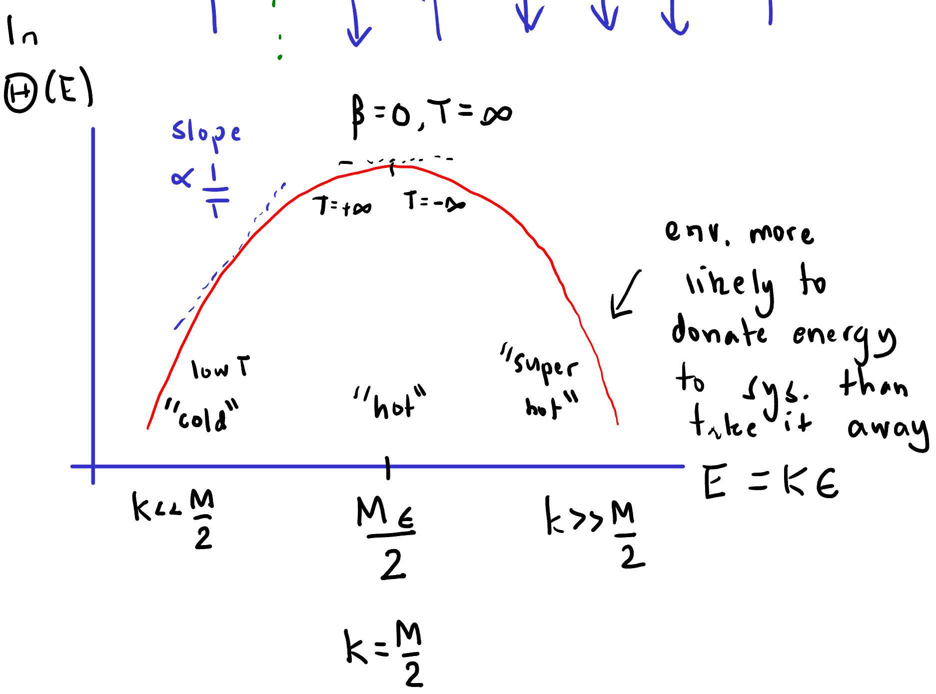
1 | 2 3 . . . . . M+1

↑ | ↓ ↑ ↓ ↓ ↓ ↑



$k = \#\ \uparrow$ spins

each $\uparrow$ spin has energy ϵ

" $\downarrow$ " " " 0

$$\beta = \frac{1}{k_B T} = \frac{\partial \ln \Theta}{\partial E}\bigg|_{E_{tot}}$$

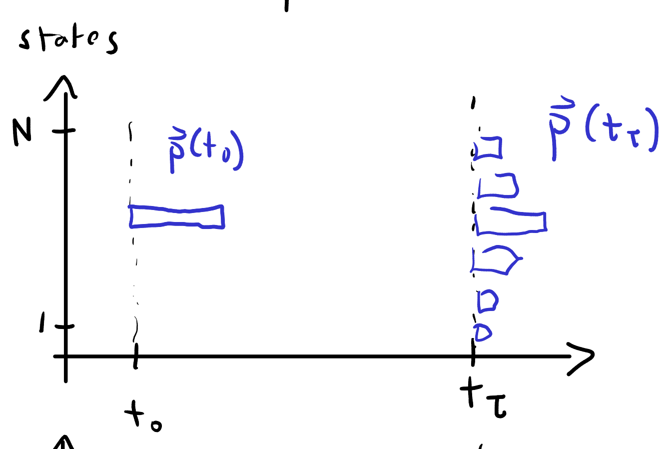
$$\approx \frac{2}{\epsilon}\left(1 - \frac{2E_{tot}}{M\epsilon}\right)$$

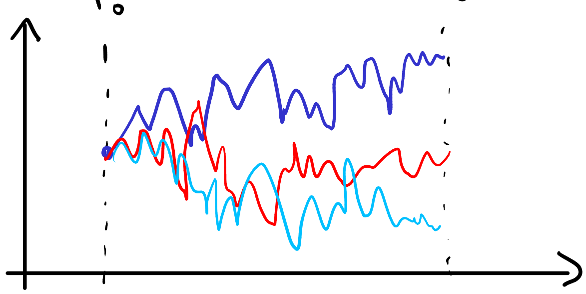
Master equation:

$$\vec{p}(t_\tau) = W\vec{p}(t_{\tau-1})$$

$$= \cdots\cdots = W^\tau \vec{p}(t_0)$$

$P_n(t_\tau)$





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

$\mathcal{P}(\nu)$ = prob. of traj. ν

$$= W_{n_\tau n_{\tau-1}} \cdots W_{n_1 n_0} p_{n_0}(t_0)$$

$$\sum_\nu \mathcal{P}(\nu) = \sum_{n_\tau} \cdots \sum_{n_0} \mathcal{P}(\nu) = 1$$

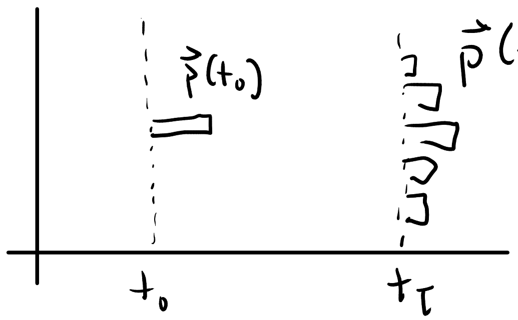
i) given a traj. ν, define "reverse" traj. $\tilde{\nu}$ (reversing seq. of states, but still going forw. in time)

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

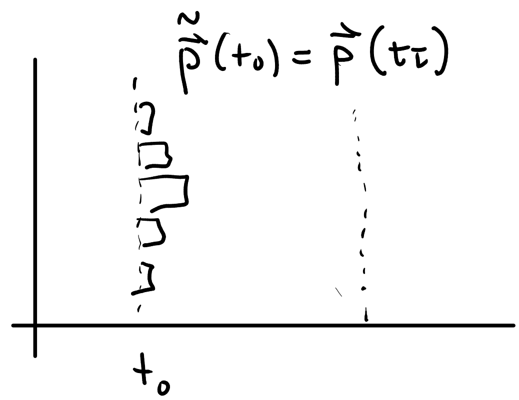
$$\tilde{\nu} = (\tilde{n}_0, \tilde{n}_1, \ldots, \tilde{n}_\tau)$$

$$\tilde{n}_0 = n_\tau,\quad \tilde{n}_1 = n_{\tau-1},\quad \ldots,\quad \tilde{n}_\tau = n_0$$

ii) reverse ensemble: initial distrib. of states is the <u>final</u> distrib of our original ensemble



original ensemble
"forward"



reverse ensemble
$\tilde{\mathcal{P}}$ ← rev. ensemble

GOAL: compare ν in forw. ensemble : $\mathcal{P}(\nu)$
to $\tilde{\nu}$ in rev. ensemble $\tilde{\mathcal{P}}(\tilde{\nu})$

rev. seq. of states

B/c W is ergodic + mixing $\Rightarrow$ LDB holds

if $W_{nm} \neq 0 \Rightarrow W_{mn} \neq 0$ (MR)

if $\mathcal{P}(\nu) \neq 0 \Rightarrow \tilde{\mathcal{P}}(\tilde{\nu}) \neq 0$

define a ratio for traj. where $\mathcal{P}(\nu) \neq 0$: "irreversibility" $I(\nu)$

$$I(\nu) \equiv k_B \ln \frac{\mathcal{P}(\nu)}{\tilde{\mathcal{P}}(\tilde{\nu})}$$

$|I(\nu)|$ is large when $\mathcal{P}(\nu) >> \tilde{\mathcal{P}}(\tilde{\nu})$

or $\tilde{\mathcal{P}}(\tilde{\nu}) >> \mathcal{P}(\nu)$

$I(\nu) = 0$ when $\mathcal{P}(\nu) = \tilde{\mathcal{P}}(\tilde{\nu})$

define an avg. over an ensemble of trajs:

$Q(\nu)$ = quantity associated w/ ν

$$Q \equiv \langle Q(\nu) \rangle = \sum_\nu \mathcal{P}(\nu) Q(\nu)$$

Calculate $\langle e^{-I(\nu)/k_B} \rangle = \sum_\nu \mathcal{P}(\nu) e^{-I(\nu)/k_B}$

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

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

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

always true!

integral fluctuation theorem

$$\boxed{\langle e^{-I(\nu)/k_B} \rangle = 1}$$

IFT

Seifert, PRL 040602 (2005);
precursors: 1990's (we will see later)

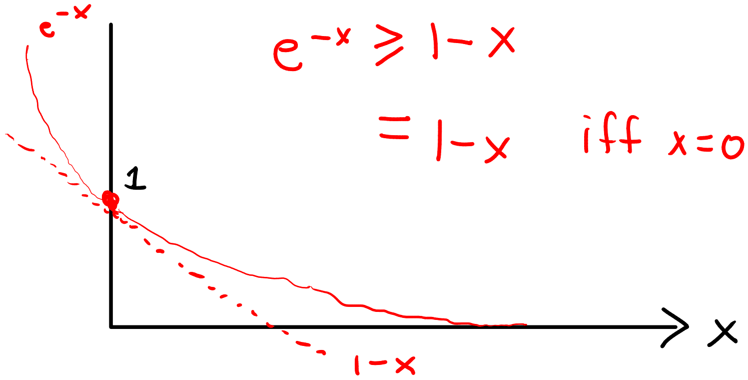
Consequences:

1) IFT $\Rightarrow$ $\langle I(\nu) \rangle = I \geq 0$ always

proof: $$1 = \left\langle e^{-I(\nu)/k_B} \right\rangle = \sum_{\nu} \mathcal{P}(\nu)\, e^{-I(\nu)/k_B}$$

$e^{-x} \geq 1-x$

$= 1-x$ iff $x=0$



$$\geq \sum_{\nu} \mathcal{P}(\nu) \left(1 - \frac{I(\nu)}{k_B}\right)$$

$$= \sum_{\nu} \mathcal{P}(\nu) - \frac{1}{k_B} \sum_{\nu} \mathcal{P}(\nu)\, I(\nu)$$

$$= 1 - \frac{1}{k_B} \underbrace{\langle I(\nu) \rangle}_{I}$$

$$1 \geq 1 - \frac{I}{k_B} \Rightarrow \boxed{I \geq 0}$$

2) you can decompose $I(\nu)$ into the irreversibilities of single time steps:

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

"concatenate"

$$= \underbrace{(n_0, n_1)}_{\mu_0} \oplus \underbrace{(n_1, n_2)}_{\mu_1} \oplus \cdots \oplus (n_{\tau-1}, n_\tau)$$

μ_i = traj. of one time step from n_i to n_{i+1}

will prove: $$I(\nu) = I(\mu_0) + I(\mu_1) + \cdots + I(\mu_{\tau-1})$$