

Condensed Matter Physics I
SOLUTION of the written test of November 8, 2017

Exercise 1: Sommerfeld model and occupation of electronic energy levels

The Fermi function gives the occupation probability of an electronic energy level:

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

$$1/\beta(T = 300K) = k_B T = 0.026 \text{ eV}$$

$$E - \mu \approx E - E_F = 0.1 \text{ eV (considering } \mu(T = 300K) \approx E_F)$$

$$\implies f(E = E_F - 0.1 \text{ eV}) = [e^{-0.1/0.026} + 1]^{-1} = 0.98$$

Exercise 2: Sommerfeld model for 2D electron gas

$$1. k_F^2 = 2\pi n \implies E_f = \frac{\pi \hbar^2 n}{m}$$

$$2. \frac{E_{tot}}{N} = \frac{E_{tot}}{nA} = \frac{u}{n} = \frac{2}{n} \int_{k < k_F} \frac{d\mathbf{k}}{(2\pi)^2} \frac{\hbar^2 k^2}{2m} = \frac{E_F}{2}, \quad \text{where } A = \text{area, and } d\mathbf{k} = k dk d\phi \text{ (2D)}$$

Alternative solution:

$$u = \frac{E_{tot}}{A} = \int_0^{E_F} E g(E) dE = g(E_F) \int_0^{E_F} E dE = g(E_F) \frac{E_F^2}{2} = \frac{m}{\pi \hbar^2} \frac{E_F^2}{2} = n \frac{E_F}{2} \implies \frac{E_{tot}}{N} = \frac{E_F}{2}$$

3. Start from:

$$\begin{aligned} n &= \int_0^\infty g(E) f(E) dE = \frac{m}{\pi \hbar^2} \int_0^\infty \frac{1}{e^{\beta(E-\mu)} + 1} dE \quad [\text{change of variable: } x = \beta(E - \mu)] \\ &= \frac{m}{\pi \hbar^2} \int_{-\beta\mu}^\infty \frac{1}{e^x + 1} dx = \frac{m}{\pi \hbar^2} k_B T [x - \ln(e^x + 1)]_{-\beta\mu}^\infty = \frac{n}{E_F} k_B T [\beta\mu + \ln(e^{-\beta\mu} + 1)] \\ &\implies \beta(E_F - \mu) = \ln(e^{-\beta\mu} + 1) \implies \ln(e^{\beta E_F} - 1) = \beta\mu \quad (*, \text{ exact form}) \end{aligned}$$

Approximations:

$$1) k_B T \ll E_F \implies e^{\beta E_F} \gg 1 \implies \ln(e^{\beta E_F} - 1) \approx \ln(e^{\beta E_F}) = \beta E_F$$

and therefore from (*): $\mu \approx E_F$

$$2) k_B T \gg E_F \implies \ln(e^{\beta E_F} - 1) \approx \ln(1 + \beta E_F - 1) \approx \ln(\beta E_F)$$

and therefore from (*): $\mu \approx k_B T \ln(\beta E_F)$

Exercise 3: Crystalline structures: family of lattice planes

1. The intercepts of the upper plane in the fig., for instance, are: $(-1, \infty, 1/2)$ in unit of a
 \implies taking the reciprocals, the Miller indices are: $(h, k, \ell) = (-1, 0, 2)$

2. The reciprocal lattice vector identifying the family of lattice planes, with reference to the SC lattice, is: $\mathbf{K}_{SC} = \frac{2\pi}{a}(-1, 0, 2) \implies d = \frac{a}{\sqrt{h^2 + k^2 + \ell^2}} = \frac{a\sqrt{5}}{5}$ (planes in the figure)

3. This is the family of lattice planes of SC; BCC and FCC have a family of lattice planes parallel to those indicated in the figures, characterized by a distance $d = \frac{a\sqrt{5}}{10}$ (for instance, there is one plane in between the two of the figure, passing through the point in the middle of the cube, and in the middle of the faces perpendicular to \mathbf{a}_2). Infact, the shortest reciprocal lattice vector of BCC and FCC parallel to \mathbf{K}_{SC} is:
 $\mathbf{K}_{FCC, BCC} = \frac{2\pi}{a}(-2, 0, 4)$

Exercise 4: Crystalline structures: Bravais lattices and primitive unit cells in 2D

1. Recognize that the underlying lattice (B, small dots) is honeycomb (see for instance the exercises in class concerning graphene): the primitive unit cell is a rhombus
2. containing 3 sites A and 2 sites B

Exercise 5: Crystalline structures: Bravais lattices and primitive unit cells in 3D

1. In plane, the unit cell is the same as in Ex. 4; consider 2 layers made of Si_2O_3 per unit cell, plus 2 additional O atoms in between the two layers (between the Si atoms): the 3D primitive unit cell contains therefore 4 Si atoms and 8 O atoms, and the formula unit of the compound is SiO_2 .
2. See above. The 3D primitive unit cell is HEX.