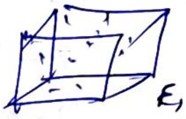
Ideal gas example in microcanonical ensemble –
or
Method of calculation of thermodynamic quantities in microcanonical ensemble ~~takin~~ by taking example of classical ideal gas —

The Hamiltonian for ideal gas is given by

$$H(\vec{r}_i, \vec{p}_i) = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m}$$



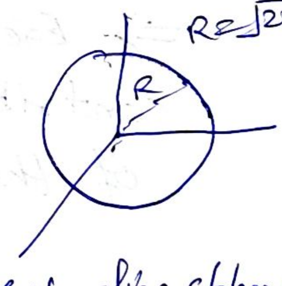
E, V, N

~~System is Isolated~~

$$\Sigma(E) = \int d\vec{r}_i \int_{H<E} d\vec{p}_i$$

$$= V^N \int d\vec{p}_1 \int d\vec{p}_2 \cdots \int d\vec{p}_N$$

$$\frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \cdots + \frac{p_N^2}{2m} < E$$



$R = \sqrt{2mE}$

or $$\Sigma(E) = V^N \Omega_{3N}(R)$$

where $R = \sqrt{2mE}$ 6N-dim sphere

In the previous class we have calculated,

$$\Omega_n(R) = \frac{\pi^{n/2}}{\left(\frac{n}{2}\right)!} R^n$$

Thus $$\Sigma(E) = V^N \frac{\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!} (2mE)^{3N/2}$$

Since we have $$S(E,V,N) = \ln \Sigma(E)$$

we take $k_B = 1$ for simplicity

$$S(E,V,N) = \ln V^N + \ln \pi^{\frac{3N}{2}} - \ln\left(\frac{3N}{2}\right)! + \ln(2mE)^{\frac{3N}{2}}$$

we use stirling Approximation

$$\text{or } S = N\ln V + \frac{3N}{2}\ln\pi - \frac{3N}{2}\ln\frac{3N}{2} + \frac{3N}{2} + \frac{3N}{2}\ln(2mE)$$

$$\text{or } \boxed{S = N\ln\left[V\left(\frac{4\pi mE}{3N}\right)^{3/2}\right] + \frac{3}{2}N}$$

$$\exp\left[\frac{1}{N}\left(S - \frac{3}{2}N\right)\right] = V\left(\frac{4\pi mE}{3N}\right)^{3/2}$$

$$\text{or } \boxed{E = \frac{3}{4\pi m}\frac{N}{V^{2/3}}\exp\left[\frac{2}{3}\frac{S}{N} - 1\right]}$$

we have $E(S,V,N)$, using first law of thermodynamics (combined with second law) we can obtain the thermodynamic parameters T, P, etc

$$T = \left.\frac{\partial E}{\partial S}\right|_{V,N} = \frac{1}{2\pi m} V^{-2/3}\exp\left[\frac{2}{3}\frac{S}{N} - 1\right]$$

$$P = -\left.\frac{\partial E}{\partial V}\right|_{T,N} = \frac{1}{2\pi m}\frac{N}{V^{5/3}}\exp\left[\frac{2}{3}\frac{S}{N} - 1\right]$$

$$\text{or } \boxed{PV = NT}$$ Ideal gas → equation of state