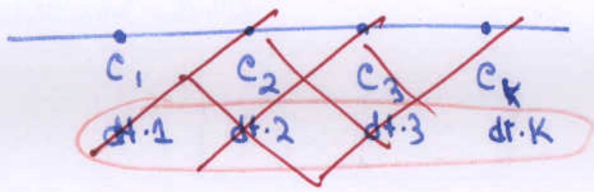
Master equation: A. Kinetic view of stat. physics: Redner, Krapivsky, Ben Naim
Van Kampen:



① Stochasticity: integrating ~~faster~~ other degrees of freedom.

[has the jump rates been calculated for real system?]

①



$$P(c_K) = \sum_{c_{K-2}}\sum_{c_{K-1}} \mathbb{P}(c_K \mid c_{K-1}, \cdots, c_1)\, P(c_{K-1}, c_{K-2}, \cdots)$$

Markov-property: finite relaxation time $dt \gg \tau$

$$\boxed{\mathbb{P}(c_K \mid c_{K-1}, c_{K-2}, \cdots) = \mathbb{P}(c_K \mid c_{K-1})}$$

transition rate.

• Master-equation:

$$\boxed{\mathbb{P}_{dt}(c_K \mid c_{K-1}) = \delta_{c_K, c_{K-1}} + dt \cdot \omega(c_K \leftarrow c_{K-1}) + \cdots}$$

$$P(c, t+dt) = \sum_{c'} \mathbb{P}_{dt}(c, t+dt \mid c', t)\, P(c', t)$$

$$= P(c,t) + dt \sum_{c'} \omega(c \leftarrow c')\, P(c', t) + \cdots$$

$$\rightarrow \boxed{\frac{\partial P(c,t)}{\partial t} = \sum_{c'} \omega(c, c')\, P(c', t)}$$

· **Condition:** $\sum_{c} P(c,t) = 1 \Rightarrow \sum_{c} \omega(c,c') = 0$

$$\Rightarrow \boxed{\omega(c',c') = -\sum_{c\neq c'} \omega(c,c')}$$

leads to

$$\frac{\partial P(c,t)}{\partial t} = \sum_{c'\neq c} \omega(c,c')\,P(c',t) + \underbrace{\omega(c,c)\,P(c,t)}$$

$$\downarrow$$

$$- P(c,t)\sum_{c''\neq c} \omega(c'',c)$$

$$\boxed{\frac{\partial P(c)}{\partial t} = \sum_{c'} M_{c,c'}\,P(c',t)}$$

$$\boxed{M = \begin{cases} \omega(c,c') & c\neq c' \\ -\sum_{c\neq c'} \omega(c,c') & c=c' \end{cases}}$$

$$= \sum_{c'\neq c} \left[\omega(c,c')\,P(c',t) - \omega(c',c)\,P(c,t)\right]$$

$$\boxed{\frac{\partial P(c)}{\partial t} = \sum_{c'} \left[\omega(c,c')\,P(c',t) - \omega(c',c)\,P(c,t)\right]}$$

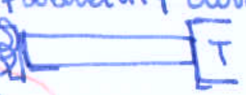
⊙ **Stationary state:** $\frac{dP(c,t)}{dt} = 0$

Equilibrium — Non-equilibrium stationary state

Equilibrium:

$$\boxed{\omega(c,c')\,P(c',t) = \omega(c',c)\,P(c,t)}$$

detailed balance: no probability current



⊙ Kolmogorov criteria

David Mukamel. Les Houches.

Non-equilibrium stationary state:

a. simple. way...

$$\sum_{c'} \left[\omega(c,c')\,P(c',t) - \omega(c',c)\,P(c,t)\right] = 0$$

"Pairwise balance"

⊛ Event chain MC. [PRL]

What choices one should have for ω?

- $\omega(c,c')\, e^{-\frac{E(c')}{T}} = \omega(c',c)\, e^{-\frac{E(c)}{T}}$

Let $E(c') = E(c) + Q$ — Q: energy current

$$\boxed{\omega_{+Q}(c',c) = \omega_{-Q}(c,c')\, e^{-Q/T}}$$

SKIP

Generalize: (derive) Exercise

$$\omega_{Q_1,Q_2}(c',c) = \omega_{-Q_1,-Q_2}(c,c')\, e^{-\frac{Q_1}{T_1}-\frac{Q_2}{T_2}}$$

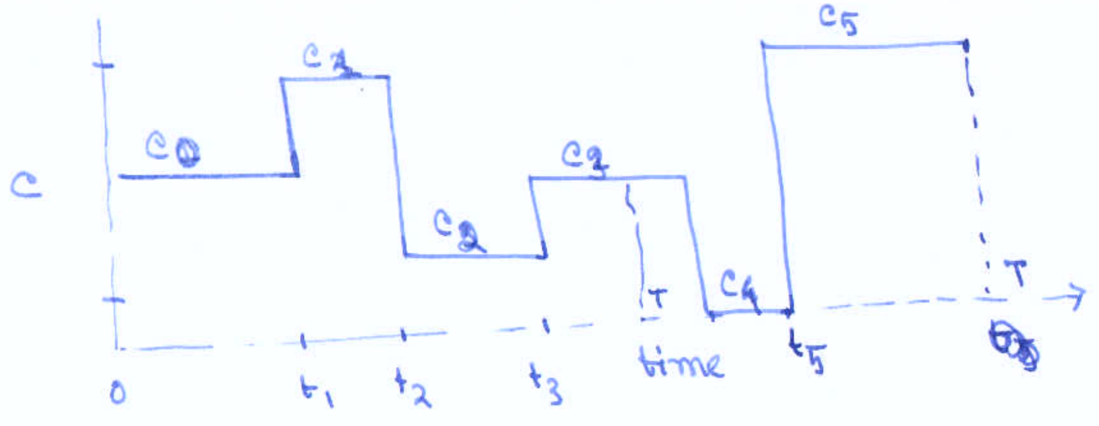
$\longrightarrow$ Gallavotti-Cohen symmetry. [Derrida, Mallick]

- Probability of a Trajectory: Detailed balance $\longleftrightarrow$ time reversal

Onsager:

> "Prob. of a ~~long history~~ trajectory $\equiv$ Prob of time reversed ~~trajectory~~"

In equilibrium



Prob of jump: $\omega(c' \leftarrow c) \equiv M(c',c)$

Prob to stay at c: $\lim_{dt\to 0} \left[1 - \sum_{c'} \omega(c' \leftarrow c)\, dt\right]^{\frac{t}{dt}} = e^{-t \cdot \sum_{c'} \omega(c' \leftarrow c)}$

$= e^{t\, M(c,c)}$

$$P[\{c\}] = e^{M(c_n,c_n)(T-t_n)} \cdots\cdots e^{(t_2-t_1)M(c_1,c_1)}\, M(c_1,c_0)\, e^{t_1 M(c_0,c_0)}\, P(c_0)$$

$\boxed{\text{Time reversed trajectory}}$:

$$P[R\{c_i\}] = e^{t_1 M(c_0,c_0)} \cdots e^{(t_n - t_{n-1}) M(c_{n-1},c_{n-1})} M(c_{n-1},c_n)\, e^{(T-t_n) M(c_n,c_n)} P(c_n)$$

Time reversal symmetry:

Exercice

$$\frac{P[\{c\}]}{P[R\{c\}]} = \frac{e^{M(c_3,c_3)(T-t_3)} M(c_3,c_2)\, e^{(t_3-t_2) M(c_2,c_2)} M(c_2,c_1)\, e^{(t_2-t_1) M(c_1,c_1)} M(c_1,c_0)\, e^{t_1 M(c_0,c_0)} P(c_0)}{\cdots\cdots e^{(T-t_3) M(c_3,c_3)} P(c_3)}$$

$$= \frac{M(c_3,c_2)\, M(c_2,c_1)\, M(c_1,c_0)\, P(c_0)}{M(c_0,c_1)\, M(c_1,c_2)\, M(c_2,c_3)\, P(c_3)}$$

use detailed balance: $\frac{M(c_3,c_2)}{M(c_2,c_3)} = \frac{P(c_3)}{P(c_2)}$

$$= \frac{P(\cancel{c_3})}{P(\cancel{c_2})} \cdot \frac{P(\cancel{c_2})}{P(\cancel{c_1})} \cdot \frac{P(\cancel{c_1})}{P(\cancel{c_0})} \cdot \frac{P(\cancel{c_0})}{P(\cancel{c_3})} = 1$$

will be used later

◎ Langevin equation, Fokker-Planck equation, Ito-Stratonovich,

Path integral for Langevin equation.

Stochastic differential equation at low noise limit. Action-formulation.

(A) Langevin equation. [Paul Langevin]

~~Originally introduced~~

Mechanical model for Brownian motion.

$$\boxed{m\frac{d^2q}{dt^2} = F(q,t) - \gamma\cdot\frac{dq}{dt} + \eta(t)}$$

→ stochastic noise ~~(energy input)~~

[due to integration over other degrees of freedom]

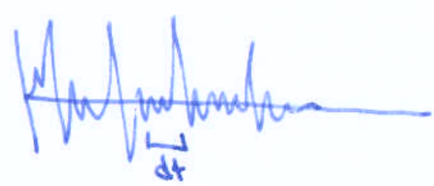
~~Energy dissipation~~

• ~~The two must be related; fluctuation-dissipation relation~~

◎ Stochastic white noise: (t ≫ τ relaxation of faster degrees of freedom!)

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

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



◎ A well defined quantity:

$$dB_t = \int_t^{t+dt} dt'\,\eta(t')$$

| Wiener process

$$P[dB_t] = \frac{1}{\sqrt{2\pi\Gamma dt}}\, e^{-\frac{(dB)^2}{2\Gamma dt}}$$

(Gaussian distribution)

[comment: all cumulant k>2 are zero]

(one may choose other type of noises)

◎ Fluctuation-dissipation relation:

Energy input = Energy dissipation

$$\cancel{\Gamma = 2\gamma k_BT}$$

$$\boxed{\frac{\Gamma}{2k_BT} = \gamma}$$

• Proof: $F(q) = 0$ Exercise

$$m \cdot \frac{dv}{dt} = -\gamma v + \eta(t)$$

$$\Rightarrow \quad v(t) = \underbrace{v(0)\, e^{-\frac{\gamma}{m} t}}_{0} + \frac{1}{m} \int_0^t dt'\, e^{-\frac{\gamma}{m}(t-t')}\, \eta(t')$$

at large time: $\langle v(t) \rangle = 0$

$$\langle v^2(t) \rangle = \frac{1}{m^2} \int_0^t dt' dt''\, e^{-\frac{\gamma}{m}(2t-t'-t'')} \langle \eta(t')\eta(t'') \rangle$$

$$= \frac{\Gamma}{2m\gamma}$$

One knows: in equilibrium: Equipartition of energy

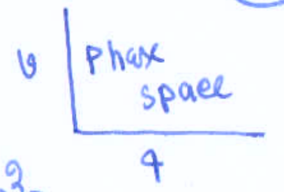
$$\frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} K_B T$$

$$\Rightarrow \langle v^2 \rangle = \frac{K_B T}{m}$$

$$\Rightarrow \quad \frac{K_B T}{m} = \frac{\Gamma}{2m\gamma} \quad \Rightarrow \quad \boxed{\frac{\Gamma}{K_B T} = 2\gamma}$$

Exercise: Derive full solution:

(B) Fokker-Planck equation: $P_t(q,v)$: $v = \frac{dq}{dt}$



SKIP

$$\frac{\partial P_t(q,v)}{\partial t} = -\frac{\partial}{\partial q}\left[v P\right] + \frac{\partial}{\partial v}\left[\frac{\gamma v - F}{m} P\right] + \frac{\Gamma}{m^2}\cdot\frac{\partial^2 P}{\partial v^2}$$

$$= \mathcal{L}_{FP} \odot P_t(q,v)$$

Master-equation for continuous configuration space.

(~~Cramers-Moyal expansion~~:

SKIP

(C) $\boxed{\text{Over-damped limit}}$: $\gamma \cdot \frac{dq}{dt} = F(q) + \eta(t)$

$$\boxed{\frac{dq}{dt} = \frac{1}{\gamma} F(q) + \eta(t)}$$

with $\langle \eta(t)\eta(t')\rangle = \frac{2k_BT}{\gamma}\delta(t-t')$

⊙ Fokker-Planck equation:

$$\boxed{\frac{\partial P(q,t)}{\partial t} = -\frac{d}{dq}\left[\frac{F(q)}{\gamma}\cdot P(q,t)\right] + \frac{k_BT}{\gamma}\cdot\frac{d^2 P}{dq^2}}$$

⊙ Langevin $\longrightarrow$ Fokker-Planck:

discretise time

$$q(t+\Delta t) = q(t) + \frac{\Delta t}{\gamma}\cdot F\left[\alpha\, q(t+\Delta t) + (1-\alpha)\, q(t)\right] + dB(t)$$

$$dB(t) \Downarrow \eta(t)\,dt$$

$(\langle dB^2\rangle \simeq dt\,\frac{2k_BT}{\gamma}$

$\Rightarrow dB \sim \sqrt{dt}\ )$

⊙ $\alpha = 0$ Ito

⊙ $\alpha = \frac{1}{2}$ Stratonovich

◎ Choose a test function $R(q(t))$ Tutorial

$$\langle R\rangle_{t+\Delta t} = \langle R(q(t+\Delta t))\rangle$$

$$= \left\langle R\left[q(t) + dB + \frac{\Delta t}{\gamma}\cdot\left\{F(q(t)) + \alpha F'(q(t))\cdot \overbrace{(q(t+\Delta t)-q(t))}^{dB + \frac{\Delta t}{\gamma}F(q(t))}\right\}\right]\right\rangle$$

$$= \left\langle R\left[q(t) + dB + \frac{dt}{\gamma}\cdot F(q(t))\right]\right\rangle + \mathcal{O}(\Delta t^{3/2})$$

$$= \langle R(q(t))\rangle + \langle dW\cdot R'(q(t))\rangle + \frac{dt}{\gamma}\langle F(q(t))R'(q(t))\rangle + \frac{1}{2}\cdot\langle dB^2\cdot R''(q(t))\rangle + \cdots$$

Tutorial

$$= \langle R\rangle_t + \frac{dt}{\gamma}\cdot\langle F(q(t))R'(q(t))\rangle + \frac{2k_BT}{2\gamma}\cdot\Delta t\cdot\langle R''(q(t))\rangle + \cdots$$

◎ $\langle R\rangle_{t+\Delta t} = \int dq\, R(q)\, P_{t+\Delta t}(q)$

$$\langle F(q)\cdot R'(q)\rangle = \int dq\, F(q)\cdot R'(q)\cdot P_t(q)$$

$$= F(q)R(q)\underbrace{P_t(q)}_{\to 0}\Big|_{-\infty}^{\infty} - \int dq\cdot\frac{d}{dq}\big(F(q)P_t(q)\big)\cdot R(q)$$

$$\langle R''(q)\rangle = \int dq\cdot\frac{d^2P_t(q)}{dq^2}\cdot R(q)$$

Putting together:

$$\int dq\cdot\left[P_{t+\Delta t}(q) - P_t(q) + \frac{\Delta t}{\gamma}\frac{d}{dq}(FP) - \frac{kT\Delta t}{\gamma}\cdot P''\right]R(q) = 0$$

[for additive noise: Ito vs Stratonovich does not matter]

⊙ General case:

$$\frac{dq}{dt} = \frac{F(q)}{\gamma} + \eta(t)$$

where $\langle \eta(t)\eta(t') \rangle = \frac{2 k_B T(q)}{\gamma}\,\delta(t-t')$

(space dependent temperature)

Multiplicative noise

(Stochastic differential equation with multiplicative noise.)

Ex: $m\frac{dv}{dt} = -\gamma v + \eta$

$$E = \frac{1}{2}mv^2 \Rightarrow \frac{dE}{dt} = -\frac{2\gamma}{m}E + \sqrt{\frac{2E}{m}}\cdot\eta$$

F-P eq^n

$$\boxed{\frac{\partial P_t(q)}{\partial t} = -\frac{\partial}{\partial q}\left[\frac{F(q)}{\gamma}P\right] + \frac{d^2}{dq^2}\left[\frac{k_B T(q)}{\gamma}P\right] - \alpha\cdot\frac{d}{dq}\left[P\cdot\frac{d}{dq}\left(\frac{k_B T(q)}{\gamma}\right)\right]}$$

The probability at time t depends on choice of α.

⊙ α can be chosen from discrete model.

⊙ Can also be chosen from physical arguments

(a) $\delta(t-t') \simeq \frac{1}{\sqrt{\pi\epsilon^2}}\cdot e^{-\frac{(t-t')}{\epsilon^2}}$ at $\epsilon \to 0$

$\equiv$ Stratonovich.

(b) $P(v) = \sqrt{\frac{m}{2\pi kT}}\, e^{-\frac{mv^2}{2kT}}$

$$P(E) = \frac{1}{2\sqrt{\pi kTE}}\, e^{-E/kT}$$

Comes if one considers the FP with $\alpha = 1/2$

Skip

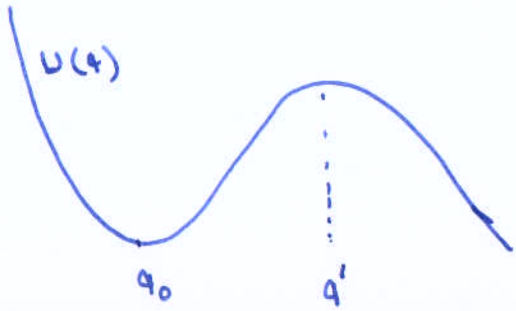
Large deviations in Langevin equation: Freidlin-Wentzell theory

[Random perturbations of dynamical systems, Springer 1984]

$$\frac{dq}{dt} = \frac{F(q)}{\gamma} + \eta(t) \; ; \quad \langle \eta(t)\eta(t')\rangle = \epsilon \, \frac{2K_BT(q)}{\gamma}\,\delta(t-t')$$

ϵ → small parameter (weak noise)

Example:



Kramer's escape problem

$$\tau_{escape} \sim e^{+\frac{1}{\epsilon}\left[\frac{U(q')-U(q_0)}{KT}\right]}$$

large-deviation form

switch

[Find a useful exercise]

General large deviation form:

$$P_t(q|q_0) \sim e^{-\frac{1}{\epsilon}\Phi_t(q)}$$

$\frac{1}{\epsilon}$ is the large parameter

[~~NB: $P_t(q) = \int dq_0\, P_t(q|q_0)\, P(q_0)$ with assumption $P(q_0) = e^{-\frac{1}{\epsilon}\Phi_0(q_0)}$~~]

Substituting in the FP equation with multiplicative noise

Exercise

$$\boxed{\frac{\partial}{\partial t}\Phi_t(q) = -\frac{F(q)}{\gamma}\cdot\frac{\partial}{\partial q}\Phi_t(q) - \frac{KT(q)}{\gamma}\cdot\left(\frac{\partial \Phi_t}{\partial q}\right)^2 + \mathcal{O}(\epsilon)}$$

Ito-Strato does not matter.

Check: For T = constant and $F(q) = -\frac{\partial U(q)}{\partial q}$

$$\Phi_t(q) \xrightarrow{t\to\infty} \boxed{\Phi(q) = \frac{U(q)-U(q_0)}{KT}}$$

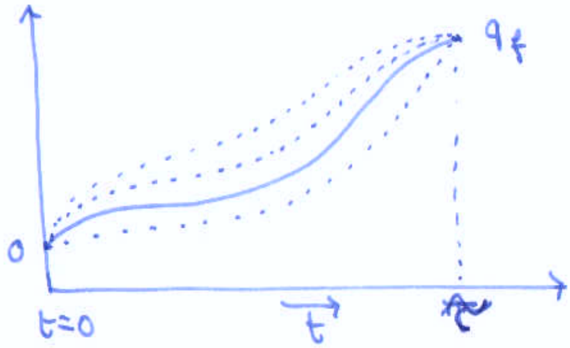
skip

Exercise: Verify that for detailed balance one needs

$$F(q) = -\frac{\partial U(q)}{\partial q}$$

Probability of Trajectories:

$$P[q_f, \tau \mid q_0, 0] = \int_{q_0}^{q_f} \mathcal{D}[q]\, e^{-\frac{1}{\epsilon} S_\tau[q(t)]}$$



Prob of trajectory

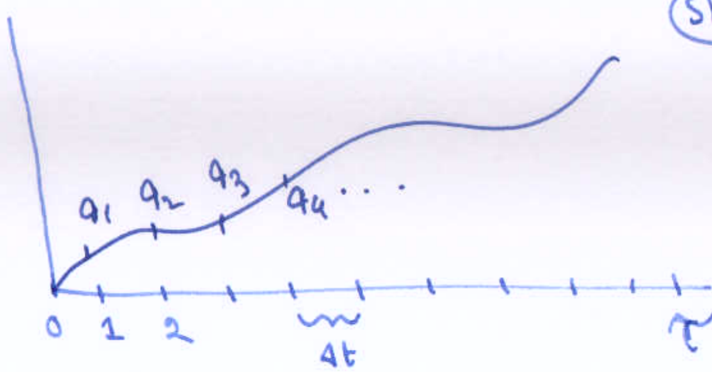
$$\boxed{\text{Prob}[q(t)] \sim e^{-\frac{1}{\epsilon} S_\tau[q(t)]} \sim e^{-\frac{1}{\epsilon} \int_0^\tau dt \frac{\left(\dot{q} - F(q)/\gamma\right)^2}{\left(\frac{2kT(q)}{\gamma}\right)}}}$$

$\left(\frac{2kT(q)}{\gamma}\right) \longrightarrow \sigma(q)$

Proof: Discretise time

Skip

Write W as B



- $\boxed{q(i\Delta t = t) \equiv q_i}$

- $q_{i+1} = q_i + \frac{\Delta t}{\gamma} F[\alpha q_{i+1} + (1-\alpha) q_i] + dB$ ← B

Additive

$$P[dB] = \frac{1}{\sqrt{2\pi\epsilon\cdot\sigma\cdot\Delta t}}\, e^{-\frac{(dB)^2}{2\sigma\epsilon\Delta t}}$$

$\langle dB^2 \rangle = \epsilon \cdot \frac{2kT}{\gamma} = \epsilon\sigma$ ← B

Simplicity: Additive noise.

$$P[B_{i+1} - B_i] = \frac{1}{\sqrt{2\pi\epsilon\sigma\Delta t}}\, e^{-\frac{(B_{i+1}-B_i)^2}{2\sigma\epsilon\Delta t}}$$

- $$\underset{dB_1 \cdots dB_N}{P[B_1, \cdots, B_N]} = \prod_{i=1}^{N} dB_i \left(\frac{1}{\sqrt{2\pi\epsilon\sigma\Delta t}}\right)^N \cdot e^{-\sum_i \frac{(B_{i+1}-B_i)^2}{2\sigma\epsilon\Delta t}}$$

Change to q_i variables

$$dB_1 \cdots dB_N = J \cdot dq_1 \cdots dq_N$$

Jacobian $J = \det \left[\frac{dB_i}{dq_j} \right]$

$$\boxed{B_{i+1} = B_i + q_{i+1} - q_i - \frac{\Delta t}{\gamma} F\left[\alpha q_{i+1} + (1-\alpha) q_i\right]}$$

$\left[\frac{dW_i}{dq_j}\right]$ is a lower triangular matrix

$$\Rightarrow \boxed{J = \prod_i \left[1 - \Delta t \cdot \frac{\alpha}{\gamma} \cdot \frac{dF(q_j)}{dq_j} \right] \simeq e^{-\Delta t \sum_{i=1}^{N} \frac{\alpha}{\gamma} \cdot \frac{dF(q_j)}{dq_j}}}$$

$$\Rightarrow \frac{P[q_1, \cdots dq_N]}{dq_1 \cdots dq_N} = dq_1 \cdots dq_N \cdot \prod_{i=1}^{N} e^{-\Delta t \cdot \sum \frac{\alpha}{\gamma} \frac{dF(q_j)}{dq_j}} \frac{e^{-\Delta t \sum_{i=1}^{N} \frac{(B_{i+1} - B_i)^2}{2\sigma \cdot \epsilon \cdot (\Delta t)^2}}}{\left(\sqrt{2\pi\epsilon\sigma\Delta t}\right)^N}$$

$$\Rightarrow P(q_f, T | q_0, 0) = \int_{q_0 = 0}^{q_{N+1} = q_f} \prod_{i=1}^{N} \frac{dq_i}{\sqrt{2\pi\epsilon\sigma\Delta t}} \, P(q_1 \cdots q_N)$$

$$\xrightarrow[N \to \infty]{\Delta t \to 0} \int_{q(0) = q_0}^{q(T) = q_f} \mathcal{D}[q] \, e^{-\frac{1}{\epsilon} \cdot \int_0^T dt \frac{\left(\dot{q} - \frac{F}{\gamma}\right)^2}{2\sigma} - \underbrace{\int_0^T dt \frac{\alpha}{\gamma} \cdot \frac{dF}{dq}}}$$

at ϵ small this term does not contribute

Remark: Same for multiplicative noise

~~Exercise: Prove Fokker-Planck equation from the action~~

$$P[q_f,T|_{q_0,0}] = \int_{q_0=0}^{q(T)=q_f} \mathcal{D}[q]\; e^{-\frac{1}{\epsilon} S_T[q(t)]}$$

where $S_T[q(t)] = \int_0^T dt\, \frac{\left(\dot{q} - \frac{F}{\gamma}\right)^2}{2\sigma}$

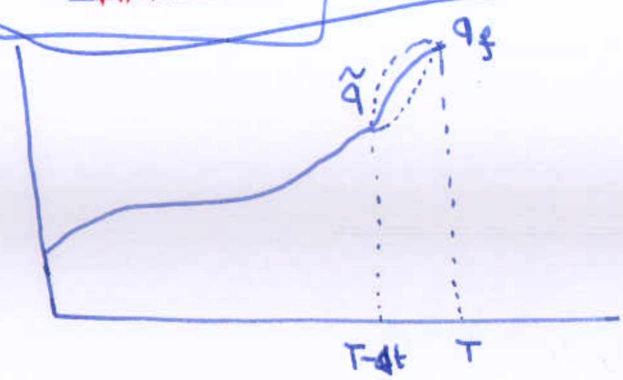
$\boxed{\text{Remark}}$: at small ϵ, the trajectory of "least action" contribute

$$P[q_f,T|_{q_0}] \simeq e^{-\frac{1}{\epsilon} W_T[q_f, q_0]} = e^{-\frac{1}{\epsilon} S_T[q_{cl}(t)]}$$

$\cancel{\Phi \equiv S_{min}}$

$\boxed{\text{Calculate } W_T(q_f)}$:

SKIP for later



$$P[q_f,T) = \int d\tilde{q}\; P(q_f,T|\tilde{q},T-\Delta t)\, P(\tilde{q},T-\Delta t)$$

$$\Rightarrow e^{-\frac{1}{\epsilon} W_T(q_f)} \simeq \int d\tilde{q}\; e^{-\Delta t \frac{(q_f - \tilde{q} - \frac{F}{\gamma}\Delta t)^2}{\epsilon\, 2\sigma(q_f)\Delta t^2}}\; e^{-\frac{1}{\epsilon} W_{T-\Delta t}(\tilde{q})}$$

$$\downarrow$$

$$e^{-\frac{1}{\epsilon} W_{T-\Delta t}(q_f) - \frac{1}{\epsilon} W'(q)(\tilde{q}-q_f)}$$

$$= e^{-\frac{1}{\epsilon} W_{T-\Delta t}(q_f)} \int d\tilde{q}\; e^{-\frac{\left(\tilde{q} - q_f + \frac{F\Delta t}{\gamma}\right)^2}{\epsilon\, 2\sigma(q_f)\Delta t} - \frac{(\tilde{q}-q_f) W'(q)}{\epsilon}}$$

$$= e^{-\frac{1}{\epsilon} W_{T-\Delta t}(q_f)} \cdot e^{-\frac{\Delta t}{\epsilon} \cdot \frac{F^2}{2\gamma^2 \sigma} + \frac{\Delta t}{2\sigma\epsilon}\left[\frac{F}{\gamma} + \Phi'(q)\cdot\sigma\right]^2}$$

$$\cdot \int d\tilde{q}\; e^{-\frac{1}{\epsilon} \frac{\left[\tilde{q} - q_f + \frac{F\Delta t}{\gamma} + \Delta t\, \sigma \cdot \Phi'(q)\right]^2}{2\sigma\Delta t}}$$

$$\Rightarrow \quad W_T(q_f) = W_{T-\Delta t}(q_f) + \Delta t \frac{F^2}{2\sigma\gamma^2} - \frac{\Delta t}{2\sigma}\left[\frac{F}{\gamma} + \sigma \cdot W'_T(q_f)\right]^2$$

$$\Rightarrow \quad \frac{dW_T(q_f)}{dT} = \frac{F^2}{2\sigma\gamma^2} - \frac{1}{2\sigma}\left[\frac{F}{\gamma} + \sigma \cdot W'_T(q_f)\right]^2$$

$$\boxed{\frac{dW}{dT} = -\frac{F}{\gamma} \cdot W'_T(q_f) - \frac{\sigma}{2} \cdot \left[W'_T(q_f)\right]^2}$$

Same as before

(*) Equation followed by minimal Action : Hamilton - Jacobi equation

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Analogy with classical mechanics : "least action Path"

$$P[q_f, T \mid q_0] \sim e^{-\frac{1}{\epsilon} S[q(t)]}$$

where $S[q(t)] = \int_0^T dt \frac{[\dot{q} - \frac{F(q)}{\gamma}]^2}{2\sigma} = \int_0^T dt\, \mathcal{L}(q, \dot{q})$

fixed

Path of least Action : [variational calculus]

$$\boxed{\frac{\partial \mathcal{L}}{\partial q} = \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}}$$

Skip

[N.B. : $S[q] = \int_0^T dt\, \mathcal{L}(q, \dot{q})$

$$S[q(t) + \delta q(t)] = \int_0^T dt\, \mathcal{L}\left(q + \delta q, \dot{q} + \frac{d\delta q}{dt}\right)$$

$$= \int_0^T dt \left\{\frac{\partial \mathcal{L}}{\partial q} \cdot \delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}} \frac{d\delta q}{dt} + \mathcal{L}(q, \dot{q})\right\}$$

$$= S[q] + \int dt \left\{\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}}\right\}\delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}} \delta q \Big|_{t=0}^{t=T} \quad]$$

⊙ Least action Path:

$$\boxed{\ddot{q} = \frac{F(q)\,F'(q)}{\gamma^2} \quad \text{with} \quad q(0) = q_0, \quad q(\tau) = q_f}$$

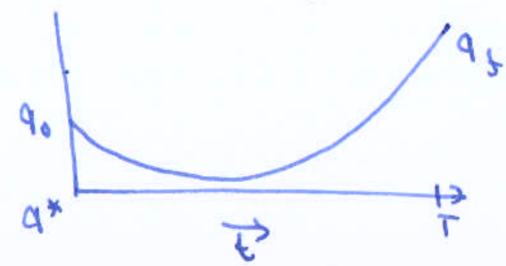
Equilibrium probability: $F(q) = -\frac{\partial U}{\partial q}$ ← convex fn

Important: $P(q_f|q_0) \xrightarrow[t\to\infty]{} q(q_f)$

AVOID

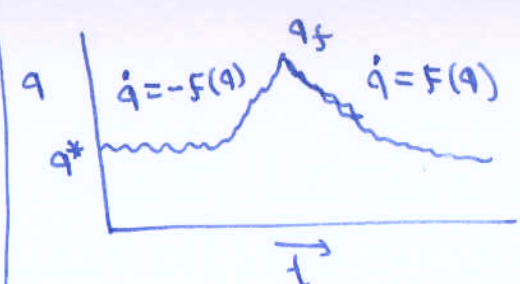
⊙ $P(q_f) = P(q_f|q^*)\,P(q^*)$
$\hookrightarrow e^{-\frac{1}{\epsilon}\cdot 0}$

$\Rightarrow P(q_f) \asymp P(q_f|q^*)$



⊙ $P(q_f|q^*) \xrightarrow{t\to\infty} P(q_f)$

$$\phi(q_f) = \min_{q(t)} S[q(t)] = W_\infty(q_f)$$



⊙ Time reversal symmetry:

Optimal trajectory = optimal trajectory for time reversed problem

$$q(t)\,\{q^* \to q_f\} = q_R(-t) \quad \{q_R(0) = q_f\,;\, q_R(\infty) = q^*\}$$

noise less equation:

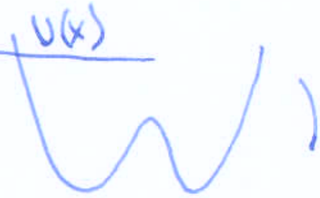
$$\frac{d q_R(\tau)}{d\tau} = \frac{F(q_R(\tau))}{\gamma} \xrightarrow[\tau=-t]{} \boxed{\frac{d}{dt} q(t) = -\frac{F(q(t))}{\gamma}}$$

⊙ $$W_\infty(q_f) = \int_{-\infty}^{0} dt\,\frac{(\dot{q} - F/\gamma)^2}{2\sigma} = -\frac{2}{\gamma\sigma}\int_{-\infty}^{0} dt\,\dot{q}(t)\frac{F(q)}{\gamma} = +\frac{2}{\gamma\sigma}\int_{q^*}^{q_f} dq\,\frac{\partial U}{\partial q}$$

$$= \frac{2}{\gamma\sigma}\cdot\left[U(q_f) - U(q^*)\right]$$

$$\Rightarrow \quad \phi(q_f) \xrightarrow{\sigma = \frac{2KT}{\gamma}} \frac{U(q_f) - U(q^*)}{k_B T}$$

~~(Q: What happens in a double well potential~~



* Exercise: check this satisfies H-J eqn

Hamiltonian Framework:

~~Legendre transform~~

Legendre transform:

① $H[p,q] = p\dot{q} - \mathcal{L}(q,\dot{q})$ with $p = \frac{\partial \mathcal{L}}{\partial \dot{q}}$

② $$\boxed{e^{-\int_0^T dt \frac{f(t)^2}{\epsilon 2\sigma}} \simeq \int \mathcal{D}[p]\, e^{+\frac{1}{\epsilon}\int_0^T dt \left\{ \frac{\sigma}{2} p^2 - p f \right\}}}$$

OR

$$\Rightarrow \boxed{P[q_f|q_0] = \int \mathcal{D}[q,p]\, e^{-\frac{1}{\epsilon}\int dt \left\{ p\dot{q} - \underbrace{\left[\frac{\sigma}{2} p^2 + p \cdot \frac{F}{\gamma} \right]}_{H[p,q]} \right\}}}$$

SKIP

③ $$P[q_f|q_0] = \int \mathcal{D}[q,\eta]\, \delta\left(\dot{q} - \frac{F}{\gamma} - \eta\right) P(\eta)$$

$$= \int \mathcal{D}[q,\eta,p]\, e^{-\int_0^t dt \frac{p}{\epsilon}\left(\dot{q} - \frac{F}{\gamma} - \eta\right)}\, e^{-\int dt \frac{\eta^2}{2\sigma\epsilon}}$$

$$= \int \mathcal{D}[q,p]\, e^{-\frac{1}{\epsilon}\int dt \left\{ p\dot{q} - H \right\}}$$

[Martin-Siggia-Rose-De-Dominicis formalism]

$p \equiv$ response field

- Least Action path:

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \text{and} \quad \dot{q} = \frac{\partial H}{\partial p}$$

- The equilibrium problem:

$$F(q) = -\frac{\partial U}{\partial q}$$

Show $$P(q_f) \approx e^{-\frac{1}{\epsilon KT}\left[U(q_f) - U(q^*)\right]}$$

minima

Same strategy: $H(p,q) = \frac{\sigma}{2}p^2 + \frac{F(q)}{\gamma}p$

p is like noise

$$\boxed{\begin{aligned} \dot{p} &= -p \cdot \frac{F'(q)}{\gamma} \\ \dot{q} &= \sigma p + F(q)/\gamma \end{aligned}}$$

with $q(-\infty) = q^*$
$q(0) = q_f$

Two boundary condition.

Solution: $\dot{q} = -\frac{F(q)}{\gamma}$ (time reversibility)

$\sigma p = -\frac{2F}{\gamma}$

Relaxation path
$p = 0$

Check: $\boxed{H[p,q] = 0 \quad \text{[Physical interpretation!]}}$

leads to

$$\phi(q_f) = \int_{-\infty}^{0} dt\, p\dot{q} = -\int_{-\infty}^{0} dt \cdot \dot{q} \cdot \frac{2F}{\gamma\sigma}$$

$$= \frac{2}{\sigma\gamma} \int_{q^*}^{q_f} dq \cdot \frac{\partial U}{\partial q} = \frac{2}{\sigma\gamma}\left[U(q_f) - U(q^*)\right]$$

$$= \frac{1}{KT}\left[U(q_f) - U(q^*)\right]$$

Physical picture: why $H=0$

$t \to \infty$ (required for $\omega \to \phi$)

* cost more if q_f ~~is~~ reached ~~and~~ at finite time and then one has to wait.*

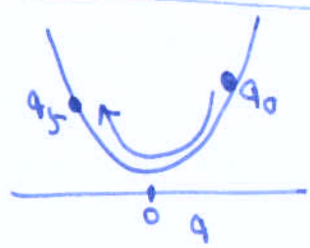
for $H = \delta \Rightarrow t \sim \frac{1}{\delta}$

Asymptotically $H \to 0 \Rightarrow t \to \infty$

Remark: $p(t) \equiv$ external ~~noise~~ force $\equiv$ A ~~correlated~~ noise realization.

$$\dot q = \frac{F}{\gamma} + \boxed{\sigma p}$$
$$\dot q = \frac{F}{\gamma} + \boxed{\eta}$$

Exercise: $U(q) = \frac{1}{2} q^2 \Rightarrow F(q) = -\omega^2 q$

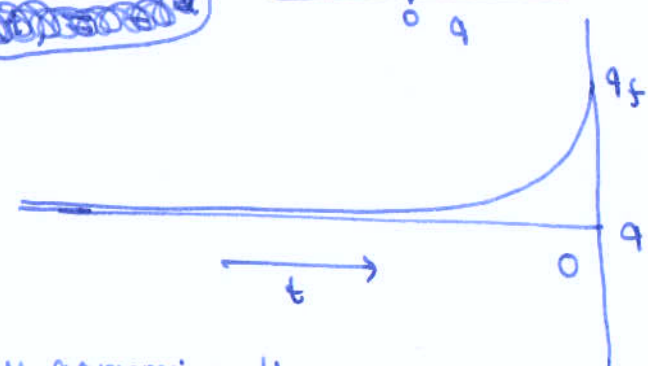


$\gamma = 1$
$\omega = 1$

Least action path:

$$q(t) = q_f \, e^{\frac{\omega^2}{\gamma} t}$$

$$p(t) = \frac{2\omega^2}{\sigma\gamma} \cdot q_f \cdot e^{\frac{\omega^2}{\gamma} \cdot t}$$

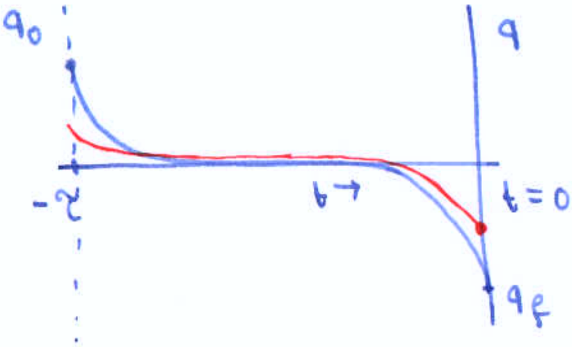


One can solve the full problem without any approximation

$$q(t) = q_f e^t \frac{1 - e^{-2(t+\tau)}}{1 - e^{-2\tau}} + q_0 e^{-(t+\tau)} \frac{1 - e^{2t}}{1 - e^{-2\tau}}$$

$$p(t) = \frac{2 q_f e^t}{\sigma(1 - e^{-2\tau})} - \frac{2 q_0 e^{t-\tau}}{\sigma(1 - e^{-2\tau})}$$

$$\omega_\tau(q_f, q_0) = \frac{(q_f - q_0 e^{-\tau})^2}{\sigma(1 - e^{-2\tau})} \xrightarrow[\tau \to \infty]{} \frac{q_f^2}{\sigma} = \frac{1}{2}\frac{q_f^2}{KT}$$



At $\tau \to \infty$:

$$q(t) = q_f e^{t}$$

$$p(t) = \frac{2}{\sigma} \cdot q_f e^{t}$$

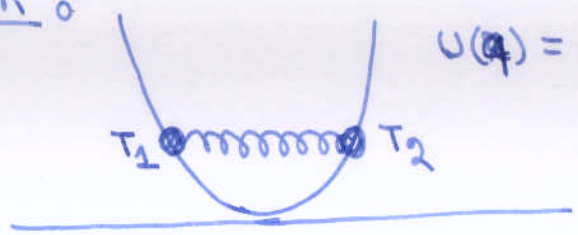
same as ~~...~~ downhill trajectory

$$q_R(t) = q_f e^{-t} = q(-t)$$

*one should have $p_R(t) = 0$

- Verify $H=0$ for $\tau \to \infty$ case

(A) A non-equilibrium problem:



$$U(q) = \frac{1}{2} q^2$$

$$E(q_1, q_2) = \frac{1}{2} q_1^2 + \frac{1}{2} q_2^2 + \frac{1}{2} (q_1 - q_2)^2$$

Eq^n of motion

$$\dot{q}_1 = -\partial_{q_1} U + \eta_1$$

$$\dot{q}_2 = -\partial_{q_2} U + \eta_2$$

Two-temp are diff.

$$\langle \eta_1(t) \eta_1(t') \rangle = \epsilon 2KT_1 \, \delta(t-t') = \epsilon \sigma_1 \delta(t-t')$$

$$\langle \eta_2 \, \eta_2 \rangle = \epsilon \sigma_2 \delta(t-t')$$

$$\langle \eta_1 \eta_2 \rangle = 0$$

- $H(q_1, q_2) = \frac{\sigma_1}{2} p_1^2 + \frac{\sigma_2}{2} p_2^2 + p_1 \cdot (-2q_1 + q_2) + p_2 (-2q_2 + q_1)$

- Solve least action trajectories: with

$$q_1(-\infty) = 0 \quad ; \quad q_1(0) = \gamma_1$$

$$q_2(-\infty) = 0 \quad ; \quad q_2(0) = \gamma_2$$

⊛ Check: $\boxed{\text{~~Then~~ downhill trajector} \neq \text{uphill trajectory.}}$

⊙ The Large deviation function

[Hint: use $x = q_1 - q_2$, $Y = q_1 + q_2$ or Mathematica

$$P(\gamma_1, \gamma_2) \sim e^{-\frac{1}{\epsilon}\phi(\gamma_1, \gamma_2)}$$

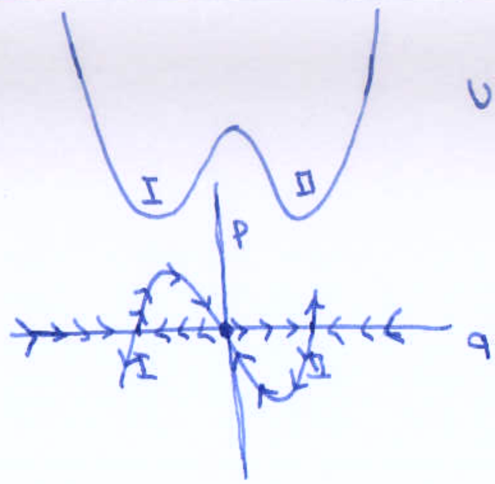
$$\Rightarrow \phi(\gamma_1,\gamma_2) = \frac{4}{\sigma_1^2 + 14\sigma_1\sigma_2 + \sigma_2^2} \cdot \Big\{ -4(\sigma_1+\sigma_2)\gamma_1\gamma_2 + (7\sigma_1+\sigma_2)\gamma_1^2 + (7\sigma_2+\sigma_1)\gamma_2^2 \Big\}$$

Plot

Equilibrium $\xrightarrow{\sigma_1=\sigma_2=\sigma}$ $\frac{2}{\sigma}\left(\gamma_1^2 - \gamma_1\gamma_2 + \gamma_2^2\right)$

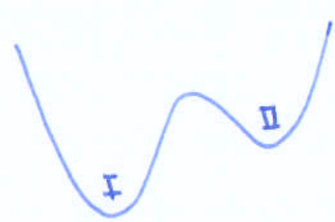
(B) Double-well potential:

$$V(q) = \frac{1}{2}q^2 - \frac{1}{4}q^4$$



$$\phi(q_f) = \min\left\{ W_\infty(q_f|q_I^*),\ W_\infty(q_f|q_{II}^*) \right\}$$

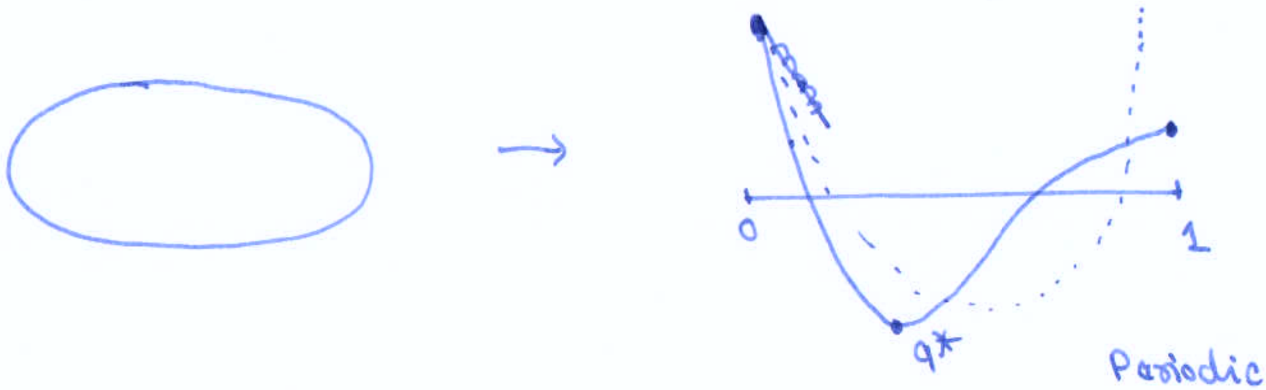
More generally



$$\phi(q_f) = \min\left\{ \phi(q_I^*) + W_\infty(q_f|q_I^*)\ ;\ \phi(q_{II}^*) + W_\infty(q_f|q_{II}^*) \right\}$$

Q: Why $\phi(q)$ is smooth in equilibrium? How is this related to time reversibility?

Non-smooth large deviation function:



$$F(q) = -\frac{\partial U}{\partial q} + f$$

Constant force:

Periodicity: $F(q+1) = F(q)$

Exact analysis: $\dot{q} = F(q) + \eta$ $\quad \langle \eta\eta \rangle = \epsilon\, \delta(t-t')$

Fokker Planck eq^n:

$$\frac{dP_t(q)}{dt} = -\frac{d}{dq}\left(F(q)\, P_t(q)\right) + \frac{\epsilon}{2}\frac{d^2 P}{dq^2}$$

Stationary state

$$\frac{dP_t(q)}{dt} = 0$$

Solution: $0 \le q \le 1$

$$P_s(q) = \mathcal{N}\left\{ \int_0^q dx\, e^{\frac{2}{\epsilon}\int_x^q dy\, F(y)} + \int_q^1 dx\, e^{\frac{2}{\epsilon}\int_x^{q+1} dy\, F(y)} \right\}$$

For small ϵ: $P_s(q) \sim e^{-\frac{1}{\epsilon}\phi(q)}$

$$P_s(q) = \mathcal{N}\, e^{\frac{2}{\epsilon}\int_{q^*}^q dy\, F(y)} \left\{ \int_0^q dx\, e^{-\frac{2}{\epsilon}\int_{q^*}^x dy\, F(y)} + e^{\frac{2}{\epsilon}\int_q^{q+1} dy\, F(y)} \int_q^1 dx\, e^{-\frac{2}{\epsilon}\int_{q^*}^x dy\, F(y)} \right\}$$

$q^* \equiv$ minimum

Define   Important

$$-\int_{q^*}^{q} dy\, F(y) = V(q) - V(q^*) = V(q) \qquad \underline{0<q<1}$$

$V(q^*)$ → get zero

$$\Rightarrow \quad e^{-\frac{1}{\epsilon}\phi(q)} \asymp N\, e^{-\frac{2}{\epsilon}[V(q)]}\left\{ \int_0^q dx\, e^{\frac{2}{\epsilon}[V(x)]} \right.$$

$$\left. + e^{-\frac{2}{\epsilon}[V(1) - V(0)]} \int_q^1 dx\, e^{\frac{2}{\epsilon}[V(x)]} \right\}$$

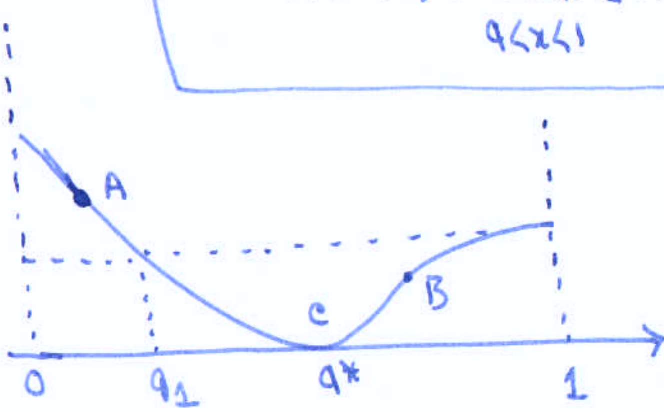
understand

$$\Rightarrow -\phi(q) = -2V(q) + 2\max\left\{ \max_{0<x<q}[V(x)],\right.$$

$$\left. -V(1)+V(0) + \max_{q<x<1}[V(x)] \right\}$$

$$\Rightarrow \boxed{\phi(q) = 2[V(q)] - 2\max\left\{ \max_{0<x<q}[V(x)],\; -V(1)+V(0) + \max_{q<x<1}[V(x)] \right\}}$$

Example:



$$\phi(q^*) = 0 - 2\max\{V(0),\, -\cancel{V(1)} + V(0) + \cancel{V(1)}\} = -2V(0)$$

Redefine: [Setting $V(q^*) = 0$]

$$\phi(q) \longrightarrow \phi(q) - 2V(0)$$

$$\boxed{\phi(q) = 2\left[V(q) + V(0)\right] - 2\max\left\{\max_{0<x<q} V(x),\ V(0) - V(1) + \max_{q<x<1} V(x)\right\}}$$

$$\phi(q^*) = 0$$

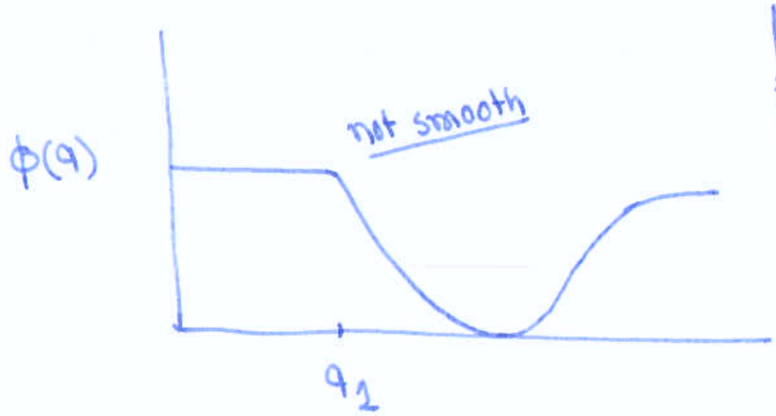
$$\phi(q_A) = 2\left[V(q_A) + V(0)\right] - 2\max\left\{V(0),\ V(0) - V(1) + V(q_A)\right\}$$

$$= 2\left[V(q_A) + V(0)\right] - 2\left[V(q_A) + V(0) - V(1)\right]$$

$$= 2V(1)$$

$$\phi(q_B) = 2\left[V(q_B) + V(0)\right] - 2\max\left\{V(0),\ V(0) - \cancel{V(1)} + \cancel{V(1)}\right\}$$

$$= 2V(q_B)$$



$\Rightarrow \cancel{\phi(q) = \min} \{$

<u>Exercise</u>: verify for $f = 0$ there is no discontinuity.

• Hamiltonian Picture:

Justification by Naive argument

• $q(-\infty) = q^*$; $q(0) = q_f$

[* of course one can solve explicitly]

Exercise

• Optimal trajectories: $H[p,q]=0$

$$\Rightarrow \frac{p^2}{2} + F(q)\cdot p = p\left[\frac{p}{2}+F\right]=0$$

• uphill trajectory. $p = -2F(q)$ | • Downhill $p = 0$

• Large deviation function S

uphill: $= \int_{t_0} dt\,\left[p\dot{q} - \overset{0}{H}\right]$

(for uphill trajectory) $= -2\int_{q_0}^{q_f} dq\, F(q)$

Downhill: 0 for downhill

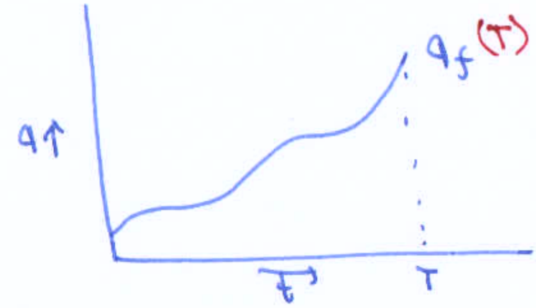
• But there are multiple such paths: which one minimise?

$$\Phi(q_f) = \min\left\{\underset{\text{Rightwards}}{-2\int_{q^*}^{q_f} dq\, F(q)}\ ,\ \underset{\text{Leftwards}}{-2\int_{q^*}^{q_f} dq\, F(q)}\right\}$$

Non analyticity due to ~~multiple~~ non-smooth switching between optimal paths.

Kafri, Baek J. Stat. Mech. 2016

Hamilton - Jacobi equation:



$$P_T(q_f) = \int \mathcal{D}[P,q]\, e^{-\frac{1}{\epsilon} S[P(t),q(t)]}$$

$$\xrightarrow{\epsilon \text{ small}} e^{-\frac{1}{\epsilon}\phi(q_f,T)}$$

What is the equation satisfied by $\phi(q_f,T)$?

- ~~Using F-P equation~~

$$\cancel{\frac{\partial \phi}{\partial T} = -\frac{\partial^2 \phi}{\partial q_f^2}} \quad -$$

* canonical transformation

[Rana & Joag]

classical mechanics

- $$\boxed{\frac{\partial \phi(q_f,T)}{\partial T} = -H\left(\frac{\partial \phi}{\partial q_f}, q_f, T\right)}$$

for any Hamiltonian

where $S = \int_0^T dt \left\{ P\dot{q} - H(P,q,T) \right\}$

~~David Tom~~

David Tong

- Example:

$$\dot{q} = F + \eta \quad \text{with} \quad \langle \eta\eta \rangle = \epsilon\, \delta(t-t')$$

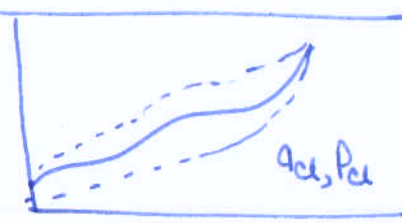
corresponding

$$H = \frac{P^2}{2} + FP$$

$$\Rightarrow \frac{\partial \phi}{\partial T} = -H\left(\frac{\partial \phi}{\partial q_f}, q_f\right) = -\frac{1}{2}\frac{\partial^2 \phi}{\partial q_f^2} - F(q_f)\cdot \frac{\partial \phi}{\partial q_f}$$

Same as obtained using FP equation

- Proof of H-J equation



$$\phi(q_f,T) = \int_0^T dt \left\{ P_{cl}(t)\dot{q}_{cl} - H(P_{cl}(t), q_{cl}(t)) \right\}$$

where
$$P_{cl}(t) = P_{cl}(t, q_f)$$
$$q_{cl}(t) = q_{cl}(t, q_f)$$

Step 1:
$$\boxed{\frac{\partial \phi}{\partial q_f} = p_a(\tau)}$$

because:
$$\delta\phi = \int dt \left[\underbrace{\dot{q}_a - \frac{\partial H}{\partial p_a}}_{0}\right]\delta p \pm \left[\underbrace{\dot{p}_a + \frac{\partial H}{\partial q_a}}_{0}\right]\delta q$$
$$+ p_a(\tau)\, \underbrace{\delta q_a(\tau)}_{\delta q_f} + p_a(0)\,\delta q_a(0)$$

Write explicitly

$$\Rightarrow \boxed{\frac{\partial \phi}{\partial q_f} = p_a(\tau)}$$

Step 2:
$$\frac{d\phi}{d\tau} = \frac{\partial \phi}{\partial \tau} + \frac{\partial \phi}{\partial q_f}\cdot \dot{q}_f = \frac{\partial \phi}{\partial \tau} + p_a^{(\tau)}\cdot \dot{q}_f$$

Step 3:
$$\frac{d\phi}{d\tau} = p_a(\tau)\,\dot{q}_a(\tau) - H\big(p_a(\tau), q_a(\tau)\big)$$
$$= p_a(\tau)\cdot \dot{q}_f - H\left(\frac{\partial \phi}{\partial q_f}, q_f\right)$$

Comparing one gets the H-J equation.

Remark: In stationary state
$$\frac{\partial \phi}{\partial \tau} = 0$$
$$\Rightarrow \boxed{H\left(\frac{\partial \phi}{\partial q_f}, q_f\right) = 0}$$

---

* Check for $F = -\frac{\partial U(q)}{\partial q}$; $\phi(q) = \left[\frac{U(q) - U(q^*)}{k_B T}\right] \to 1$

* Same-equation obtained from Fokker-Planck equation.

<u>Large deviation of an observable:</u> $\boxed{\text{Additivity principle}}$

$$Q_T = \int_0^T dt\, q(t)$$

$\boxed{\text{Non-local function of the history. Non-trivial!}}$

$$\dot q = F(q) + \eta(t) \qquad \text{with } \langle \eta(t)\eta(t')\rangle = \epsilon\, \delta(t-t')$$

<u>Question:</u> what is the probability

$$e^{-\frac{1}{\epsilon}\phi(Q_T)} \swarrow \quad P(Q_T)\, ? \qquad \boxed{\text{when starting } q(0) = 0}$$

$$\cancel{\sim e^{-\frac{T}{\epsilon}\phi(\gamma)}}$$

$$\left[P\left(\frac{Q_T}{T} = \gamma\right) \sim e^{-\frac{T}{\epsilon}\phi(\gamma)} \right]$$

<u>Generating function:</u>

$$\langle e^{\frac{\lambda}{\epsilon} Q_T} \rangle = \int \mathcal{D}[p,q]\, e^{\frac{\lambda}{\epsilon}\int_0^T dt\, q(t) - \frac{1}{\epsilon}\int_0^T dt \{p\dot q - H(p,q)\}}$$

why?

$$H(p,q) \to \frac{p^2}{2} + F\cdot p$$

$$= \int \mathcal{D}[p,q]\, e^{-\frac{1}{\epsilon} S[p,q]}$$

where
$$S[p,q] = \int_0^T dt\, p\dot q - \tilde H[p,q]$$

$$\tilde H \hookrightarrow \frac{p^2}{2} + F p + \lambda q$$

For small ϵ

$$\langle e^{\frac{\lambda}{\epsilon} Q_T} \rangle \sim e^{\frac{1}{\epsilon} G(\lambda)}$$

where
$$\boxed{G(\lambda) = -\min_{(p,q)} \left[\int dt\, p\dot q - \tilde H \right]}$$

~~Least action paths~~

Variational calculus:

$$\delta S = \int_0^T dt \left(\dot q - \frac{\delta H}{\delta p}\right)\delta q + \int_0^T dt \left(\dot p + \frac{\delta H}{\delta q}\right)\delta p + p\,\delta q \Big|_0^T$$

Least action paths:

$$\dot q = \frac{\delta H}{\delta p} = p + F$$

$$\dot p = -\frac{\delta H}{\delta q} = -p \cdot F'(q) - \lambda$$

boundary condition

$q(0) = 0$ given

$p(T) = 0$

leads to

$$a(\lambda) = -\int_0^T dt \left\{ p_\alpha \dot q_\alpha - \frac{p_\alpha^2}{2} - F p_\alpha - \lambda q_\alpha \right\}$$

$$= -\int_0^T dt \left\{ p^2 + \cancel{pF} - \frac{p^2}{2} - \cancel{pF} - \lambda q \right\}$$

$$= -\int_0^T dt \left\{ \frac{p^2}{2} - \lambda q \right\}$$

Special example:

$$W(q) = \frac{1}{2} q^2$$

$$\Rightarrow F(q) = -q$$

leads to

$$\dot q = p - q$$

$$\dot p = p - \lambda$$

Sol^n $q(t) = e^{-t} \int_0^t d\tau \, e^{\tau} p(\tau)$

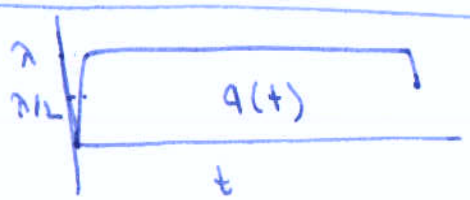
$$p(t) = \lambda e^{t} \int_t^T d\tau \, e^{-\tau}$$

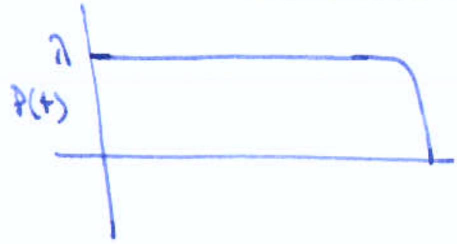
$$= \lambda e^{t} \left[e^{-t} - e^{-T} \right]$$

$$= \lambda \left[1 - e^{-(T-t)} \right]$$

$$\Rightarrow \boxed{q(t) = \lambda \left\{ 1 - e^{-t} - \frac{e^{-T}}{2} \left(e^{t} - e^{-t} \right) \right\}}$$

$$\Rightarrow \boxed{p(t) = \lambda \left(1 - e^{-(T-t)} \right)}$$





$\boxed{\text{mostly-time independent}}$

Then $G(\lambda) \simeq - T \cdot \left\{ \frac{\lambda^2}{2} - \lambda^2 \right\}$ for large T

$$= T \cdot \frac{\lambda^2}{2}$$

The large deviation function :

$$\cancel{P\left(\frac{Q_T}{T} = \gamma\right) \sim e^{-\frac{T}{\epsilon}\phi(\gamma)}}$$

$$\cancel{\left\langle e^{+\frac{\lambda}{\epsilon} Q_T} \right\rangle \simeq \int dQ_T \, e^{+\frac{\lambda}{\epsilon} \cdot T \cdot \gamma - \frac{T}{\epsilon}\phi(\gamma)}}$$

$$\cancel{\simeq e^{\frac{T}{\epsilon} \max_\gamma \{\lambda\gamma - \phi(\gamma)\}}}$$

$$\Rightarrow \cancel{\boxed{G(\lambda) = \max\{\lambda\gamma - \phi(\gamma)\}}}$$

Inverse Legendre transform

$$\phi(\gamma) = \max_\lambda \{\lambda\gamma - G(\lambda)\}$$

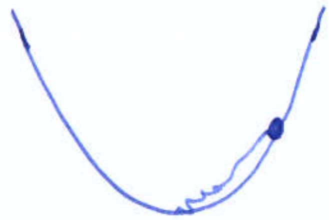
$$\Rightarrow \gamma = G'(\lambda) = \lambda$$

$$\Rightarrow \phi(\gamma) = \lambda\gamma - G(\lambda) = \gamma^2 - \frac{\gamma^2}{2}$$

$$\Rightarrow \boxed{\phi(\gamma) = \frac{\gamma^2}{2}} = \frac{1}{2} F(\gamma)^2$$

"Additivity" conjecture: For general potential

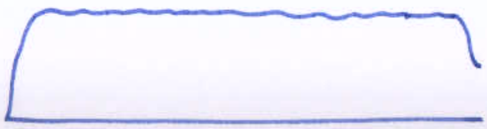
$$F(q) = -\partial_q V$$



$$P\left(\int_0^T dt\, q(t) = T\cdot\gamma\right) \asymp e^{-\frac{T}{\epsilon}\Phi(\gamma)}$$

$$= \int \mathcal{D}[q]\, e^{-\int_0^T dt\, \frac{(\dot q - F(q))^2}{2\epsilon}}$$

Optimal profile time independent: $q(t) = \gamma$



$$\Rightarrow \dot q = 0 \Rightarrow \boxed{P(T\gamma) \asymp e^{-\frac{T}{\epsilon}\cdot\frac{F(\gamma)^2}{2}}}$$

"Additivity conjecture"

* Important for interacting particle systems.