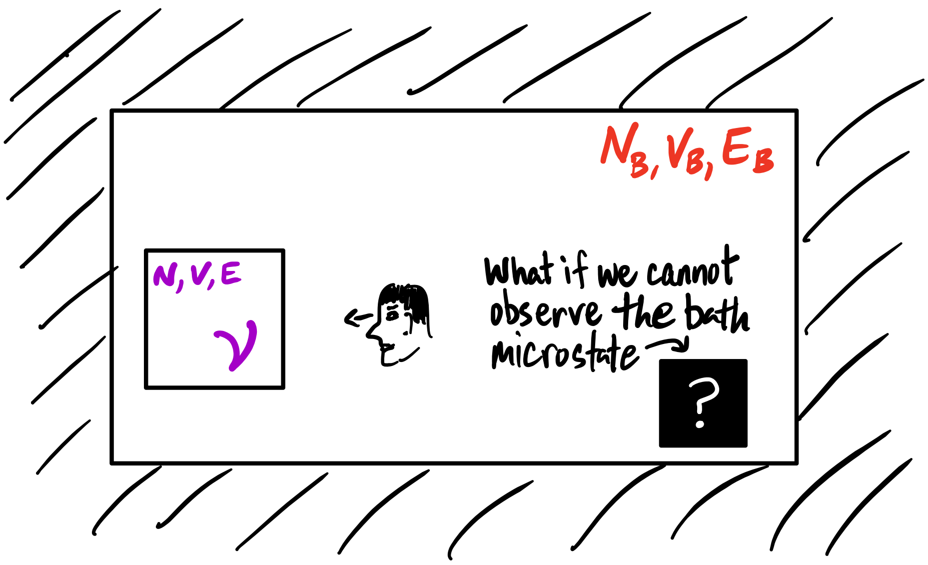
Lecture 3

Recall from last lecture...

System + (Thermal) Bath

Microstate of the full system + bath is defined by

$$\nu_T = \{\nu, \nu_B\}$$



Variables with no flow:

$$N_T = N + N_B$$
$$V_T = V + V_B$$

Variable with flow:

$$E_T = \underbrace{E(\nu)}_{\text{System microstate}} + \underbrace{E_B(\nu_B)}_{\text{Bath microstate}}$$

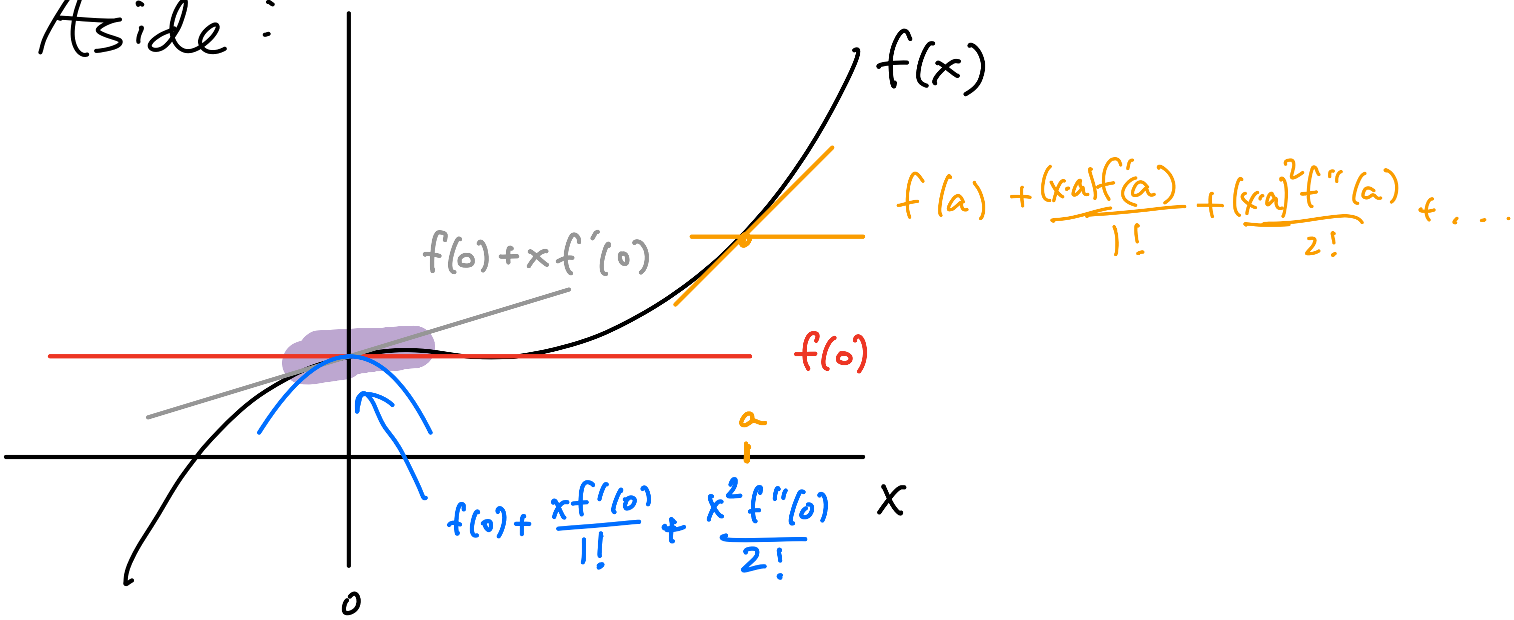
Probability of system microstate ν $\Longleftrightarrow$ How many bath microstates have energy $E_T - E(\nu)$

$$P(\nu) \propto \Omega_B(E_T - E(\nu)) \qquad \text{(Marginalization)}$$

What is $\Omega_B(E_T - E)$ in the limit of small E?

Taylor Expand!

Aside:



(Let's actually Taylor expand $\ln \Omega_B(E_T - E)$ not $\Omega_B(E_T - E)$)

$$\ln \Omega_B(E_T - E) \simeq \ln \Omega_B(E_T) + E \left(\frac{\partial \ln \Omega_B}{\partial E} \right) \Bigg|_{E=0} + \dots$$

How do the # of bath microstates change (on a log scale) with a change in system energy E?

Notice that $E_T - E = E_B \Rightarrow$

$$\left(\frac{\partial \ln \Omega_B}{\partial E}\right)\Bigg|_{E=0} = \left(\frac{\partial \ln \Omega_B}{\partial E_B}\right)\underbrace{\left(\frac{\partial E_B}{\partial E}\right)}_{\Rightarrow -1}$$

Chain Rule

$$= -\left(\frac{\partial \ln \Omega_B}{\partial E_B}\right)_{N_B, V_B}$$

The BIG INSIGHT...

$\left(\frac{\partial \ln \Omega_B}{\partial E_B}\right)_{N_B, V_B}$ has nothing to do with the system. It is a property of the bath!

Let's just define (for now) that bath property as

$$\beta = \left(\frac{\partial \ln \Omega_B}{\partial E_B}\right)_{N_B, V_B}$$

The Taylor expansion becomes

$$\ln \Omega_B(E_T - E) \approx \ln \Omega_B(E_T) + E\left(\frac{\partial \ln \Omega_B}{\partial E}\right)\bigg|_{E=0} + \ldots$$

chain

$$\ln \Omega_B(E_T - E) \approx \ln \Omega_B(E_T) - \beta E + \ldots ?$$

The system's energy is much smaller than the bath's

Exponentiating both sides yields

$$\Omega_B(E_T - E) = \Omega_B(E_T)\, e^{-\beta E} \propto e^{-\beta E}$$

The system-dependent part is of greatest interest to us

$$P(\nu) \propto \Omega_B(E_T - E(\nu)) \propto e^{-\beta E}$$

(Marginalization) (Taylor expansion)

$$\boxed{P(\nu) \propto e^{-\beta E}}$$

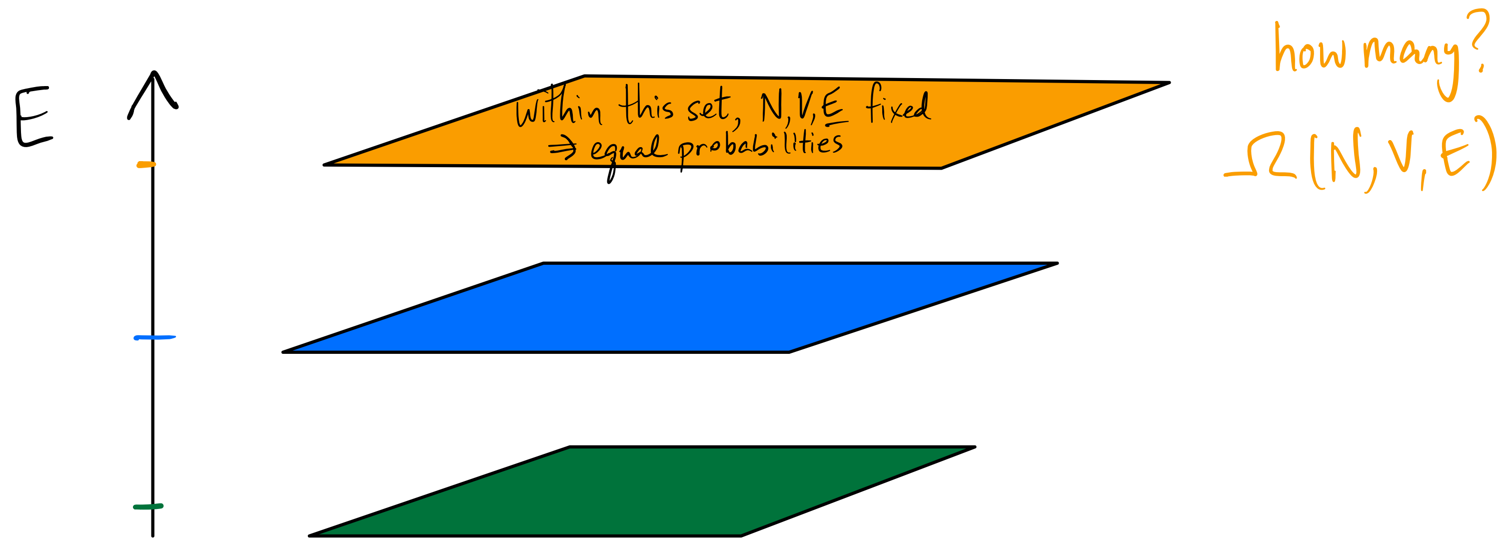
Boltzmann Distribution!

E is no longer fixed. It fluctuates!

Are the system microstates ν equally likely?

In the microcanonical ensemble — constrained (N, V, E) — two microstates ν_1 and ν_2 had equal probability.

(ν_1 and ν_2 had to have equal energy due to the constraint.)



Q: Why the $\propto$ sign? $\left(P(\nu) \propto e^{-\beta E}\right)$ $P(\nu) = \frac{e^{-\beta E}}{Q}$

A: We would need to normalize the distribution

(Normalization Factor)

Depends on β? on ν?

$e^{-\beta E(\nu)}$ Boltzmann Factor

$$1 = \sum_\nu P(\nu) = \sum_\nu \frac{e^{-\beta E}}{Q} = \frac{1}{Q}\sum_\nu e^{-\beta E} \Rightarrow$$

$$Q(\beta) = \sum_\nu e^{-\beta E}$$

dummy variable

Depends on ν?

No, ν is a dummy variable being summed over.

$$\Rightarrow \quad P(\nu) = \begin{cases} \dfrac{e^{-\beta E(\nu)}}{Q(\beta, V, N)}, & \text{if } N_\nu = N, V_\nu = V \\ 0, & \text{otherwise} \end{cases}$$

What is $P(E)$?

All of those possible ν's with $E_\nu = E$ have the same probability and combine together to give the probability of E.

$$P(E) = \sum_{\substack{\nu \text{ with} \\ E_\nu = E}} P(\nu) \propto e^{-\beta E} \sum_{\substack{\nu \text{ with} \\ E_\nu = E}} (1)$$

$$= e^{-\beta E}\,\Omega(E) \qquad e^{+N\ln\omega}$$

"large deviation form"

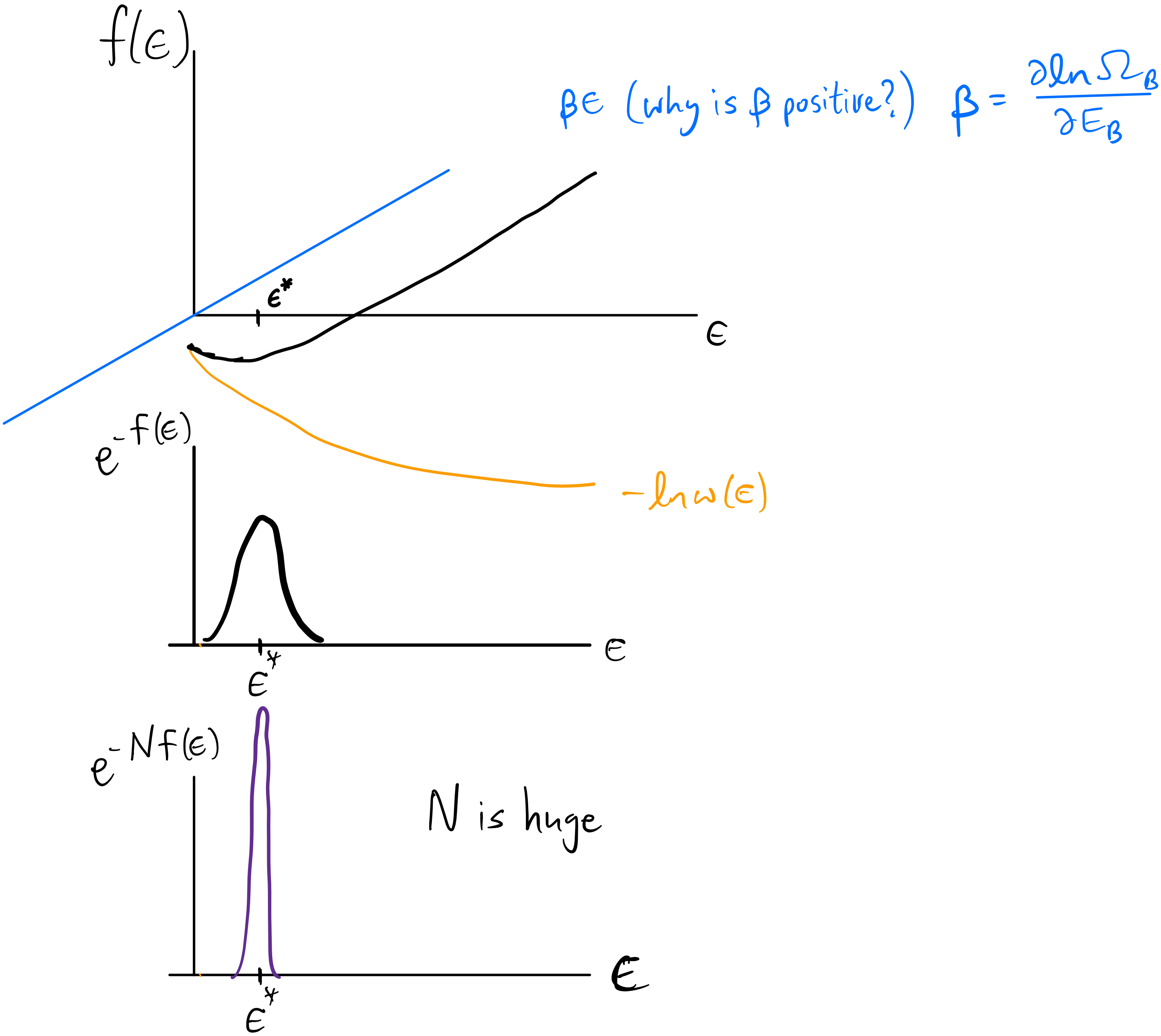
$$\Rightarrow \quad P(E) \propto \exp\Big[-\underbrace{N}_{\text{extensive}}\big(\underbrace{\beta\epsilon - \ln\omega}_{\text{intensive}}\big)\Big]$$

another "large deviation form"

$$\left(\epsilon = \frac{E}{N}\right)$$

Let's study this distribution in the limit of a big system. $(N \to \infty)$

Define $f(\epsilon) = \beta\epsilon - \ln\omega \quad \Rightarrow \quad P(E) \propto e^{-N f(\epsilon)}$



In the macroscopic limit, only one value of $\epsilon = \epsilon^*(\beta)$ has non-negligible weight.

Things look boring at the macroscopic scale.
(no detected fluctuations)

We've said a little about the distribution $P(E)$.
How do we compute the typical E, i.e. $\langle E \rangle$?