4-3 Other Examples

⊙ phonon

a solid consisting of N atoms

ith atom : mass m_i

equilibrium position $\vec{r}_i^{(0)} = (x_{i1}^{(0)}, x_{i2}^{(0)}, x_{i3}^{(0)})$

$1, 2, 3 \rightarrow x, y, z$

diplacement $\vec{\xi}_i = \vec{r}_i - \vec{r}_i^{(0)}$

$$\xi_{i\alpha} = x_{i\alpha} - x_{i\alpha}^{(0)}$$

→ kinetic energy $K = \frac{1}{2}\sum_{i=1}^{N}\sum_{\alpha=1}^{3} m_i \dot{x}_{i\alpha}^2 = \frac{1}{2}\sum_{i=1}^{N}\sum_{\alpha=1}^{3} m_i \dot{\xi}_{i\alpha}^2$

potential energy $V = V_0 + \underbrace{\sum_{i\alpha}\left[\frac{\partial V}{\partial x_{i\alpha}}\right]_0 \xi_{i\alpha}}_{=0} + \frac{1}{2}\sum_{i\alpha, j\gamma}\left[\frac{\partial^2 V}{\partial x_{i\alpha}\partial x_{j\gamma}}\right]_0 \xi_{i\alpha}\xi_{j\gamma} + \cdots$

($\because$ V has a minimum value at $\vec{r}_i^{(0)}$)

$$\simeq V_0 + \frac{1}{2}\sum_{i\alpha, j\gamma} A_{i\alpha, j\gamma}\,\xi_{i\alpha}\xi_{j\gamma}$$

↓ normal mode transformation (diagonalization)

$$\xi_{i\alpha} = \sum_{r=1}^{3N} B_{i\alpha, r}\, q_r$$

total # of normal mode ~ fixed as $3N$.

"collective excitation"

$\Rightarrow H_{tot} = K + V$

$$= V_0 + \frac{1}{2}\sum_{r=1}^{3N}(\dot{q}_r^2 + \omega_r^2 q_r^2)$$

quantization $\Rightarrow$ $[a_i, a_j^\dagger] = 1\cdot\delta_{ij}$, bosonic excitation

$$E_{n_1,\dots,n_{3N}} = V_0 + \sum_{r=1}^{3N}(n_r + \tfrac{1}{2})\hbar\omega_r$$

$\because\left(H_r = \frac{1}{2}(\dot{q}_r^2 + \omega_r^2 q_r^2) \longrightarrow \epsilon_r = (n_r + \tfrac{1}{2})\hbar\omega_r \quad n_r = 0, 1, 2, \dots\right)$

$$= -N\eta + \frac{1}{2}\sum_r \hbar\omega_r n_r$$

η ⟶ binding energy per atom in the solid at $T=0$.

$\Rightarrow Z = \sum_{n_1, n_2, \dots} e^{-\beta[-N\eta + n_1\hbar\omega_1 + n_2\hbar\omega_2 + \cdots + n_{3N}\hbar\omega_{3N}]}$

$$= e^{\beta N\eta}\prod_{r=1}^{3N}\left(\frac{1}{1 - e^{-\beta\hbar\omega_r}}\right)$$

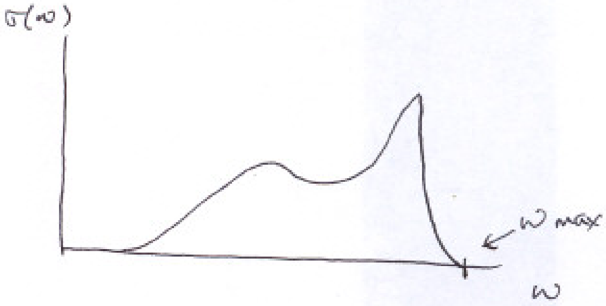
$$\Rightarrow \ln Z = \beta N q - \sum_{r=1}^{3N} \ln(1-e^{-\beta\hbar\omega_r})$$

continuum approximation (spacing between $\omega_r \ll kT$)

$$= \beta N q - \int_0^\infty \ln(1-e^{-\beta\hbar\omega_r})\, \underbrace{\sigma(\omega)}_{\text{phonon densities of state}}\, d\omega$$

$$\bar{E} = -\frac{\partial \ln Z}{\partial \beta} = -Nq + \int_0^\infty \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}\,\sigma(\omega)\,d\omega$$

$$C_V = \left(\frac{\partial \bar{E}}{\partial T}\right)_V = -k\beta^2\left(\frac{\partial \bar{E}}{\partial \beta}\right)_V = +k\int_0^\infty \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}(\beta\hbar\omega)^2\,\sigma(\omega)\,d\omega$$



$\sigma(\omega) = 0$ if $\omega > \omega_{max}$

if $\beta\hbar\omega_{max} \ll 1$

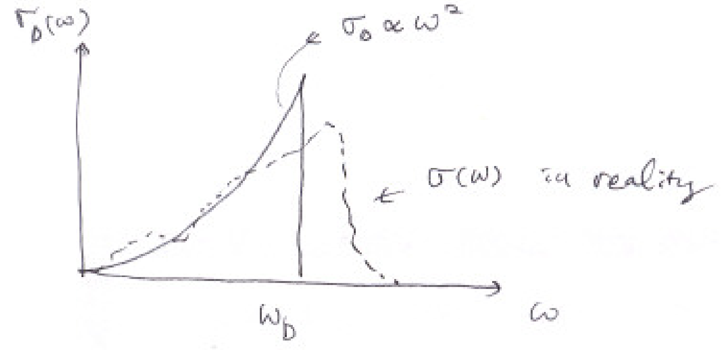
$$e^{\beta\hbar\omega} \simeq 1 + \beta\hbar\omega$$

$$\Rightarrow \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}\cdot(\beta\hbar\omega)^2 \simeq 1.$$

$$\Rightarrow C_V = k\underbrace{\int_0^\infty \sigma(\omega)\,d\omega}_{=3N} = 3Nk.$$

(* equipartition theorem. → $\frac{1}{2}kT \times 2 \times 3N = \bar{E}$)

Debye approximation



λ : normal mode (phonon) wave length
a : lattice spacing

$\lambda \gg a$ → phonon ≃ normal mode of elastic continuum.

→ Sound wave $\omega = c_s k$

$$\sigma_D(\omega)\,d\omega = 3 \cdot \frac{V}{(2\pi)^3} 4\pi k^2\,dk = 3 \cdot \frac{V}{2\pi^2 c_s^3}\,\omega^2 d\omega$$

↑
2 ⊗ transverse mode
1 ⊗ longitudinal

$\lambda \lesssim a$ → no mode

$$\Rightarrow \sigma_D(\omega) = \begin{cases} 3 \cdot \dfrac{V}{2\pi^2 c_s^3}\,\omega^2 & \text{for } \omega < \omega_D \\ 0 & \text{for } \omega > \omega_D \end{cases}$$

"Debye approximation"

$$\int_0^\infty \sigma_D(\omega)\,d\omega = 3N \Rightarrow \frac{3V}{2\pi^2 c_s^3}\int_0^{\omega_D} \omega^2 d\omega = \frac{V\omega_D^3}{2\pi^2 c_s^3} = 3N$$

$$\rightarrow \omega_D = c_s \left(6\pi^2 \frac{N}{V}\right)^{1/3}$$

$$C_V = \left(\frac{\partial \bar{E}}{\partial T}\right)_V = k\int_0^\infty \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}(\beta\hbar\omega)^2\,\sigma(\omega)\,d\omega$$

$$= k\int_0^{\omega_D} \frac{e^{\beta\hbar\omega}(\beta\hbar\omega)^2}{(e^{\beta\hbar\omega}-1)^2}\,\frac{3V}{2\pi^2 C_s^3}\,\omega^2\,d\omega$$

$$= k\cdot\frac{3V}{2\pi^2(C_s\beta\hbar)^3}\int_0^{\beta\hbar\omega_D}\frac{e^x x^4}{(e^x-1)^2}\,dx \qquad x=\beta\hbar\omega$$

using $\omega_D = C_s\left(6\pi^2\frac{N}{V}\right)^{1/3}$, $\left(\Rightarrow\ V = 6\pi^2 N\cdot\left(\frac{C_s}{\omega_D}\right)^3\right)$

$$C_V = 3Nk\, f_D\left(\frac{\Theta_D}{T}\right)$$

$$\left(\begin{array}{l} f_D(y) \equiv \dfrac{3}{y^3}\displaystyle\int_0^y \frac{e^x x^4}{(e^x-1)^2}\,dx \quad \sim \text{Debye function} \\ k\Theta_D = \hbar\omega_D \quad \sim \text{Debye temperature}\end{array}\right.$$

- high temperature limit. $\frac{\Theta_D}{T} \ll 1$.

$$\Rightarrow f_D\left(\frac{\Theta_D}{T}\right) \simeq \frac{3}{y^3}\int_0^y x^2\,dx = 1.$$

$$\Rightarrow C_V = 3Nk \quad \sim \text{classical result.}$$

- low temperature limit. $\frac{\Theta_D}{T} \gg 1$

$$f_D\left(\frac{\Theta_D}{T}\right) \simeq 3\left(\frac{T}{\Theta_D}\right)^3\cdot\underbrace{\int_0^\infty \frac{e^x x^4}{(e^x-1)^2}\,dx}_{=\frac{4\pi^4}{15}}$$

(see Appendix A.11)

$$\Rightarrow C_V \propto T^3$$

$$\left(C_V = \frac{12\pi^4}{5}Nk\left(\frac{T}{\Theta_D}\right)^3\right)$$

$$C_V = \underbrace{\alpha T}_{\text{electron contribution}} + \underbrace{\gamma T^3}_{\text{phonon contribution}}$$

⊙ Ferromagnetism

A solid consisting of N identical atoms arranged in a regular lattice.

$\vec{S}_i$: a net electronic spin of the ith atom

$\vec{\mu}_j$: magnetic moment. $\vec{\mu}_j = g\mu_0 \vec{S}_j$

(g : g-factor
μ_0 : Bohr magneton

external magnetic field $\vec{H}_0$

⇒ Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$

$$\mathcal{H}_0 = -\sum_{j=1}^{N} \vec{\mu}_j \cdot \vec{H}_0 = -g\mu_0 H_0 \sum_{j=1}^{N} S_{jz}$$

$$\mathcal{H}_1 = -J \sum \vec{S}_j \cdot \vec{S}_k$$

↳ exchange coupling :

originated from the Pauli exclusion principle

(Not from magnetic dipole-dipole interaction, which is negligible compared to the exchange coupling.)

(ex) two electronic spins, each at the same orbital of neighboring atoms

e ($\sigma = \uparrow$) e ($\sigma = \downarrow$)
× ×
atomic site 1 atomic site 2

~ no exclusion they can come close to each other
⇒ higher Coulomb ~~intera~~ interaction.

e ($\sigma = \uparrow$) e ($\sigma = \uparrow$) ~ exclusion
× ×

⇒ $\mathcal{H}_{12} = -J\vec{S}_1 \cdot \vec{S}_2$ ~ parallel spin alignment results in lower energy.

$J > 0$

※ J falls off rapidly with increasing separation between atoms.

∵ overlap between electrons ↓ as the separation ↑

⇒ One can consider only the nearest-neighbor interaction

Consider only z-directional spin : "Ising model"

$$\mathcal{H}_{12} \rightarrow \mathcal{H}_{12}' = -J \sum_{j,k} S_{jz} S_{kz}$$

$\rightarrow$ j and k ~ nearest-neighbor pair

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{12}'$$

~ Ising model

1 dimensional Ising model ~ exactly solvable

2 dimensional Ising model ⊕ $H_0 = 0$ ~ exactly solvable

3-dimensional Ising model - not yet exactly solved.

~ graduate-course level.

⊕ Weiss molecular-field approximation

Focus on a particular atom j.

$$\mathcal{H}_j = -g\mu_0 H_0 S_{jz} - 2J S_{jz} \sum_{k=1}^{n} S_{kz}$$

n : # of nearest neighboring atoms.

$$g\mu_0 H_m \equiv 2J \overline{\sum_{k=1}^{n} S_{kz}}$$ as an approximation. "mean field theory"

~ "molecular" field

$$\Rightarrow \mathcal{H}_j = -g\mu_0 (H_0 + H_m) S_{jz}$$

$\Rightarrow \quad E_m = -g\mu_0 (H_0 + H_m)\, m_s ,$

$$m_s = -S,\ (-S+1),\ (-S+2),\ \cdots,\ S$$

$$\Rightarrow \quad \overline{S_{jz}} = \frac{1}{g\mu_0}\, \overline{\mu_{jz}} = \frac{1}{g\mu_0}\, \frac{1}{\beta}\frac{\partial \ln Z_j}{\partial H_0}$$

$$Z_j = \sum_{m_s=-S}^{S} e^{-\beta E_m(m_s)} ,$$

consider : why do we use the canonical partition function for the fermionic systems?

$$\Rightarrow \quad \overline{S_{jz}} = S B_s(\eta)$$

$$\left(\begin{array}{l} \eta \equiv \beta g \mu_0 (H_0 + H_m) \\ B_s(\eta) \equiv \frac{1}{S}\left[\left(S+\frac{1}{2}\right)\coth\left(S+\frac{1}{2}\right)\eta - \frac{1}{2}\coth\frac{1}{2}\eta \right] \end{array} \right.$$

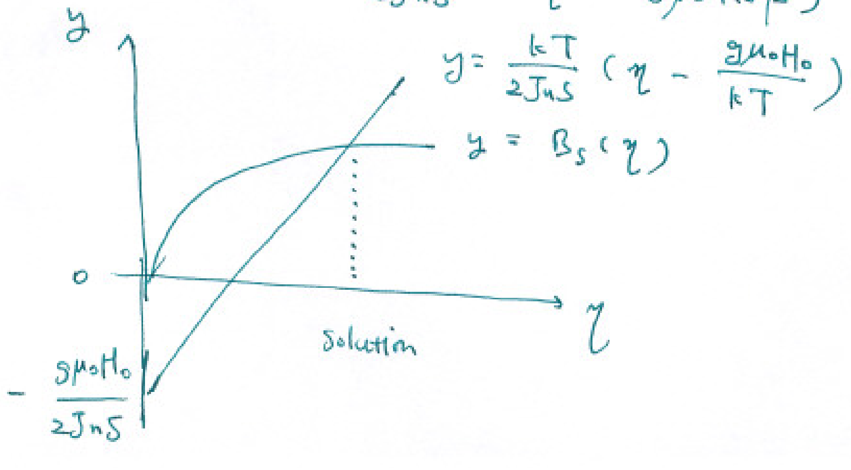
see Reif eq. (7.8.14)

Put this result into $g\mu_0 H_m \equiv 2J \overline{\sum_{k=1}^{n} S_{kz}}$

$$\Rightarrow \quad 2JnS\, B_s(\eta) = g\mu_0 H_m .$$

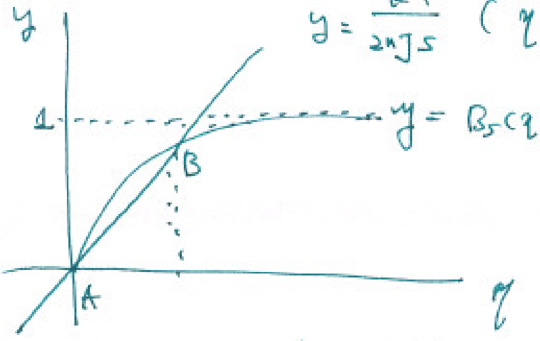
$$= kT\,(\eta - \beta g\mu_0 H_0)$$

$$\Rightarrow \quad B_s(\eta) = \frac{kT}{2JnS}\,(\eta - g\mu_0 H_0 \beta)$$



① the case of $H_0 = 0$

$$y = \frac{kT}{2nJS}\left(\eta - \frac{g\mu_0 H_0}{kT}\right) \to 0$$



$y = B_S(\eta)$

two solutions A and B.

A : no magnetization

B : spontaneous magnetization even at $H_0 = 0$

(no external field)

→ ferromagnetism

To have the solution B,

$$\left.\frac{dB_S(\eta)}{d\eta}\right|_{\eta=0} > \frac{kT}{2nJS}$$

When $\eta \ll 1$, $B_S(\eta) \simeq \frac{1}{3}(S+1)\eta$

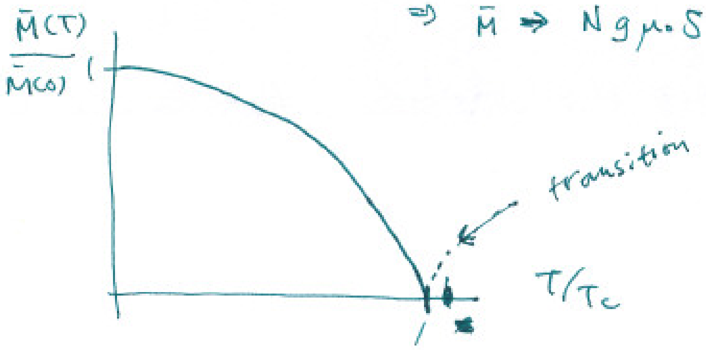
$$\Rightarrow \quad \frac{1}{3}(S+1) > \frac{kT}{2nJS}$$

$$\Rightarrow \quad kT < kT_c = \frac{2nJS(S+1)}{3}$$

~ possibility of ferromagnetism below T_c, "Curie temperature"

When $T \to 0$ $(\eta \to \infty)$, $B_S(\eta) \to 1$

$$\Rightarrow \bar{M} \to Ng\mu_0 S$$



∘ (At small H_0 / above $T>T_c$) $\Rightarrow$ $\eta \sim$ small

$$\Rightarrow \frac{1}{3}(S+1)\eta = \frac{kT}{2nJS}\left(\eta - \frac{g\mu_0 H_0}{kT}\right)$$

(from $B_S(\eta) = \frac{kT}{2nJS}\left(\eta - \frac{g\mu_0 H_0}{kT}\right)$, $B_S(\eta) \to \frac{1}{3}(S+1)\eta$)

$\Rightarrow$ using $kT_c = \frac{2nJS(S+1)}{3}$,

$$\eta = \frac{g\mu_0 H_0}{k(T-T_c)}$$

$$\bar{M} = \frac{1}{3} N g \mu_0 S(S+1)\eta \qquad (\because \bar{M} = N g \mu_0 \bar{S}_{jz} , \ \bar{S}_{jz} = S B(\eta))$$

$$\Rightarrow \chi = \frac{\bar{M}}{H_0} = \frac{N g^2 \mu_0^2 S(S+1)}{3k(T-T_c)}$$, magnetic susceptibility

$\sim$ " Curie-Weiss Law "

$\chi \to \infty$ as $T \to T_c$.

∘※∘ (Experimental results show different T_c , i.e. $T_c \neq \frac{2nJS(S+1)}{3}$ / The above results are not so correct.)

$\because$ the crude approximation
mean-field

∘※∘ discuss ∙ Goldstone mode

∙ low energy excitation . skyrmion

2f) Skyrmion.