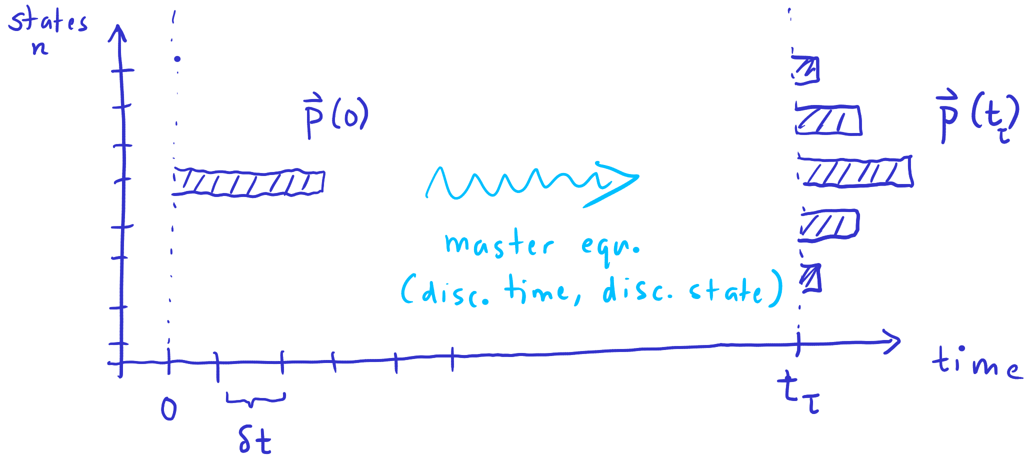
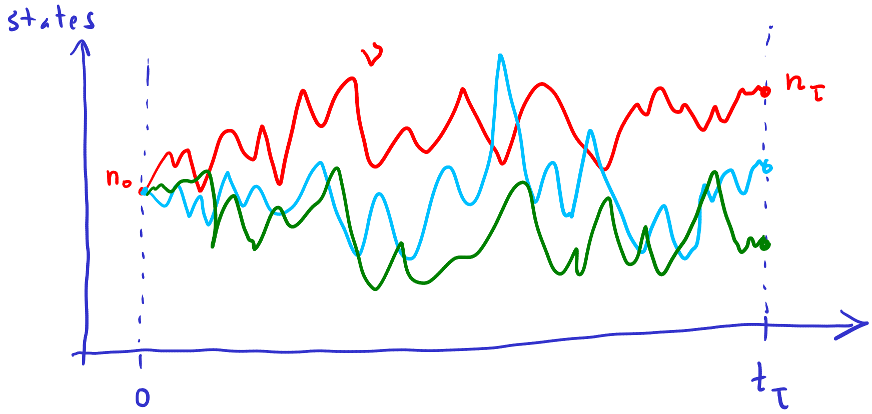
PHYS 414: 4-8-20



traj. picture



$\nu = (n_0, n_1, \ldots, n_\tau)$

note: $\mathcal{P}(\nu)$ is always defined w/ respect to a given initial distrib.

last time: $\Delta E(\nu) = E(\nu, t_\tau) - E(\nu, 0) = E_{n_\tau} - E_{n_0}$

$$\int_0^t dt\, \dot{S}^i(\nu,t) = \Delta S^i(\nu) = k_B \ln\left[\frac{W_{n_\tau,n_{\tau-1}} W_{n_{\tau-1},n_\tau} \cdots W_{n_1,n_0}\, p_{n_0}}{W_{n_0,n_1} W_{n_1,n_2} \cdots W_{n_{\tau-1},n_\tau}\, p_{n_\tau}}\right]$$

$$\dot{S}^i(\nu,t_\tau) \equiv \frac{k_B}{\delta t} \ln \frac{W_{n_\tau,n_{\tau-1}}\, p_{n_{\tau-1}}}{W_{n_{\tau-1},n_\tau}\, p_{n_\tau}} \qquad = k_B \ln\left[\frac{\mathcal{P}(\nu)}{\tilde{\mathcal{P}}(\tilde{\nu})}\right]$$

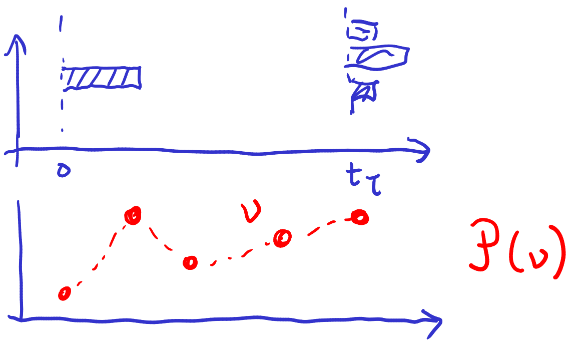
$$\sum_\nu \mathcal{P}(\nu) = 1$$

$$\sum_{\tilde{\nu}} \tilde{\mathcal{P}}(\tilde{\nu}) = 1$$

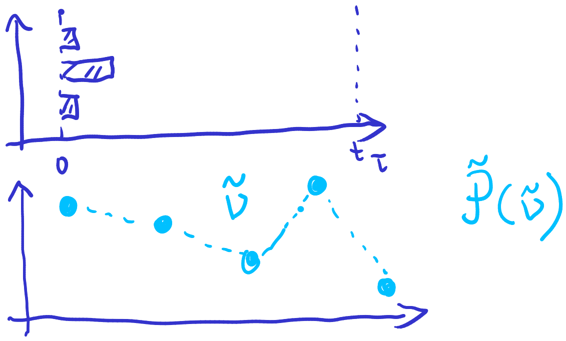
reverse of ν: $\tilde{\nu} \equiv (\tilde{n}_0, \tilde{n}_1, \ldots, \tilde{n}_\tau)$

$\tilde{n}_0 \equiv n_\tau$, $\tilde{n}_1 \equiv n_{\tau-1}$, ..., $\tilde{n}_\tau \equiv n_0$

forward traj



backw. traj.



Special case: if you start initially in stat. state

then $\vec{p}(0) = \vec{p}^{\,s} = \vec{p}(t_\tau)$

then $$\Delta S^i(\nu) = k_B \ln \frac{\mathcal{P}(\nu)}{\tilde{\mathcal{P}}(\tilde{\nu})} = k_B \ln \frac{\mathcal{P}(\nu)}{\mathcal{P}(\tilde{\nu})}$$

ensemble for back. traj. is now same as ensemble for forw. ones

rewriting: $$\boxed{\frac{\mathcal{P}(\tilde{\nu})}{\mathcal{P}(\nu)} = e^{-\Delta S^i(\nu)/k_B}}$$

this special case result in stat. state was discovered first

$\Rightarrow$ Gallavotti - Cohen fluc. theorem (1995)

our formulation: Lebowitz - Spohn (1999)

More special case: stat. state is an equil. stat. state

$$W_{n_i n_{i-1}} P^s_{n_{i-1}} = W_{n_{i-1} n_i} P^s_{n_i} \qquad \text{det. balance}$$

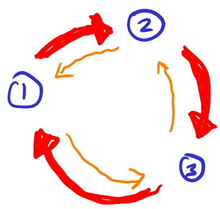
$$\dot{S}(\nu, t_i) = \frac{k_B}{\delta t} \ln \frac{W_{n_i n_{i-1}} P^s_{n_{i-1}}}{W_{n_{i-1} n_i} P^s_{n_i}} = 0$$

$$\Delta S^i(\nu) = \int_0^t dt\, \dot{S}(\nu, t) = 0$$

$\Rightarrow$ $\mathcal{P}(\nu) = \mathcal{P}(\tilde{\nu})$ in an ESS

no "arrow of time" in ESS

NESS:



(1, 2, 3, 1, 2, 3) more likely

(3, 2, 1, 3, 2, 1) in this NESS

but in this you have entropy production

Return to more general form (not necessarily a stat. state)

$$\boxed{\frac{\tilde{\mathcal{P}}(\tilde{\nu})}{\mathcal{P}(\nu)} = e^{-\Delta S^i(\nu)/k_B}}$$

generalized Crooks fluct. theorem

(orig. version: 1998)

average both sides over all paths: $A(\nu)$

$$\langle A(\nu)\rangle = \sum_\nu \mathcal{P}(\nu)\, A(\nu)$$

$\tilde{\nu}(\nu)$

$$\underbrace{\sum_\nu \mathcal{P}(\nu)\frac{\tilde{\mathcal{P}}(\tilde{\nu})}{\mathcal{P}(\nu)}}_{\sum_\nu \tilde{\mathcal{P}}(\tilde{\nu})} = \left\langle e^{-\Delta S^i(\nu)/k_B}\right\rangle$$

$$= \sum_{\tilde{\nu}} \tilde{\mathcal{P}}(\tilde{\nu})$$

$$= 1$$

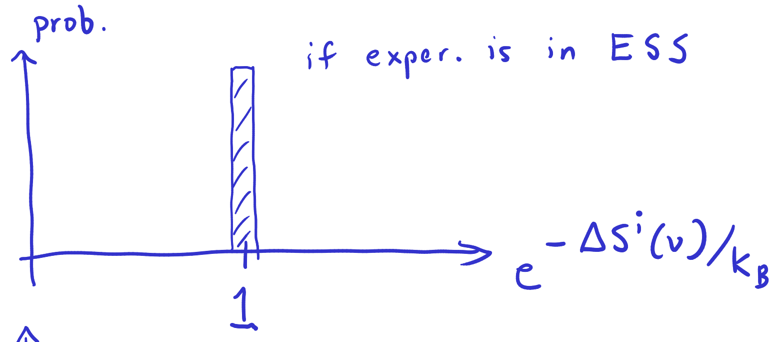
$$\Rightarrow \boxed{1 = \left\langle e^{-\Delta S^i(\nu)/k_B}\right\rangle}$$

universally valid relation (not just in stat. state)

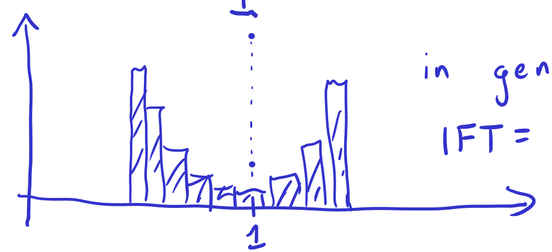
$\Rightarrow$ integral fluctuation theorem (IFT)

imagine running an experiment many times, + you were able to collect $\Delta S^i(\nu)$ for each traj. ν + hence we can also get $e^{-\Delta S^i(\nu)/k_B}$ for each ν

histogram of $e^{-\Delta S^i(\nu)/k_B}$ results



if exper. is in ESS



in general IFT = mean of this dist = 1 always