Physics 481: Condensed Matter Physics - Homework Solutions 9

(3)

Problem 1 :

a) $\psi = \frac{1}{\sqrt{L}} \frac{1}{a} e^{ikz} \sin\left(n_x \pi \frac{x}{a}\right) \sin\left(n_y \pi \frac{y}{a}\right)$

$k = \frac{2\pi}{L} n$

ground state in x,y - direction $\frac{1}{a} \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{\pi y}{a}\right)$

b) states with lowest energy are filled

- for small a, gap between states in x,y direction is large

$\Rightarrow$ only x-y ground state is occupied

- for larger a several x,y - states are occupied

c) Fermi energy in 1D :

$$\frac{N}{L} = 2 \cdot 2 \int_0^{k_F} \frac{dk}{2\pi} = \frac{4 k_F}{2\pi}$$

$$k_F = \frac{\pi}{2} \frac{N}{L} \qquad \varepsilon_F = \frac{\hbar^2}{2m} \left(\frac{\pi}{2} \frac{N}{L}\right)^2$$

$$N = L a^2 \rho \qquad \rho = 8.49 \cdot 10^{22} \mathrm{cm}^{-3}$$

④

distance between x,y ground state and 1st excited state ΔE =

$$\frac{\hbar^2}{2m}\left[\left(\frac{2\pi}{a}\right)^2 - \left(\frac{\pi}{a}\right)^2\right] = \frac{\hbar^2 3\pi^2}{2m\, a^2}$$

if $\varepsilon_F < \Delta E$, only x-y ground state occupied

$$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{\pi}{2}a^2\rho\right)^2 \overset{!}{\leq} \Delta E = \frac{\hbar^2 3\pi^2}{2m\, a^2}$$

$$\left(\frac{\pi}{2}a^2\rho\right)^2 \leq 3\pi^2/a^2$$

$$\frac{\pi^2}{4}a^4\rho^2 \leq \frac{3\pi^2}{a^2}$$

$$a^6 \leq \frac{12}{\rho^2}$$

$$a < 3.44\cdot 10^{-8}\,\mathrm{cm}$$

d) $$D(\varepsilon) = \frac{\sqrt{2m}}{\pi\hbar}\frac{1}{\sqrt{\varepsilon}}$$

$$C = \frac{\pi^2}{3}k_B^2 T\, D(\varepsilon_F)$$

$$= \frac{\pi^2}{3}k_B^2 T\frac{\sqrt{2m}}{\pi\hbar}\frac{1}{\sqrt{\varepsilon_F}} = \frac{\pi^2}{3}k_B^2 T\frac{\sqrt{2m}}{\pi\hbar}\frac{1}{\sqrt{\frac{\hbar^2}{2m}\left(\frac{\pi}{2}\rho a^2\right)^2}}$$

$$= \frac{4}{3}k_B^2 T\frac{m}{\hbar^2}\frac{1}{\rho a^2}$$

Problem 2

1D:
$$D(\varepsilon) = \frac{2}{2\pi}\int_{-\infty}^{\infty} dk \;\; \delta(\varepsilon - \varepsilon_k) = \frac{1}{\pi}\int dk \;\; \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right)$$

$$x = \frac{\hbar^2 k^2}{2m_e} \;, \quad k = \sqrt{\frac{2m_e}{\hbar^2}x} \;, \quad dk = \sqrt{\frac{m_e}{2\hbar^2 x}}\, dx$$

$$D(\varepsilon) = \frac{2}{\pi}\int_0^{\infty} \sqrt{\frac{m_e}{2\hbar^2 x}}\, dx \;\; \delta(\varepsilon - x)$$

$$D(\varepsilon) = \frac{\sqrt{2m_e}}{\pi\hbar} \; \frac{1}{\sqrt{\varepsilon}}$$

2D
$$D(\varepsilon) = \frac{2}{(2\pi)^2}\int d^2k \;\; \delta(\varepsilon - \varepsilon_k) = \frac{1}{\pi}\int_0^{\infty} dk\, k \;\; \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right)$$

$$= \frac{1}{\pi}\int_0^{\infty} \frac{m_e}{\hbar^2}\, dx \;\; \delta(\varepsilon - x)$$

$$D(\varepsilon) = \frac{m_e}{\pi\hbar^2}$$

Van-Hove singularity

1D $\quad \sim \frac{1}{\sqrt{\varepsilon}}\,\Theta(\varepsilon) \swarrow$ step function

2D $\quad \mathrm{Const}\cdot\Theta(\varepsilon)$ (singularity from $\frac{\partial \varepsilon}{\partial k} = 0$ exactly cancelled by measure of integral)

Problem 3

ground state energy

$$\frac{E_0}{V} = \frac{2}{(2\pi)^3} \int_0^{k_F} d^3k \; \frac{\hbar^2 k^2}{2m} = \frac{1}{\pi^2} \int_0^{k_F} dk\, k^2 \frac{\hbar^2 k^2}{2m}$$

$$= \frac{1}{\pi^2} \frac{\hbar^2}{2m} \frac{1}{5} k_F^5 \qquad\qquad k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}}$$

$$\frac{E_0}{V} = \frac{1}{\pi^2} \frac{\hbar^2}{10m} \left(3\pi^2 \frac{N}{V}\right)^{5/3} = \frac{3}{10} \frac{\hbar^2}{m} \frac{N}{V} \underbrace{\left(3\pi^2 \frac{N}{V}\right)^{2/3}}_{k_F^2} = \frac{3}{5} \frac{N}{V} \varepsilon_F$$

$$E_0 = \frac{3}{10} \frac{\hbar^2}{m} N^{5/3} (3\pi^2)^{2/3} V^{-2/3}$$

$$p = -\left(\frac{\partial E_0}{\partial V}\right)_N = \frac{1}{5} \frac{\hbar^2}{m} N^{5/3} (3\pi^2)^{2/3} V^{-\frac{5}{3}}$$

$$p = \frac{2}{3} E_0/V = \frac{2}{5} \frac{N}{V} \varepsilon_F$$