$\rho(q,p)$

$$\Omega = \frac{\omega}{\omega_0}$$

$$\{\rho, H\} = 0 \qquad \omega_0 = h^{3N}$$

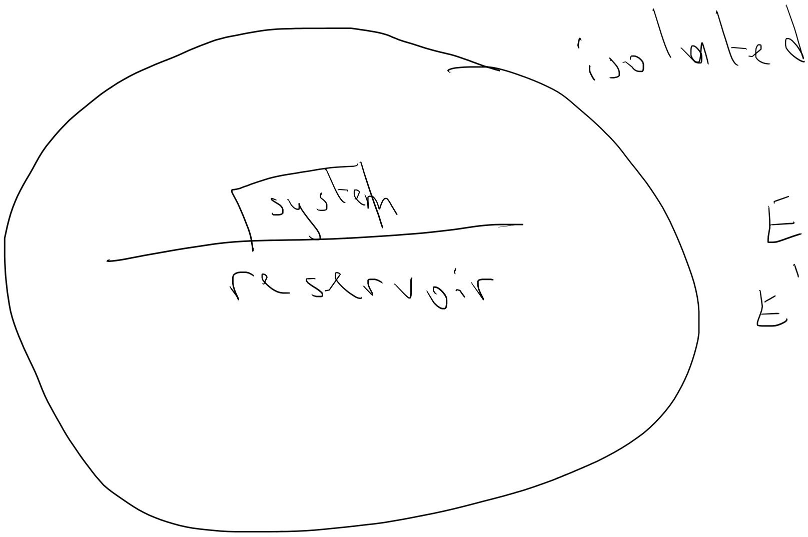
$\ln\rho$ : additive conserved quantity

$\rho = \text{const} \equiv \frac{1}{\omega}$ : microcanonical ensemble

$\ln\rho = \text{const} - \beta E$ : canonical ensemble

$\ln\rho = \text{const} - \beta \underline{E} + \beta\mu\underline{N}$ : grand canonical ensemble

$U \equiv \langle E \rangle$




$E^{(0)} = E + E'$

$E$: energy of the system

$E'$: energy of the reservoir

$P_r$: probability that the system is in a state of energy $E_r$?

$$P_r = \frac{1 \cdot \Omega_R(E')}{\Omega_c(E^{(0)})} = \frac{1 \cdot \Omega_R(E^{(0)} - E_r)}{\Omega_c(E^{(0)})} \Leftarrow$$

$$\ln\Omega_R(E^{(0)} - E_r) = \left[\ln\Omega_R(E^{0})\right] + \frac{\partial \ln\Omega_R(E)}{\partial E}\bigg|_{E=E_0}(-E_r) + \dots$$

$$= \text{const} - E_r \frac{1}{kT} + \cdots$$

$$\Omega_R(E^{(0)} - E_r) = \text{const}\, e^{-\frac{E_r}{kT}}$$

$$P_r = \text{const}\, e^{-\frac{E_r}{kT}} = \boxed{\frac{e^{-\frac{E_r}{kT}}}{\sum_r e^{-\frac{E_r}{kT}}} = P_r}$$

$$\sum_r e^{-\frac{E_r}{kT}} \equiv Z \quad \text{partition function}$$

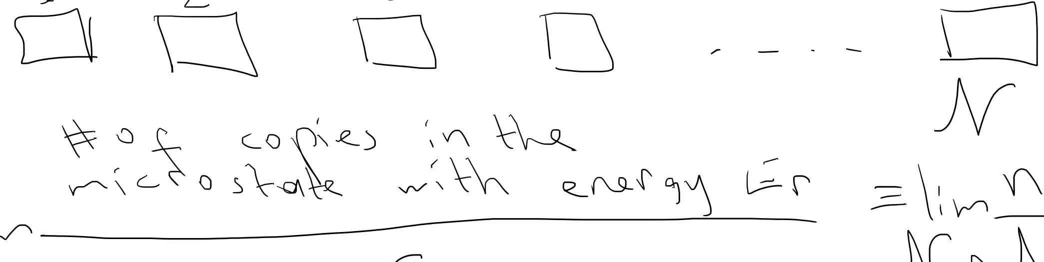
$$U = \sum_r E_r P_r = \sum_r \frac{E_r e^{-\beta E_r}}{Z} \qquad \beta \equiv \frac{1}{kT}$$

$$= \frac{1}{Z} \sum E_r e^{-\beta E_r}$$

$$= \frac{1}{Z} \sum_r \left(-\frac{\partial}{\partial \beta}\right) e^{-\beta E_r} = \frac{1}{Z}\left(-\frac{\partial}{\partial \beta}\right) Z$$

$$\boxed{U = -\frac{\partial \ln Z}{\partial \beta}}$$

<u>Derivation using ensembles</u>




$$P_r = \lim_{N \to \infty} \frac{\#\text{ of copies in the microstate with energy } E_r}{N} \equiv \lim_{N \to \infty} \frac{n_r}{N}$$

$\{n_r\}$

$$W(\{n_r\}) = \frac{N!}{n_0!\, n_1! \ldots n_M!}$$

most probable $\{n_r\} = \{n_r^*\}$?

$$\sum_r n_r = N \qquad \frac{1}{N}\sum_r E_r n_r \equiv \langle E \rangle \equiv U$$

$$\ln W = \ln N! - \sum_r \ln n_r!$$

$N \to \infty$ $\quad = (N \ln N - \cancel{N}) - \sum_r (n_r \ln n_r - \cancel{n_r})$

$n_r \to \infty$

$$\ln W = N \ln N - \sum_r n_r \ln n_r$$

$$\delta \ln W = -\sum_r \left[(\delta n_r) \ln n_r + \cancel{n_r} \frac{\delta n_r}{\cancel{n_r}}\right]$$

$$\delta \ln W = -\sum_r (\ln n_r + 1)\, \delta n_r = 0$$

$$\sum n_r = N \Rightarrow \sum_r \delta n_r = 0$$

$$\sum E_r n_r = NU \Rightarrow \sum_r E_r \delta n_r = 0$$

$$\sum_r (\ln n_r + 1 + \alpha + \beta E_r)\, \delta n_r = 0 \Leftarrow$$

$\alpha, \beta$: Lagrange multipliers.

$$\ln n_r^* + 1 + \alpha + \beta E_r = 0$$

$$n_r^* = \text{const}\, e^{-\beta E_r}$$

$$P_r \propto e^{-\beta E_r} \Leftarrow$$

$$\left.\begin{aligned} \langle n_r \rangle &= n_r^* \\ \frac{\Delta n_r}{\langle n_r \rangle} &\propto \frac{1}{\sqrt{N}} \to 0 \end{aligned}\right\}$$

$$\langle n_r \rangle = \frac{\sum_{\{n_r\}} n_r W(\{n_r\})}{\sum W(\{n_r\})}$$

$$= \left.\frac{\sum n_r \frac{N!}{n_0! n_1! \ldots} w_0^{n_0} w_1^{n_1} \ldots}{\sum W(\{n_r\})}\right|_{w_r = 1} \Leftarrow$$

$$= \left.\frac{1}{\sum W(\{n_r\})} w_r \frac{\partial}{\partial w_r} \sum \frac{N!\, w_0^{n_0} w_1^{n_1} \ldots}{n_0! n_1! \ldots}\right|_{w=1}$$

$$\langle n_r \rangle = w_r \frac{\partial}{\partial w_r} \ln \Gamma(N, U, \{w_r\})$$

$$\Gamma = \sum_{\{n_r\}} \frac{N!}{n_0! n_1! \ldots} w_0^{n_0} w_1^{n_1} \ldots$$

$\Leftarrow$

$$\sum n_r = N$$

$$\sum n_r E_r = NU$$

$$\Gamma' = \sum_{\substack{\{n_r\} \\ \sum n_r = N}} \frac{N!}{n_0!\, n_1! \dots} w_0^{n_0} w_1^{n_1} \dots$$

$$= (w_0 + w_1 + \dots)^N$$

$$\Gamma(N,z) = \sum_U \Big( \underbrace{\sum_{\substack{\{n_r\} \\ \sum n_r = N \\ \sum E_r n_r = NU}} \frac{N!}{n_0!\, n_1! \dots} w_0^{n_0} w_1^{n_1} \dots}_{\Gamma(N,U)} \Big) z^{NU}$$

$$= \sum_{\substack{\{n_r\} \\ \sum n_r = N}} \frac{N!}{n_0!\, n_1! \dots} (w_0^{n_0} w_1^{n_1} \dots) z^{\sum n_r E_r}$$

$$\Gamma(N,z) = \left( w_0 z^{E_0} + w_1 z^{E_1} + w_2 z^{E_2} \dots \right)^N = [f(z)]^N$$

$$\Gamma(N,z) = \sum_{U'} \Gamma(N,U') z^{NU'} \Leftarrow$$

$$\Gamma(N,U) = \frac{1}{2\pi i} \oint dz \frac{\Gamma(N,z)}{z^{NU+1}}$$

$$\Gamma(N,U) = \frac{1}{2\pi i} \oint_C dz \frac{[f(z)]^N}{z^{NU+1}}$$

$C$ is a contour that

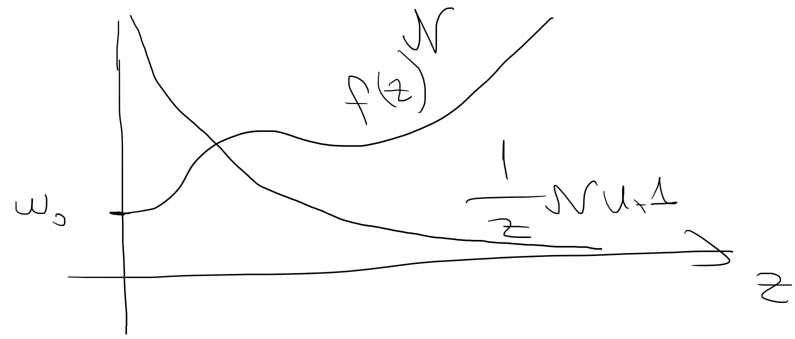
i) go around $z = 0$

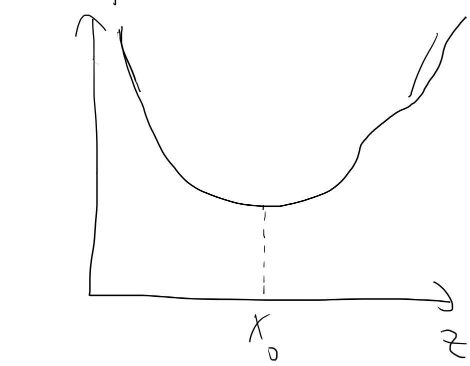
ii) radius should be smaller than the convergence radius of $f(z)$

integrand $\dfrac{[f(z)]^N}{z^{Nu+1}}$

$$f(z) = w_0 z^{E_0} + w_1 z^{E_1} + w_2 z^{E_2} \cdots$$

$$0 = E_0 < E_1 < E_2 \cdots$$




$$\Gamma(N, u) = \frac{1}{2\pi i} \oint_C dz \, \frac{[f(z)]^N}{z^{Nu+1}}$$

$$= \frac{1}{2\pi i} \oint dz \, e^{-g(z)}$$

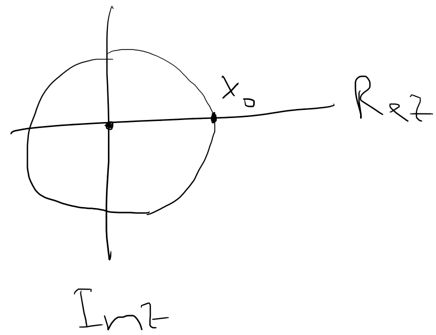
$$g(z) = -\ln \frac{[f(z)]^N}{z^{Nu+1}} = -N \ln f(z) + (Nu+1) \ln z$$

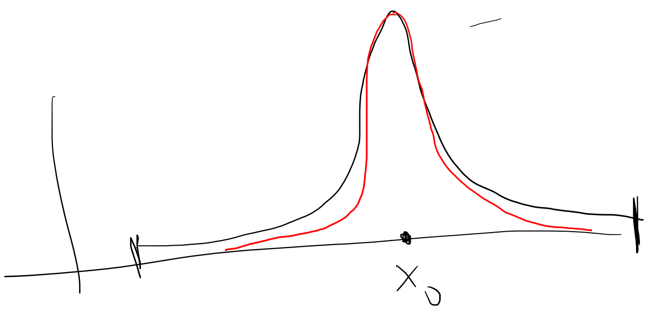
$$g(z) = -N \ln f(z) + (Nu+1) \ln z$$

$$\Gamma(N,U) = \frac{1}{2\pi i}\oint dz\, e^{+g(z)}$$

$$g(z) = +N \ln f(z) - (NU+1)\ln z$$

$g(z)$ (as an analytical function of complex $z$) can not have a local maximum or local minimum.


$$g'(x_0) = 0$$

$$g(z) = +N \ln f(z) - (NU+1)\ln z$$

$$g'(x_0) = N\frac{f'(x_0)}{f(x_0)} - \frac{(NU+1)}{x_0} = 0$$

$$NU \gg 1$$

$$\frac{f'(x_0)}{f(x_0)} = \frac{U}{x_0} \Rightarrow \boxed{x_0 = U\frac{f(x_0)}{f'(x_0)}}$$

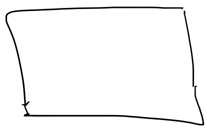
$$g(z) = g(x_0) + g''(x_0)(z-x_0)^2\frac{1}{2!} + \dots$$

$$\Gamma(N,U) \simeq \frac{1}{2\pi i}\oint dz\, e^{g(x_0) + g''(x_0)(z-x_0)^2\frac{1}{2!}}$$

$$\Gamma(N,U) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} dz\, e^{g(x_0)+\frac{1}{2!}g''(x_0)\,y^2}$$

$\langle n_r\rangle \propto e^{-\beta E_r}$ $\qquad x_0 \equiv e^{-\beta}$

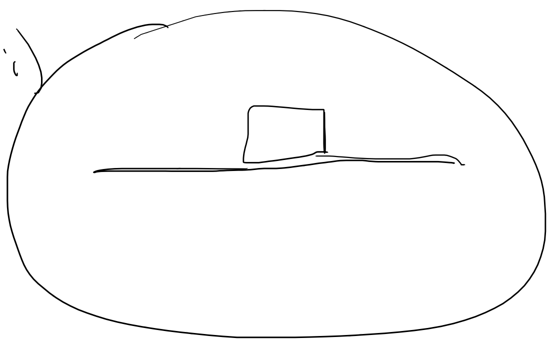
$$P_r = \frac{e^{-\beta E_r}}{Z}$$



$T \Longleftrightarrow U$ fixed

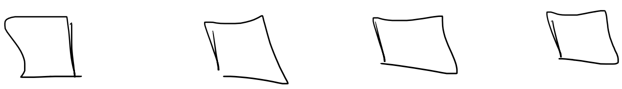
$\sum E_r P_r = U \Rightarrow$ determines $\beta$ in terms of $U$

i)



microcanonical ensemble

ii)



$$\{n_r\} \Longleftrightarrow W(\{n_r\})$$

$$n_r^* \propto e^{-\beta E_r}$$

iii) $\langle n_r\rangle = n_r^*$