

1. Density Matrix

①

time dependent Schrödinger Equation:

$$i\hbar \frac{\partial \psi_i(t)}{\partial t} = H \psi_i(t)$$

density operator: $\hat{\rho}(t)$

matrix elements: $\langle H | \psi_i \rangle = E_i | \psi_i \rangle$

$\Downarrow$

$$\langle \psi_i | \hat{\rho}(t) | \psi_j \rangle = \langle \psi_i(t) | \hat{\rho} | \psi_j(t) \rangle$$

time-dependence: $\langle \dot{\psi}_i(t) | \hat{\rho} | \psi_j(t) \rangle + \langle \psi_i(t) | \dot{\hat{\rho}} | \psi_j(t) \rangle$

one can write:

$$i\hbar \left[\langle \dot{\psi}_i(t) | \hat{\rho} | \psi_j(t) \rangle + \langle \psi_i(t) | \dot{\hat{\rho}} | \psi_j(t) \rangle \right]$$
$$= -\langle \psi_i(t) | H \hat{\rho} | \psi_j(t) \rangle + \langle \psi_i(t) | \hat{\rho} H | \psi_j(t) \rangle$$

$\Downarrow$

$$i\hbar \dot{\rho} = [\hat{\rho}, \hat{H}]$$

classical analog: Liouville equation

$$i\hbar \dot{\rho} = \{H, \rho\}$$

ρ - density

$\{, \}$ - Poisson brackets

- for the microcanonical ensemble:

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$$S_{mn} = S_n \delta_{mn}$$

$$S_n = 1/\Gamma$$

Γ = total volume of
state space (states with
same energy)

$\Downarrow$

if S_{mn} is diagonal at $t=0$

- it should be diagonal for all other times
- diagonal elements should remain constant

$$S_{mn} = \frac{1}{N} \sum_{k=1}^N a_m^k a_n^{k*} = ?$$

if a priori probabilities are equal

we can write

$$S_{mn} = \frac{1}{N} \sum_{k=1}^N |a|^2 e^{i(\varphi_m^k - \varphi_n^k)} = \langle e^{i(\varphi_m^k - \varphi_n^k)} \rangle$$

since wavefn. is undetermined up to a phase

$$S_{mn} \text{ is diagonal if } \langle e^{i(\varphi_m^k - \varphi_n^k)} \rangle = \delta_{mn}$$

$\Downarrow$

equal a priori phase approximation

easiest to switch to momentum representation

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$$q \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial p}$$

Hamiltonian: $\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + \frac{m\omega^2}{2} q^2$

$$\hat{H} = \frac{1}{2m} p^2 + \frac{m\omega^2 \hbar^2}{2} \frac{\partial^2}{\partial p^2} = -\frac{\hbar^2}{2m' \omega'^2} + \frac{m' \omega'^2}{2} p^2$$

Hamiltonian has the same form in p space as in q -space
only the constants are different

this means that we can write the density matrix in
momentum space, but we only need the diagonal
element
↓

$$\langle p | \exp(-\beta \hat{H}) | p \rangle = A \exp[-B p^2] = A \exp\left[-\frac{m' \omega'^2}{\hbar} \tanh\left(\frac{\beta \hbar \omega'}{2}\right) p^2\right]$$

$$m' = \frac{1}{m\omega^2}$$

$$\omega' = \omega$$

$$= A \exp\left[-\frac{1}{\hbar m \omega} \tanh\left(\frac{\beta \hbar \omega}{2}\right) p^2\right]$$

$$= A \exp[-B p^2]$$

$$B = \frac{\tanh\left(\frac{\beta \hbar \omega}{2}\right)}{\hbar m \omega}$$

$$\langle p^2 \rangle = \frac{\hbar m \omega}{2 \tanh\left(\frac{\beta \hbar \omega}{2}\right)}$$

2 Chemical Equilibrium

(4)

- H_2 $I_H = \frac{1}{2}$ for H-atom
combined nuclear spin $I_{H_2} = 1, 0 \Rightarrow$ bosons
- D_2 - $I_D = 1 \Rightarrow I_{D_2} = 2, 1, 0 \Rightarrow$ bosons
- HD $\rightarrow \frac{1}{2}, \frac{1}{2} \Rightarrow$ fermions
- Born-Oppenheimer approximation: potential obtained from fixed nuclei $\Rightarrow$ masses of nuclei do not matter

as a result: 1) equilibrium bond-length for H_2, D_2, HD can be taken to be the same

2) spring constant (harmonic approx.)

can be taken to be the same for all three

$$B_{H_2} = \frac{\hbar^2}{2I_{H_2}}$$

$$I_{H_2} = 2m_H \left(\frac{r_{eq}}{2}\right)^2$$

$$m_D = 2m_H$$

$$B_{D_2} = \frac{\hbar^2}{2I_{D_2}}$$

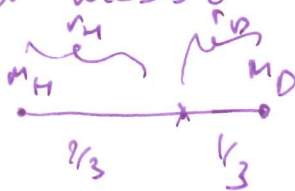
$$I_{D_2} = 2m_D \left(\frac{r_{eq}}{2}\right)^2 = 2I_{H_2}$$

$$B_{HD} = \frac{\hbar^2}{2I_{HD}}$$

$$I_{HD} = m_H r_H^2 + m_D r_D^2 = m_H \left(\frac{2r_{eq}}{3}\right)^2 + 2m_H \left(\frac{r_{eq}}{3}\right)^2$$

center of mass of HD

$$= \left(\frac{4m_H}{9} + \frac{2m_H}{9} \right) r_{eq}^2 = \frac{6m_H}{9} r_{eq}^2 = \frac{2m_H}{3} r_{eq}^2$$



$$I_{HD} = \frac{2}{3} I_{H_2}$$

take $B_{H_2} = 1 \Rightarrow$

$$\frac{B_{D_2}}{B_{H_2}} = 1/2$$

$$\frac{B_{HD}}{B_{H_2}} = 3/4$$

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- for ω (frequency):

$$k = \mu \omega^2 = \mu_{H_2} \omega_{H_2}^2 \pm \mu_{D_2} \omega_{D_2}^2 \pm \mu_{HD} \omega_{HD}^2$$

take $\omega_{H_2} = 1 \Rightarrow$

μ = reduced mass

$$\mu_{H_2} = \frac{m_H}{2} = \frac{m_H}{2}$$

$$\mu_{D_2} = \frac{m_D}{2} = m_H$$

$$\mu_{HD} = \frac{m_H m_D}{m_H + m_D} = \frac{2m_H^2}{3m_H} = \frac{2m_H}{3}$$

take $\omega_{H_2} = 1$

$$\mu_{H_2} \omega_{H_2}^2 = \mu_{D_2} \omega_{D_2}^2 = \mu_H$$

$$\frac{m_H}{2} \omega_{H_2}^2 = m_H \omega_{D_2}^2$$

$$\Rightarrow \omega_{D_2} = \sqrt{\frac{1}{2}} \omega_{H_2}$$

$$\mu_{H_2} \omega_{H_2}^2 = \mu_{HD} \omega_{HD}^2$$

$$\frac{m_H}{2} \omega_{H_2}^2 = \frac{2}{3} m_H \omega_{HD}^2$$

$$\omega_{HD} = \sqrt{\frac{3}{4}} \omega_{H_2}$$

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$$K(T) = \frac{(q_{HD}/V)^2}{\frac{q_{D_1} q_{H_2}}{V^2}} = \frac{q_{HD}^2}{q_{H_2} q_{D_2}}$$

$$q_{HD} = q_{HD}^{(tr)} q_{HD}^{(tr)} q_{HD}^{(rot)} q_{HD}^{(vib)}$$

$$q_{HD}^{(tr)} = \frac{4\pi}{h^3} \int_0^\infty d\mathbf{h} h^2 \ln(1 + e^{-\frac{h^2}{2m_{HD} kT} - \beta \epsilon_k})$$

$$q_{HD}^{(tr)} = ?$$

$$-kT \ln q_{HD} = \Omega \quad (\text{Grand potential})$$

$$q_{HD} = e^{-\Omega/kT}$$

$$\frac{\Omega_{HD}}{kT} = -\frac{q_{HD} V}{(2\pi h)^3} - \frac{pV}{kT} = \frac{2V}{\lambda_T^3} f_{5/2}(e^{\beta \mu_F})$$

$$\lambda_{HD} = \left(\frac{2\pi h^2}{m_{HD} kT} \right)^{1/2}$$

$$q_{HD}^{(tr)} = e^{-\Omega_{HD}/kT}$$

$$\frac{\Omega_{HD}}{kT} = \frac{2V}{\lambda_{HD}^3} f_{5/2}(z) \quad z = e^{\beta \mu_F}$$

$$q_{HD}^{(rot)} = \sum_J (2J+1) e^{-\beta B_{HD} J(J+1)}$$

$$q_{HD}^{(vib)} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega_{HD} (n+1/2)} = \frac{e^{-\beta \hbar \omega_{HD}/2}}{1 - e^{-\beta \hbar \omega_{HD}}}$$

$$q_{D_1}^{(tr)} = e^{-\Omega_{D_1}/kT}$$

$$\frac{\Omega_{D_1}}{kT} = + \ln(1-z) - \frac{V}{\lambda_{D_1}^3} g_{5/2}(z)$$

$$q_{D_1}^{(rot)} = 6 \sum_{J=1}^{\infty} (2J+1) e^{-\beta B_{D_1} J(J+1)} + 3 \sum_{J=1}^{\infty} e^{-\beta B_{D_1} J(J+1)}$$

$$q_{D_1}^{(vib)} = \frac{e^{-\beta \hbar \omega_{D_1}/2}}{1 - e^{-\beta \hbar \omega_{D_1}}}$$

$$q_{H_2}^{(tr)} = e^{-\Omega_{H_2}/kT}$$

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$$\Omega_{H_2} = \ln(1-f) - \frac{V}{\lambda_{H_2}^3} q_{H_2}(T)$$

$$q_{H_2}^{(rot)} = \sum_S^{(even)} (15+1) e^{-\beta B S(S+1)} + 3 \sum_S^{(odd)} (15+1) e^{-\beta B S(S+1)}$$

$$q_{H_2}^{(vib)} = \frac{e^{-\beta \hbar \omega_{H_2}}}{1 - e^{-\beta \hbar \omega_{H_2}}}$$

$$k(T) = e^{-\frac{(\Omega_{HD} - \Omega_{H_2} - \Omega_{D_2})}{kT}} \frac{(q_{H_2}^{rot})^2}{q_{H_2}^{rot} q_{D_2}^{rot}} \frac{e^{-\beta \left[\hbar \omega_{HD} + \frac{\omega_{H_2} - \omega_{D_2}}{2} \right]}}{(1 - e^{-\beta \hbar \omega_{HD}})} \times (1 - e^{-\beta \hbar \omega_{H_2}}) (1 - e^{-\beta \hbar \omega_{D_2}})$$

$$2\mu_{HD} = \mu_{H_2} + \mu_{D_2}$$

• $H_2 \rightarrow \text{~~1, 0~~ nuclear spin: 1, 0}$

degeneracy 3, 1 $\Rightarrow$ 4 components

$D_2 \rightarrow$ has lower T_c since mass is bigger

$$(recall T_c \approx \left(\frac{205^2}{m_{H_2}} \right) \left(\frac{\langle \ln \rangle}{g_{3H_2}(1)} \right)^{2/3})$$

$\Rightarrow$ at same $\langle \ln \rangle$ D_2 would have lower T_c

3 1D Ising model

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ground state energy:

$$E = -NJ$$

Flip one spin:

$$E = -NJ + 4J \rightarrow$$

possible energies determined $\Rightarrow$ has same energy $\Rightarrow$

$\uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \dots$

$\uparrow \uparrow \downarrow \uparrow \uparrow \dots$

Switch to bond representation

$\uparrow \uparrow \downarrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow$

bonds connecting parallel spins: p

anti-parallel: a

both have same number of anti-parallel bonds

$$E = -pJ + aJ = J(a - p) = Ja - J(N - a) = -JN + 2Ja$$

number of anti-parallel bonds always even

$$E(a) = J(a - p) \quad a = 0, 2, 4, \dots$$

For a particular number of bonds connecting antiparallel spins we have

$$\Omega(a) = \frac{N!}{a! p!} \approx \frac{N!}{a! (N-a)!}$$

$$S = k \ln \Omega \approx k N \ln N - a \ln a - (N-a) \ln (N-a)$$

$$E = -JN + 2Ja \Rightarrow a = \frac{E + JN}{2J} \rightarrow N-a = \frac{N}{2} - \frac{E}{2J}$$

$$S = k N \ln N - \left(\frac{N}{2} + \frac{E}{2J} \right) \ln \left(\frac{N}{2} + \frac{E}{2J} \right) - \left(\frac{N}{2} - \frac{E}{2J} \right) \ln \left(\frac{N}{2} - \frac{E}{2J} \right)$$

- calculate dimer-dimer c.f.

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$$D_{ijkl} = \langle \sigma_i \sigma_{i+1} \sigma_j \sigma_{j+1} \rangle - \langle \sigma_i \sigma_{i+1} \rangle \langle \sigma_j \sigma_{j+1} \rangle$$

- solved using idea of transfer matrix

$$Q = \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{+J \sigma_1 \sigma_2} \dots e^{+J \sigma_{N-1} \sigma_N}$$

for P.B.C.

$$Q = \text{Tr}[T^N]$$

$$T = \begin{pmatrix} e^J & e^{-J} \\ 0 & e^J \end{pmatrix}$$

diagonalize:

$$(e^J - \lambda)^2 = e^{-2J}$$

$$e^J - \lambda = \pm e^{-J}$$

$$\lambda = \underbrace{2 \cosh J}_{\lambda_0}, \underbrace{2 \sinh J}_{\lambda_1}$$

$$Q = \lambda_0^N + \lambda_1^N$$

$$N \rightarrow \infty \quad Q \sim \lambda_0^N$$

$$\begin{aligned} \langle \sigma_i \sigma_{i+1} \rangle &= \frac{1}{Q} \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{+J \sigma_1 \sigma_2} \dots e^{+J \sigma_{i-1} \sigma_i} \sigma_i e^{+J \sigma_i \sigma_{i+1}} \sigma_{i+1} e^{+J \sigma_{i+1} \sigma_{i+2}} \dots e^{+J \sigma_{N-1} \sigma_N} \\ &= \frac{\text{Tr}[T^{i-1} F T^{N-i}]}{\text{Tr}[T^N]} = \frac{\text{Tr}[F T F T^{N-1}]}{\text{Tr}[T^N]} \xrightarrow{\text{cyclic invariance of trace}} \frac{\text{Tr}[F]}{\text{Tr}[T]} \end{aligned}$$

diagonal in F, not diagonal in T

need eigenvectors of T

$$\begin{pmatrix} e^J & e^{-J} \\ 0 & e^J \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\begin{aligned} e^J x + e^{-J} y &= \lambda x \\ e^J y &= \frac{\lambda - e^J}{e^{-J}} \Rightarrow \frac{1}{\sqrt{e^J + (\lambda - e^J)^2}} \begin{pmatrix} e^{-J} \\ \lambda - e^J \end{pmatrix} \end{aligned}$$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\sqrt{e^{-2\tau} + (\lambda - e^{\tau})^2}} \begin{pmatrix} e^{-\tau} \\ \lambda - e^{\tau} \end{pmatrix}$$

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$$\lambda_0 \Rightarrow \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} = \frac{1}{\sqrt{e^{-2\tau} + e^{-2\tau}}} \begin{pmatrix} e^{-\tau} \\ e^{-\tau} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\lambda_1 \Rightarrow \begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \frac{1}{\sqrt{2e^{-2\tau}}} \begin{pmatrix} e^{-\tau} \\ -e^{-\tau} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$\begin{aligned} & \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} e^{\tau} & e^{-\tau} \\ e^{-\tau} & e^{\tau} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 2\cosh\tau & 2\sinh\tau \\ 2\cosh\tau & -2\sinh\tau \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 4\cosh\tau & 0 \\ 0 & 4\sinh\tau \end{pmatrix} = \begin{pmatrix} 2\cosh\tau & 0 \\ 0 & 2\sinh\tau \end{pmatrix} \end{aligned}$$

transform F

$$\begin{aligned} & \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\ &= \frac{1}{2} \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \end{aligned}$$

$$\langle \sigma_i, \sigma_{i+1} \rangle = \frac{\text{Tr} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix}^{n-1}}{Q}$$

$$= \text{Tr} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0^{n-1} & 0 \\ 0 & \lambda_1^{n-1} \end{pmatrix}$$

$$= \frac{\text{Tr} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & \lambda_1^{n-1} \\ \lambda_0^{n-1} & 0 \end{pmatrix}}{Q} = \frac{\text{Tr} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda_0 \lambda_1^{n-1} \\ \lambda_1 \lambda_0^{n-1} & 0 \end{pmatrix}}{Q} = \frac{\lambda_1 \lambda_0^{n-1} + \lambda_0 \lambda_1^{n-1}}{Q}$$

$$\langle \sigma_i \sigma_{i+m} \rangle = \frac{\lambda_1 \lambda_0^{m-1} + \lambda_0 \lambda_1^{m-1}}{\lambda_0^m + \lambda_1^m} \quad \approx$$

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as $N \rightarrow \infty$

$$\langle \sigma_i \sigma_{i+1} \rangle = \frac{\lambda_0}{\lambda_1}$$

for dimer-dimer c.t.

$$\langle \sigma_i \sigma_{i+1} \sigma_j \sigma_{j+1} \rangle = \langle \sigma_1 \sigma_2 \sigma_j \sigma_{j+1} \rangle$$

$$= \frac{\text{Tr}(F T F T^{j-2} F T F T^{N-j})}{\text{Tr} T^N}$$

$$= \text{Tr} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0^{j-2} & 0 \\ 0 & \lambda_1^{j-2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0^{N-j} & 0 \\ 0 & \lambda_1^{N-j} \end{pmatrix} \right]$$

Q

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$$F T F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \lambda_0 & 0 \\ 0 & \lambda_1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \lambda_0 \\ \lambda_1 & 0 \end{pmatrix} \\ = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_0 \end{pmatrix}$$

$$= \text{Tr} \left[\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_0 \end{pmatrix} \begin{pmatrix} \lambda_0^{j-2} & 0 \\ 0 & \lambda_1^{j-2} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_0 \end{pmatrix} \begin{pmatrix} \lambda_0^{N-j} & 0 \\ 0 & \lambda_1^{N-j} \end{pmatrix} \right]$$

Q

$$= \frac{\lambda_1 \lambda_0^{j-2} \lambda_1 \lambda_0^{N-j} + \lambda_0 \lambda_1^{j-2} \lambda_0 \lambda_1^{N-j}}{\lambda_0^N + \lambda_1^N} = \frac{\lambda_1^2 \lambda_0^{N-2} + \lambda_0^2 \lambda_1^{N-2}}{\lambda_0^N + \lambda_1^N}$$

as $N \rightarrow \infty$

$$\left(\frac{\lambda_1}{\lambda_0} \right)^2$$

$$\langle \sigma_i \sigma_{i+1} \sigma_j \sigma_{j+1} \rangle = \langle \sigma_i \sigma_{i+1} \rangle \langle \sigma_j \sigma_{j+1} \rangle = 0$$

4. Landau theory of phase transitions

(12)

$$G(\eta, T) = A_0(\eta, T) + A_1(\eta, T)\eta + A_2(\eta, T)\eta^2 + A_3(\eta, T)\eta^3 + A_4(\eta, T)\eta^4$$

$$\bullet \quad \frac{\partial G}{\partial \eta} = A_1 + 2A_2\eta + 3A_3\eta^2 + 4A_4\eta^3 = 0 \quad (\text{minimum})$$

no minimum exists at $\eta = 0 \Rightarrow$ but disordered state corresponds to $\eta = 0$ (definition of order parameter), well unless $A_1 = 0$

$$\bullet \quad A_3 = 0$$

$$G = A_0 + A_2\eta^2 + A_4\eta^4$$

$A_4 > 0 \Rightarrow$ otherwise order parameter (η) can diverge

if $A_2 > 0$ function will have one minimum $\eta = 0$

if $A_2 < 0$ two minima at finite η , one maximum at $\eta = 0$

$$\frac{\partial G}{\partial \eta} = 2A_2\eta + 4A_4\eta^3 = 0$$

$$A_2 + 2A_4\eta^2 = 0 \quad \eta = \pm \sqrt{\frac{-A_2}{2A_4}}$$

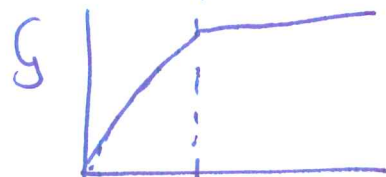
for $A_2 = 0$ extremes become one minimum

$$\text{below } T_c \quad \eta = \pm \sqrt{\frac{a(T_c - T)}{2A_4}}$$

$$G = A_0 + \frac{A_2 a(T_c - T)}{2A_4} + \frac{a^2 (T_c - T)^2}{4A_4^2}$$

above T_c

$$G = A_0$$



at T_c G changes slope! only (no latent heat)

• free energy:

$$G = A_0 + A_2 \eta^2 + A_3 \eta^3 + A_4 \eta^4$$

$A_4 > 0$ so η cannot diverge

$$\frac{\partial G}{\partial \eta} = 2A_2 \eta + 3A_3 \eta^2 + 4A_4 \eta^3 = 0$$

$\eta = 0$ one solution

other solutions:

$$2A_2 + 3A_3 \eta + 4A_4 \eta^2 = 0$$

$$\eta = \frac{-3A_3 \pm \sqrt{9A_3^2 - 4(4A_4)(2A_2)}}{8A_4}$$

$$= \frac{-3A_3 \pm \sqrt{9A_3^2 - 32A_2A_4}}{8A_4}$$

three extrema:

$$\eta = 0, \quad \frac{-3A_3 \pm \sqrt{9A_3^2 - 32A_2A_4}}{8A_4}$$

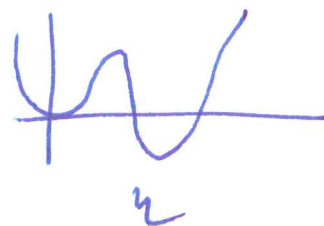
Function G ~~goes to~~ $\rightarrow \infty$ as $\eta \rightarrow \infty$, or $\eta \rightarrow -\infty$

$\rightarrow$ three extrema can be

one minimum, one maximum, one minimum

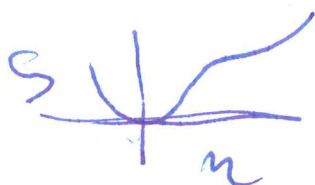
$$\Rightarrow T < T_{PT}$$

T_{PT} = phase transition T

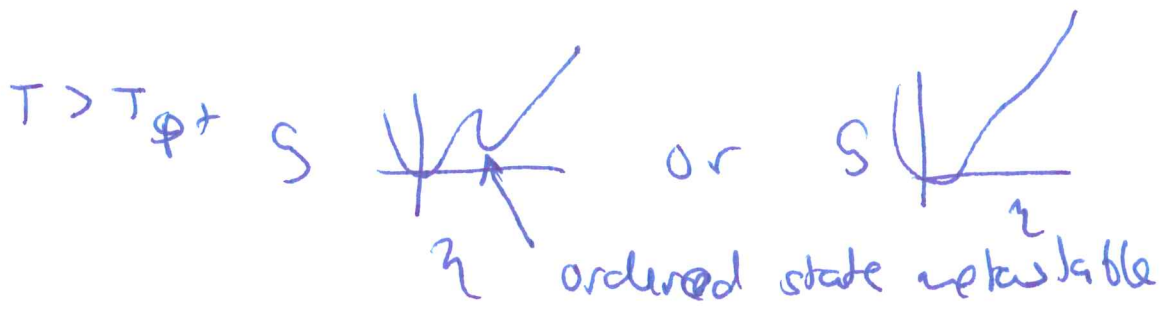
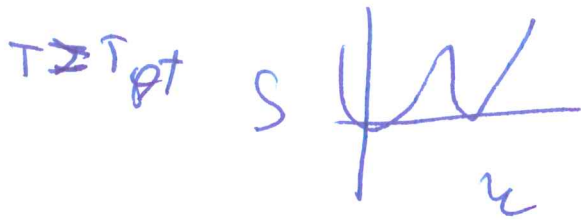


if $\sqrt{9A_3^2 - 32A_2A_4} = 0$

then the maximum and minimum form inflection point

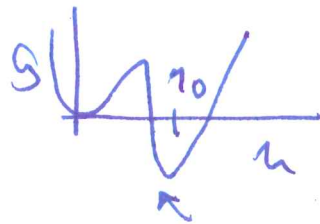


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- hysteresis is a result of metastability, since the system remains in the minimum in which the experiment was started, even though after passing the critical point, that minimum may not be the global minimum

example: suppose we are at some T where



in this case system would be in state q_0 (global minimum)

if we change $T \Rightarrow$

system may remain in q_0 , even though q_0 is no longer the global minimum

$\Rightarrow$ 1st order p.t.

• 3D

$$E = \int \delta(\epsilon) h(\epsilon) d\epsilon$$

$h(\epsilon)$ - FD distribution

$$f(\epsilon) = \frac{1}{1 + e^{\beta(\epsilon - \mu)}}$$

$$h(\epsilon) = 4\pi \left(\frac{2m}{h^2} \right)^{3/2} V \epsilon^{3/2} \quad (\text{density of states } \epsilon)$$

$$E = - \int_0^\infty f'(\epsilon) H(\epsilon) d\epsilon$$

$$H(\epsilon) = \int_0^\epsilon h(\epsilon') d\epsilon' = 4\pi \left(\frac{2m}{h^2} \right)^{3/2} V \frac{\epsilon^{5/2}}{5/2}$$

$$f'(\epsilon) = \frac{-\beta e^{\beta(\epsilon - \mu)}}{(1 + e^{\beta(\epsilon - \mu)})^2} = \underbrace{\frac{8\pi}{5} \left(\frac{2m}{h^2} \right)^{3/2} V}_{A} \epsilon^{5/2}$$

$$E = - \int_0^\infty d\epsilon A \epsilon^{5/2} \frac{e^{\beta(\epsilon - \mu)}}{(1 + e^{\beta(\epsilon - \mu)})^2}$$

expand $H(\epsilon) \approx H(\epsilon_F) + (\epsilon - \epsilon_F) H'(\epsilon_F) + \frac{(\epsilon - \epsilon_F)^2}{2} H''(\epsilon_F)$

$$E = - H(\epsilon_F) + \frac{\beta H''(\epsilon_F)}{2} \int_0^\infty \frac{d\epsilon (\epsilon - \epsilon_F)^2 e^{\beta(\epsilon - \epsilon_F)}}{(1 + e^{\beta(\epsilon - \epsilon_F)})^2}$$

$$x = \beta(\epsilon - \epsilon_F)$$

$$dx = \beta d\epsilon \Rightarrow d\epsilon = \frac{dx}{\beta}$$

$$= H(\epsilon_F) + \frac{H''(\epsilon_F)}{\beta^2 2} \int_{-\infty}^\infty \frac{dx x^2 e^x}{(1 + e^x)^2}$$

$$= H(\epsilon_F) + \frac{H''(\epsilon_F)}{202} \frac{\pi^2}{3}$$

$$E = H(\epsilon_f) + \frac{\pi^2}{6\beta^2} H^4(\epsilon_f)$$

$$H(\epsilon_f) = A \epsilon_f^{5/2}$$

$$H'(\epsilon_f) = \frac{5A}{2} \epsilon_f^{3/2}$$

$$H''(\epsilon_f) = \frac{15A}{4} \epsilon_f^{1/2}$$

$$A = \frac{8\pi}{5} \left(\frac{2m}{h^2} \right)^{3/2} V$$

$$E = A \left(\epsilon_f^{5/2} + \frac{15}{24} \frac{\pi^2}{\beta^2} \epsilon_f^{1/2} \right)$$

$$= A \left(\epsilon_f^{5/2} + \frac{5\pi^2}{8\beta^2} \epsilon_f^{1/2} \right)$$

$$C_V = \frac{\partial E}{\partial T} = A \epsilon_f^{1/2} \frac{5\pi^2}{4} \frac{T}{k^2} = \frac{28\pi}{5} \left(\frac{2m}{h^2} \right)^{3/2} V \epsilon_f^{1/2} \frac{5\pi^2}{4} \frac{T}{k^2}$$

$$= \frac{2\pi^3 V \epsilon_f^{1/2} (2m)^{3/2}}{h^3 k^2} T$$

for ~~two~~ 2D

$$h(\epsilon) = 2\pi m \epsilon$$

$$H(\epsilon_f) = \frac{4\pi m \epsilon_f^2}{2} = 2\pi m \epsilon_f^2$$

$$E = 4\pi m \epsilon_f^2$$

$$\cancel{C_V \sim 0 \text{ as } T \rightarrow 0}$$

$$E = 2\pi m \epsilon_f^2 + \frac{2\pi m}{2} \int_{-\infty}^{\infty} d\epsilon (\epsilon - \epsilon_f)^2 \delta'(\epsilon)$$

$$= 2\pi m \epsilon_f^2 + \pi m \int_{-\infty}^{\infty} d\epsilon (\epsilon - \epsilon_f)^2 \frac{e^{\beta(\epsilon - \epsilon_f)}}{(e^{\beta(\epsilon - \epsilon_f)} + 1)^2}$$

$$= 2\pi m \epsilon_f^2 + \frac{\pi m}{\beta^2} \frac{\pi^2}{3} = 2\pi m \epsilon_f^2 + \frac{\pi^3 m}{3\beta^2}$$

$$C_V = \frac{2\pi^3 m T}{3h^2}$$

$$\langle S^x | n(i) n(i') | K S \rangle$$

$$= \langle KS | C_r^\dagger C_r C_{r'}^\dagger C_{r'} | KS \rangle$$

$$= \sum_{k, k', k'', k'''} \langle \psi | c_k^\dagger c_{k'} c_{k''}^\dagger c_{k'''} | \psi \rangle e^{i(k-k') \cdot r + (k''-k''') \cdot r'}$$

Two since Fermi Sea is $C_{n_1}^\dagger \dots C_{n_N}^\dagger |FS\rangle$

with $h_i \leq h_k \quad \forall i=1, \dots, n$

~~we can write~~

we know that only two ways give a contribution

either $k \sim k'$ $k'' = k'''$

Or $h = h''' \quad k' = h''$

$$= \sum_{nh'} \langle ks | c_n^\dagger c_n c_{n'}^\dagger c_{n'} | ks \rangle = \langle ks | c_n^\dagger c_{n'} c_{n'}^\dagger c_n | ks \rangle \times$$

$$\times e^{i(k-h') \cdot (r-r')}$$

$$= \left(\sum_n \eta_n \right)^2 + \left(\sum_n \eta_n e^{ik(r-r')} \right)^2$$

In thermodynamic limit

In thermodynamic limit

$$\left[\frac{1}{(2\pi)^3} \int d^3k \, n_k \right]^2 - \left(\frac{1}{(2\pi)^3} \right)^2 \left[\int d^3k \, n_k e^{i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \right]^2$$

$n_k \approx 1$
 ω

$k < k_F$
 $k > k_F$

6. Renormalization group theory

- $\sigma_I' = A(\sigma_i; i \in I)$

- $e^{-\beta H'(\sigma_I')} = \sum_{\sigma_i \in \Omega_i'} e^{-\beta H(\sigma_i)}$

$\sigma_i \rightarrow$ sum over configurations consistent

with renormalization group transformation

- $\vec{k}' = \vec{R}(\vec{k})$

fixed points: $\vec{k}^* = \vec{R}(\vec{k}^*)$

- attractive fixed points: points nearby tend
toward fixed point

examples: ordered / disordered states (high-T
low-T)

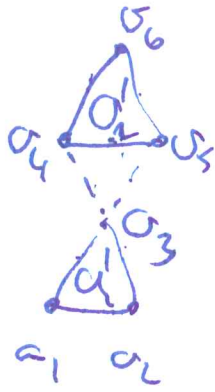
- repulsive fixed points: points nearby tend away from
fixed point

- mixed fixed points

• attractive in some directions
repulsive in other directions

- locally critical point on critical surface
is a mixed fixed point

• RGr of triangular lattice



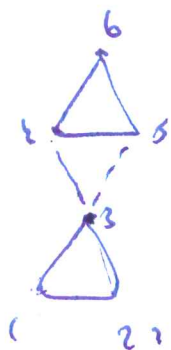
σ_1'	σ_2'	σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	
1	1	1	1	1	1	1	1	$e^{-8\gamma}$
		1	1	1	1	1	1	$e^{-4\gamma}$
		1	1	1	1	1	1	$e^{-2\gamma}$
		1	1	1	1	1	1	$e^{-2\gamma}$
		1	1	1	1	1	1	1
		1	1	1	1	1	1	$e^{-4\gamma}$
		1	1	1	1	1	1	$e^{-4\gamma}$
		1	1	1	1	1	1	$e^{4\gamma}$
		1	1	1	1	1	1	$e^{2\gamma}$
		1	1	1	1	1	1	$e^{2\gamma}$
		1	1	1	1	1	1	1
		1	1	1	1	1	1	$e^{2\gamma}$
		1	1	1	1	1	1	$e^{2\gamma}$
		1	1	1	1	1	1	$e^{2\gamma}$
		1	1	1	1	1	1	$e^{2\gamma}$

$$Z(\gamma) e^{-\gamma'} = e^{-8\gamma} + 3e^{-4\gamma} + 7e^{-2\gamma} + 3e^{2\gamma} + e^{4\gamma}$$

2

$f(s)e^{s'}$

a_1'	a_2'	a_1	a_2	a_3	a_4	a_5	a_6	
1	-1	1	1	1	1	-1	-1	e^{-4s} e^{-7s}
		1	1	1	-1	1	-1	e^{-7s}
		1	1	1	-1	-1	1	1
		1	1	1	-1	-1	-1	e^{-4s}
		1	1	-1	1	-1	-1	e^{+2s}
		1	1	-1	-1	1	-1	e^{+2s}
		1	1	-1	-1	-1	1	1
		1	1	-1	-1	-1	-1	e^{-4s}
		1	-1	1	-1	-1	-1	e^{2s}
		1	-1	1	-1	1	-1	e^{2s}
		1	-1	1	-1	-1	1	e^{4s}
		1	-1	1	-1	-1	-1	1
		-1	1	1	1	-1	-1	e^{2s}
		-1	1	1	-1	1	-1	e^{7s}
		-1	1	1	-1	-1	1	e^{4s}
		-1	1	1	-1	-1	-1	1



$$f(s)e^{s'} = 2e^{-4s} + 7e^{-7s} + 4 + 6e^{2s} + 7e^{4s}$$

$$e^{-2s'} = \frac{e^{-8s} + 3e^{-4s} + 7e^{-7s} + 3 + 6e^{7s} + e^{4s}}{2e^{-4s} + 7e^{-7s} + 4 + 6e^{7s} + 7e^{4s}}$$

$$\sigma' = \frac{1}{2} \ln \left[\frac{2e^{-4s} + 7e^{-7s} + 4 + 6e^{7s} + 7e^{4s}}{e^{-8s} + 3e^{-4s} + 7e^{-7s} + 3 + 6e^{7s} + e^{4s}} \right]$$

fixed pts.

$$T = 0$$

$$T' = \frac{1}{2} \ln 1 = 0 \quad (\text{high-}T \text{ fixed pt.})$$

$$T \rightarrow \infty \quad \text{no fixed pt.}$$

but

$$T \rightarrow -\infty \quad T' \rightarrow -\infty \quad (\text{low-}T \text{ fixed pt.})$$

for ferromagnetic model

$$T'_c \sim -.37$$