Key points of 03/02 lecture

Define classical trace and classical density matrix (canonical ensemble):

$$Q(N,T,V) = \frac{1}{N!\,h^{3N}} \int e^{-\beta \mathcal{H}(\vec{p},\vec{q})}\, d^{3N}\vec{p}\, d^{3N}\vec{q}$$

$$\xrightarrow{\text{def}} = \mathrm{Tr}\left(\exp(-\beta \mathcal{H}(\vec{p},\vec{q}))\right)$$

$$\rho_{can}(\vec{p},\vec{q}) = \frac{\exp(-\beta \mathcal{H}(\vec{p},\vec{q}))}{Q(N,T,V)}$$

$$\langle f \rangle = \mathrm{Tr}(\rho_{can} f)$$

Quantum statistical mechanics (canonical ensemble):

$$e^{-\beta \hat{\mathcal{H}}} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} (\beta \hat{\mathcal{H}})^n$$

For complete set $\{|\psi_n\rangle\}$: $\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I}$
(orthonormal)

identity operator

$$e^{-\beta \hat{\mathcal{H}}} = \sum_m e^{-\beta E_m} |\psi_m\rangle\langle\psi_m| \quad \text{where } \{|\psi_m\rangle\} \text{ energy eigen basis}$$

$$\mathrm{Tr}(\hat{A}) = \sum_\ell \langle\phi_\ell|\hat{A}|\phi_\ell\rangle \quad \text{where } \{|\phi_\ell\rangle\} \text{ complete set}$$

$$\mathrm{Tr}(e^{-\beta\hat{\mathcal{H}}}) = \sum_m e^{-\beta E_m}$$

$$\langle\hat{A}\rangle = \sum_m p_m \langle\psi_m|\hat{A}|\psi_m\rangle \quad \text{where } p_m = \frac{e^{-\beta E_m}}{\sum_\ell e^{-\beta E_\ell}}$$