

Exercise 1

8-05-13

$\hbar = m = e = 1$

$$\textcircled{1} \quad \epsilon_{\sigma} = \frac{\sum_{|k_{\sigma}| < k_{FO}} k^2/2}{\sum_{|k_{\sigma}| < k_{FO}} 1} = \frac{\frac{1}{2} \int_0^{k_{FO}} dk \, k \, k^2}{\int_0^{k_{FO}} dk \, k} = \frac{\frac{1}{2} \frac{k_{FO}^4}{4}}{\frac{k_{FO}^2}{2}} = \frac{1}{4} k_{FO}^2$$

$$\boxed{\epsilon_{\sigma} = \frac{1}{2} \epsilon_{FO} = \frac{1}{4} k_{FO}^2}$$

$$\frac{\pi k_{FO}^2}{(2\pi)^2} = N_{\sigma} = \frac{k_{FO}^2}{4\pi} A \Rightarrow \boxed{k_{FO}^2 = 4\pi \frac{N_{\sigma}}{A} = 4\pi n_{\sigma}}$$

$$t = \frac{\sum_{\sigma} N_{\sigma} \epsilon_{\sigma}}{N} = \sum_{\sigma} \frac{n_{\sigma} \epsilon_{\sigma}}{n} = \sum_{\sigma} \frac{n_{\sigma}}{n} \frac{1}{4} 4\pi n_{\sigma}$$

$$t = \pi \left[\frac{n_{\uparrow}^2}{n} + \frac{n_{\downarrow}^2}{n} \right]$$

$$\begin{aligned} \textcircled{3} \quad e(n, \mathcal{J}, B) &= \frac{1}{N} \left\{ Nt + \frac{U N_{\uparrow} N_{\downarrow}}{N} + \mu_B B (N_{\uparrow} - N_{\downarrow}) \right\} \\ &= t + U n_{\uparrow} n_{\downarrow} + \mu_B B (n_{\uparrow} - n_{\downarrow}) \frac{1}{n} \\ &= \pi \left(\frac{n_{\uparrow}^2}{n} + \frac{n_{\downarrow}^2}{n} \right) + \frac{U n_{\uparrow} n_{\downarrow}}{n^2} + \mu_B B \left(\frac{n_{\uparrow}}{n} - \frac{n_{\downarrow}}{n} \right) \\ e(n, \mathcal{J}, B) &= \frac{\pi}{4} n \left((1+\mathcal{J})^2 + (1-\mathcal{J})^2 \right) + \frac{1}{4} U (1+\mathcal{J})(1-\mathcal{J}) \\ &\quad + \frac{\mu_B B}{2} (1+\mathcal{J} - 1+\mathcal{J}) \end{aligned}$$

$$n = n_{\uparrow} + n_{\downarrow}, n\mathcal{J} = n_{\uparrow} - n_{\downarrow} \Rightarrow n_{\sigma} = \frac{n}{2} (1 + \sigma \mathcal{J}) \quad \sigma = \pm 1$$

$$e(n, \gamma, B) = \frac{\pi}{2} n (1 + \gamma^2) + \frac{U}{4} (1 - \gamma^2) + \mu_B B \gamma$$

④ Let's minimize $e(n, \gamma, B)$ with respect to γ , $-1 \leq \gamma \leq 1$

$$e(n, \gamma, B) = \frac{\pi}{2} n + \frac{U}{4} + \left(\frac{\pi}{2} n - \frac{U}{4} \right) \gamma^2 + \mu_B B \gamma$$

$$\frac{\partial e}{\partial \gamma} = 0 = \gamma \left(\pi n - \frac{U}{2} \right) + \mu_B B$$

$$\Rightarrow \gamma(n, B) = - \frac{\mu_B B}{\pi n - \frac{U}{2}} \quad B > 0$$

$$\frac{\partial^2 e}{\partial \gamma^2} = \pi n - \frac{U}{2} \geq 0 \quad \text{for } n \geq \frac{U}{2\pi}$$

- there is a local minimum when $n > \frac{U}{2\pi}$ at

$$\gamma^* = - \frac{\mu_B B}{\pi n - \frac{U}{2}} \geq -1 \quad \Rightarrow \quad B \leq \frac{1}{\mu_B} \left(\pi n - \frac{U}{2} \right)$$

$$e(n, \gamma^*, B) = \frac{\pi}{2} n + \frac{U}{4} + \left(\frac{\pi}{2} n - \frac{U}{4} \right) \frac{(\mu_B B)^2}{\left(\pi n - \frac{U}{2} \right)^2} - \frac{(\mu_B B)^2}{\pi n - \frac{U}{2}}$$

$$e(n, B) = \frac{\pi}{2} n + \frac{U}{4} - \frac{1}{2} \frac{(\mu_B B)^2}{\pi n - \frac{U}{2}} \quad B \leq \frac{\mu_B}{\pi n - \frac{U}{2}} = B_1$$

$$B > B_1 \quad e(n, B) = \frac{\pi}{2} n + \frac{U}{4} + \left(\frac{\pi}{2} n - \frac{U}{4} \right) (-1)^2 - \mu_B B$$

$$e(n, B) = \pi n - \mu_B B \quad B > \mu_B / \left(\pi n - \frac{U}{2} \right)$$

- When $n < U/2\pi$ there is no local minimum at J^* and it is evident that e is minimum at $J = -1$, the polarization that makes minima both

$$\left(\frac{\pi}{2}n - \frac{U}{4}\right)J^2 \text{ and } \mu_B B J!$$

$$e(n, B) = \pi n - \mu_B B \quad | \quad n < U/2\pi$$

$$\textcircled{5} \quad J = -\frac{\mu_B}{\pi n - \frac{U}{2}} B \quad \left. \begin{array}{l} B < \frac{\mu_B}{\pi n - \frac{U}{2}} \\ B > \frac{\mu_B}{\pi n - \frac{U}{2}} \end{array} \right\} n > \frac{U}{2\pi}$$

$$J = -1$$

$$\textcircled{6} \quad J = -1 \quad n < \frac{U}{2\pi}$$

$$\textcircled{2} \quad \frac{U}{n} \sigma(\bar{r}_i - \bar{r}_j) = \frac{U}{n} \delta(\bar{r}_i - \bar{r}_j)$$

$$\tilde{V} = \frac{1}{2} \sum_{i \neq j} \sigma(\bar{r}_i - \bar{r}_j) \quad V = \frac{U}{n} \tilde{V}$$

$$\langle SD | \tilde{V} | SD \rangle = \frac{1}{2} \sum_{\alpha \beta} \{ \langle \alpha \beta | \sigma | \alpha \beta \rangle - \langle \beta \alpha | \sigma | \alpha \beta \rangle \} \equiv \langle V \rangle$$

$$\alpha \equiv (\sigma, \bar{k}_\sigma) \quad \beta \equiv (\sigma', \bar{q}_{\sigma'})$$

$$\psi_{\sigma \bar{k}_\sigma}(s, \bar{r}) = \frac{1}{\sqrt{A}} \delta_{\sigma s} e^{i \bar{k}_\sigma \cdot \bar{r}}$$

$$\langle \tilde{V} \rangle = \frac{1}{2} \sum_{\substack{\sigma \sigma' \\ \bar{k}_\sigma, \bar{q}_{\sigma'}}} \sum_{s s'} \int d\bar{r}_1 \int d\bar{r}_2 \times \frac{1}{A^2} \delta(\bar{r}_1 - \bar{r}_2)$$

$$\left[\delta_{\sigma s}^2 \delta_{\sigma' s'}^2 e^{i(\bar{k}_\sigma \cdot \bar{r}_1 + \bar{q}_{\sigma'} \cdot \bar{r}_2 - \bar{k}_\sigma \cdot \bar{r}_1 - \bar{q}_{\sigma'} \cdot \bar{r}_2)} \right. \\ \left. - \delta_{\sigma s} \delta_{\sigma' s'} \delta_{\sigma' s} \delta_{\sigma s'} e^{i(\bar{k}_\sigma \cdot \bar{r}_1 + \bar{q}_{\sigma'} \cdot \bar{r}_2 - \bar{q}_{\sigma'} \cdot \bar{r}_1 - \bar{k}_\sigma \cdot \bar{r}_2)} \right]$$

$$= \frac{1}{2A^2} \int d\bar{r} \sum_{\substack{\sigma \sigma' \\ \bar{k}_\sigma, \bar{q}_{\sigma'}}} [1 - \delta_{\sigma \sigma'}]$$

$$= \frac{1}{2A} \left\{ \sum_{\bar{k}_\sigma} \sum_{\sigma' \bar{q}_{\sigma'}} - \sum_{\sigma} \sum_{\bar{k}_\sigma} \sum_{\bar{q}_{\sigma}} \right\}$$

$$= \frac{1}{2A} \left\{ N^2 - \sum_{\sigma} N_\sigma^2 \right\} = \frac{1}{2A} \left\{ (N_\uparrow + N_\downarrow)^2 - N_\uparrow^2 - N_\downarrow^2 \right\}$$

$$= \frac{1}{2A} \cdot 2 N_\uparrow N_\downarrow = \frac{N_\uparrow N_\downarrow}{A}$$

$$\langle V \rangle = \frac{U}{n} \langle \tilde{V} \rangle = \frac{U}{n} \frac{N_\uparrow N_\downarrow}{A} = U \frac{N_\uparrow N_\downarrow}{n}$$

Exercise 2

8-5-13

① An insulator, as the valence band is full and the conduction band is empty (2 electrons/unit cell).

$$\begin{aligned} \textcircled{2} \quad E_v(\bar{q}) &\approx 2\gamma_v \left[-3 + 1 - \frac{q_x^2 a^2}{2} + 2 \left(1 - \frac{q_x^2 a^2}{8} \right) \times \left(1 - \frac{3q_y^2 a^2}{8} \right) \right] \\ &\approx 2\gamma_v \left[-\frac{3}{4} q_x^2 a^2 - \frac{3}{4} q_y^2 a^2 \right] \end{aligned}$$

$$\boxed{E_v(\bar{q}) \approx -\frac{3}{2} \gamma_v a^2 q^2}$$

$$-2\Delta + E_c(\bar{q}) = -2\gamma_c \left[-\frac{3}{4} a^2 (q_x^2 + q_y^2) \right]$$

$$\boxed{E_c(\bar{q}) = 2\Delta + \frac{3}{2} \gamma_c a^2 q^2}$$

③

$$g_v(E) = \frac{2}{A} \sum_{\bar{q}} \delta(E - (-\frac{3}{2} \gamma_v a^2 q^2))$$

$$= \frac{2}{A} \int \frac{d\bar{q}}{(2\pi)^2} \delta(E + \frac{3}{2} \gamma_v a^2 q^2)$$

$$g_v(E) = \frac{1}{\pi} \int dq q \delta(E + \frac{3}{2} \gamma_v a^2 q^2)$$

(2)

$$\Rightarrow E = -\frac{3}{2} \kappa a^2 \rho^2$$

$$q^* = \sqrt{-\frac{2E}{3\kappa a^2}} \quad E < 0$$

$$\left[g_0(E) = \frac{1}{\pi} \frac{q \partial(-E)}{|3\kappa a^2 q|} \Big|_{q^*} = \frac{\partial(-E)}{3\pi \kappa a^2} \right]$$

$$g_c(E) = \frac{2}{A} \int_{\frac{1}{\rho}} \delta(E - 2\Delta - \frac{3}{2} \kappa a^2 \rho^2)$$

$$= \frac{1}{\pi} \int d\rho q \delta(E - 2\Delta - \frac{3}{2} \kappa a^2 \rho^2)$$

$$E = 2\Delta + \frac{3}{2} \kappa a^2 \rho^2$$

$$q^* = \sqrt{\frac{E - 2\Delta}{\frac{3}{2} \kappa a^2}} \quad E \geq 2\Delta$$

$$\left[g_c(E) = \frac{1}{\pi} \frac{q}{|3\kappa a^2 q|} \partial(E - 2\Delta) = \frac{1}{3\pi \kappa a^2} \partial(E - 2\Delta) \right]$$

$$(4) \quad n_c(\tau) = N_c(\tau) e^{-\beta(\epsilon_c - \mu)}$$

$$N_c = \int g_c(\epsilon) e^{-\beta(\epsilon - \epsilon_c)} d\epsilon$$

$$= \int_{2\Delta}^{\infty} d\epsilon e^{-\beta(\epsilon - 2\Delta)} \frac{1}{3\pi\hbar v d^2}$$

$$= \int_0^{\infty} d\epsilon' e^{-\beta\epsilon'} \frac{1}{3\pi\hbar v d^2} = \frac{k_B \tau}{3\pi\hbar v d^2} \int_0^{\infty} dx e^{-x}$$

$$N_c = \frac{k_B \tau}{3\pi\hbar v d^2}$$

$$p_s(\tau) = P_s(\tau) e^{-\beta(\mu - \epsilon_s)} \quad \epsilon_s = 0$$

$$P_s = \int g_s(\epsilon) e^{+\beta(\epsilon - \epsilon_s)} d\epsilon$$

$$= \int_{-\infty}^0 d\epsilon \frac{1}{3\pi\hbar v d^2} e^{\beta\epsilon} = \frac{k_B \tau}{3\pi\hbar v d^2}$$

$$P_s = \frac{k_B \tau}{3\pi\hbar v d^2}$$

(4)

(5)

$$n_c = p_r$$

$$\Rightarrow n_c e^{-\beta(2\Delta - \mu)} = p_r e^{-\beta\mu}$$

$$e^{2\beta\mu} = \frac{p_r}{n_c} e^{2\beta\Delta} = \frac{r_c}{r_o} e^{2\beta\Delta}$$

$$\beta\mu = \frac{1}{2} \ln \frac{r_c}{r_o} + \beta\Delta$$

$$\boxed{\mu = \frac{k_B T}{2} \ln \frac{r_c}{r_o} + \Delta}$$

(6)

$$\mu = \Delta + 2k_B T$$

$$\Rightarrow \frac{1}{2} \ln \frac{r_c}{r_o} = 2$$

$$\ln \frac{r_c}{r_o} = 4$$

$$\boxed{r_c = r_o e^4}$$