Equilibrium density matrix and "evolution" in Imaginary time

$$e^{-\frac{i}{\hbar}\hat{H}t} \longrightarrow e^{-\beta\hat{H}}$$

for time independent Hamiltonians

it is natural to define

$$\frac{it}{\hbar} = \tau \qquad \text{imaginary "time"}$$

is indeed an inverse of energy

$$e^{-\beta\hat{H}} = \left[e^{-\frac{i}{\hbar}\hat{H}t}\right]_{t=-i\hbar\beta}$$

one can think at

$$e^{-\beta\hat{H}}|\psi\rangle = |\psi, -i\hbar\beta\rangle_S \qquad \text{evolution in imaginary "time"}$$

now define the thermal "evolution" operator

$$U_T(\tau,0) = e^{-\tau\hat{H}} = U_S(-i\hbar\tau, 0)$$

Schrödinger evolution

best perturbation theory results to the resummed

$$\boxed{U_T(\tau,0) = e^{-\tau\hat{H}} = e^{-\tau H_0}\, T_{\tau'}\, e^{-\int_0^{\tau} d\tau'\, V_I(\tau')}}$$

$$\boxed{V_I(\tau) = e^{\tau H_0} V e^{-\tau H_0}}$$

interaction picture in imaginary "time"

Now equilibrium density matrix is

$$e^{-\beta \hat{H}} = e^{-\beta H_0} T_\tau e^{-\int_0^\beta d\tau V_I(\tau)}$$

and therefore the basis of stat mech perturbation theory is the calculation of

$$\boxed{Z = \mathrm{tr}\, e^{-\beta \hat{H}} = \mathrm{tr}\, e^{-\beta H_0} \underbrace{T_\tau e^{-\int_0^\beta d\tau V_I(\tau)}}_{S_T(\beta)}}$$

thermal S-matrix

$$Z = \mathrm{tr}\, e^{-\beta H_0} S_T(\beta)$$

$$Z = Z_0 \langle S_T(\beta) \rangle_0$$

$$S_T(\beta) = 1 - \int_0^\beta d\tau V_I(\tau) + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \, T_\tau V_I(\tau) V_I(\tau') + \dots$$

τ ordering unnecessary for only 1 time

Free Energy to first order

$$S_T = 1 + S^{(1)} + O(V^2)$$

$$F = -\frac{1}{\beta} \ln Z_0 \langle S_T(\beta) \rangle_0$$

$$\boxed{F = F_0 - \underbrace{\frac{1}{\beta} \ln \langle S_T(\beta) \rangle_0}}$$ exact

$$\ln(1 + \langle S^{(1)} \rangle) \simeq \langle S^{(1)} \rangle$$

$$F = F_0 + \frac{1}{\beta} \int_0^\beta d\tau \, \langle V_I(\tau) \rangle_0$$

$$\langle V_I(\tau) \rangle_0 = \frac{\mathrm{tr}\, e^{-\beta H_0} e^{\tau H_0} V e^{-\tau H_0}}{\mathrm{tr}\, e^{-\beta H_0}}$$ cyclic properties of trace

$$= \langle V \rangle_0 \quad \text{indep } \tau$$

to first order

$$\boxed{F = F_0 + \langle V \rangle_0}$$

average of an operator to first order

$$\langle \hat{A} \rangle = \frac{\mathrm{tr}\, e^{-\beta H_0} S_T(\beta) \hat{A}}{\mathrm{tr}\, e^{-\beta H_0} S_T(\beta)} \frac{Z_0}{Z_0}$$

$$\langle \hat{A} \rangle = \frac{\langle S_T \hat{A} \rangle_0}{\langle S_T \rangle_0}$$ to first order

$$\frac{\langle (1+S^{(1)}) \hat{A} \rangle_0}{\langle (1+S^{(1)}) \rangle_0} \simeq \langle (1+S^{(1)}) \hat{A} \rangle_0 \left(1 - \langle S^{(1)} \rangle\right)$$

$$\langle \hat{A} \rangle = \langle \hat{A} \rangle_0 + \langle S^{(1)} \hat{A} \rangle_0 - \langle \hat{A} \rangle_0 \langle S^{(1)} \rangle_0 + \mathcal{O}(V^2)$$

$$\boxed{\underbrace{\langle \hat{A} \rangle - \langle \hat{A} \rangle_0}_{\text{deviation from 0 due to "external" } V} = -\int_0^\beta d\tau \, \underbrace{\left[\langle \hat{V}_I(\tau) \hat{A} \rangle_0 - \langle \hat{V}_I(\tau) \rangle_0 \langle \hat{A} \rangle_0 \right]}_{\text{correlation function at equilibrium}}}$$

Classical limit is attained for large temperatures i.e. $\beta \to 0$

$$\boxed{\langle \hat{A} \rangle - \langle \hat{A} \rangle_0 = -\beta \left[\langle \underbrace{VA}_{\text{functions}} \rangle_0 - \langle V \rangle_0 \langle A \rangle_0 \right]}$$

Constant field case

$$\hat{V} = -\underset{\text{constant field}}{h} \cdot \hat{B} \leftarrow \text{operator on system variables}$$

$$\langle \hat{A} \rangle_h - \langle \hat{A} \rangle_0 = h \int_0^\beta d\tau \left[\langle \hat{B}_I(\tau) \hat{A}(0) \rangle_0 - \langle \hat{B}_I(\tau) \rangle_0 \langle \hat{A}(0) \rangle_0 \right]$$

for small h

$$\boxed{\frac{d\langle \hat{A} \rangle}{dh} = \int_0^\beta d\tau \left[\langle \hat{B}_I(\tau) \hat{A}(0) \rangle_0 - \langle \hat{B}_I(\tau) \rangle_0 \langle \hat{A}(0) \rangle_0 \right]}$$

$V = -hB$

Homogeneous linear Response

Response Function

correlation function

classical limit

$$\boxed{\frac{d\langle A \rangle}{dh} = \beta \left[\langle \hat{B} \hat{A} \rangle_0 - \langle B \rangle_0 \langle A \rangle_0 \right]}$$

$$\boxed{\chi_{A,h} = \beta\, C_{BA}}$$

$V = -hB$