

## Solutions to the problems in Chapter 6

### 6.3 Pressure of a Fermi gas at zero temperature

The number of electrons  $N$  and the internal energy  $U$ , in the volume  $V$ , are

$$N = V \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon, \quad U = V \int_0^\infty \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon, \quad (1)$$

The Fermi distribution function  $f(\varepsilon)$  and the density of states (per unit volume)  $D(\varepsilon)$  are

$$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}, \quad D(\varepsilon) = A\sqrt{\varepsilon}, \quad A = \frac{\sqrt{2m^3}}{\pi^2 \hbar^3}. \quad (2)$$

At zero temperature

$$f(\varepsilon) = \theta(\varepsilon_F - \varepsilon), \quad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \quad k_F = (3\pi^2 n)^{1/3} \quad (3)$$

Introducing the step function and  $D(\varepsilon) = A\sqrt{\varepsilon}$  in (1), we may determine  $U(0)$  and an alternative expression for  $A$ :

$$N = V \int_0^{\varepsilon_F} A\sqrt{\varepsilon} d\varepsilon = \frac{2}{3} V A \varepsilon_F^{3/2} \Rightarrow A = \frac{3n}{2\varepsilon_F^{3/2}}, \quad U(0) = V \frac{2}{5} A \varepsilon_F^{5/2} = \frac{3}{5} N \varepsilon_F \quad (4)$$

i.e.  $U \propto \varepsilon_F \propto k_F^2 \propto V^{-2/3}$  and the pressure at zero temperature is

$$P = -\frac{\partial U(0)}{\partial V} = \frac{2}{3} \frac{U}{V} = \frac{2}{5} n \varepsilon_F = \frac{(3\pi^2)^{2/3} n^{5/3} \hbar^2}{5m} \quad (5)$$

in sharp contrast to a classical gas, where the zero-temperature pressure is zero.

### 6.4 Density of states in low dimensions

The density of states in  $\vec{k}$ -space is  $D_{\vec{k}} = 2/(2\pi)^d$  in  $d$  dimensions (6.34)

$$D(\varepsilon) = \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{\vec{k}}) \equiv \int D_{\vec{k}} \delta(\varepsilon - \varepsilon_{\vec{k}}) d\vec{k} = \frac{2}{(2\pi)^d} \int \delta(\varepsilon - \varepsilon_{\vec{k}}) d\vec{k} \quad (1)$$

Introducing ‘‘spherical coordinates’’ in  $d$  dimensions and  $k = |\vec{k}|$ , then

$$d\vec{k} = \begin{cases} 2 dk & , \quad d = 1 \\ 2\pi k dk & , \quad d = 2 \\ 4\pi k^2 dk & , \quad d = 3 \end{cases} \quad (2)$$

The factor 2 in the one-dimensional case appears because the one-dimensional wave vector may assume both positive and negative values, whereas  $k \geq 0$  per definition.

$$\varepsilon_{\vec{k}} = \varepsilon_k = \frac{\hbar^2 k^2}{2m} \Rightarrow k = \frac{\sqrt{2m\varepsilon_k}}{\hbar}, \quad dk = \left( \frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k \Rightarrow \quad (3)$$

$$D(\varepsilon) = \begin{cases} \frac{2}{2\pi} \int_0^\infty 2 \delta(\varepsilon - \varepsilon_k) \left( \frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{\sqrt{2m}}{\pi \hbar} \varepsilon^{-1/2}, & d = 1 \\ \frac{2}{(2\pi)^2} \int_0^\infty 2\pi \frac{\sqrt{2m\varepsilon_k}}{\hbar} \delta(\varepsilon - \varepsilon_k) \left( \frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{m}{\pi \hbar^2}, & d = 2 \\ \frac{2}{(2\pi)^3} \int_0^\infty 4\pi \frac{2m\varepsilon_k}{\hbar^2} \delta(\varepsilon - \varepsilon_k) \left( \frac{m}{2\hbar^2 \varepsilon_k} \right)^{1/2} d\varepsilon_k = \frac{\sqrt{2m^3}}{\pi^2 \hbar^3} \varepsilon^{1/2}, & d = 3 \end{cases}$$

### 6.5 Fermi pancakes

Thin layer of Ag:  $L_x = L_y = L = 10^6 \text{ \AA}$  and  $L_z = d$ .

The density of electrons is the same as the density of atoms (one conduction electron per Ag atom), i.e.  $n = 5.86 \cdot 10^{22} \text{ cm}^{-3} = 0.0586 \text{ \AA}^{-3}$ , according to the properties given in the periodic table on the front page of Marder. The wave function of the “free” electrons should vanish at the boundaries  $z = 0$  and  $z = d$ . This condition is fulfilled if assuming the one-electron wave function to be

$$\psi(x, y, z) \propto e^{i(k_x x + k_y y)} \sin(pqz), \quad q = \frac{\pi}{d}, \quad p = 1, 2, \dots \quad (1)$$

The electron states are characterized by the two-dimensional wave vector  $\vec{k} = (k_x, k_y, 0)$  and the “band index”  $p$ . The eigenenergies are ( $k^2 = k_x^2 + k_y^2$ ):

$$\varepsilon_{p\vec{k}} = \frac{\hbar^2}{2m} (k^2 + p^2 q^2) \geq \varepsilon_{1\vec{0}} = \frac{\hbar^2 q^2}{2m} \quad (2)$$

At  $T = 0$  ( $T \ll T_F$ ), as assumed implicitly in the exercise, the occupied states are all those with energies smaller than  $\varepsilon_F$ . The number of electrons in the  $p$ th band,  $N_p$ , is zero if  $\varepsilon_{p\vec{0}} > \varepsilon_F$ . In the opposite case:

$$N_p = L^2 \int_0^{k_p} \frac{2}{(2\pi)^2} 2\pi k dk = L^2 \frac{k_p^2}{2\pi} \quad (3)$$

where  $k_p$  is the Fermi wave number of the  $p$ th band, i.e. the largest value of  $k$  of occupied states in the  $p$ th band, as determined by

$$\varepsilon_{pk_p} = \frac{\hbar^2}{2m} (k_p^2 + p^2 q^2) = \varepsilon_F \quad \Rightarrow \quad k_p^2 = \frac{2m\varepsilon_F}{\hbar^2} - p^2 q^2 = q^2 \left( \frac{\varepsilon_F}{\varepsilon_{1\vec{0}}} - p^2 \right) \quad (4)$$

(a) In the first case  $d = 4.1 \text{ \AA}$  or  $q = \pi/d = 0.76624 \text{ \AA}^{-1}$ , and

$$\varepsilon_{1\vec{0}} = \frac{\hbar^2 q^2}{2m} = \frac{(1.054572 \cdot 10^{-27} \times 0.76624 \cdot 10^8)^2}{2 \times 9.109389 \cdot 10^{-28} \times 1.602177 \cdot 10^{-12}} \text{ eV} = 2.2369 \text{ eV} \quad (5)$$

Assuming the Fermi energy to be smaller than the lowest energy of the ( $p = 2$ ) band,  $\varepsilon_F < \varepsilon_{2\vec{0}} = 4\varepsilon_{1\vec{0}}$ , then only the ( $p = 1$ ) states are occupied, in which case  $N_1$  has to be equal the total number  $N$  of free electrons:

$$N = L^2 d n = N_1 = L^2 \frac{k_1^2}{2\pi} \quad \Rightarrow \quad k_1 = \sqrt{2\pi d n} = 1.22866 \text{ \AA}^{-1} \quad (6)$$

Introducing this result in (3) we get the Fermi energy and the band width  $W$  of the occupied states:

$$\varepsilon_F = \varepsilon_{1k_1} = \varepsilon_{1\vec{0}} \left[ (k_1/q)^2 + 1 \right] = 7.99 \text{ eV}, \quad W = \varepsilon_F - \varepsilon_{1\vec{0}} = \underline{5.75 \text{ eV}} \quad (7)$$

which is in accordance with our starting assumption of  $\varepsilon_F < \varepsilon_{2\vec{0}} = 8.948 \text{ eV}$ . These results may be compared with that obtained for bulk Ag:

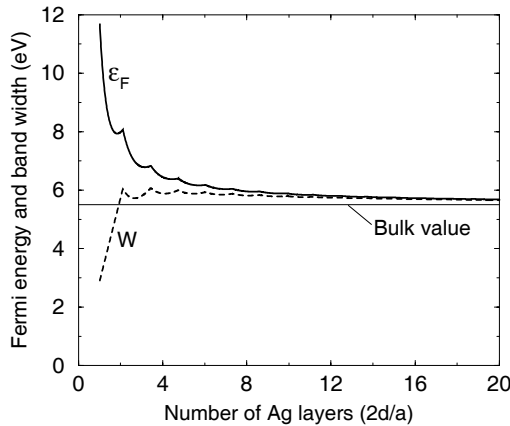
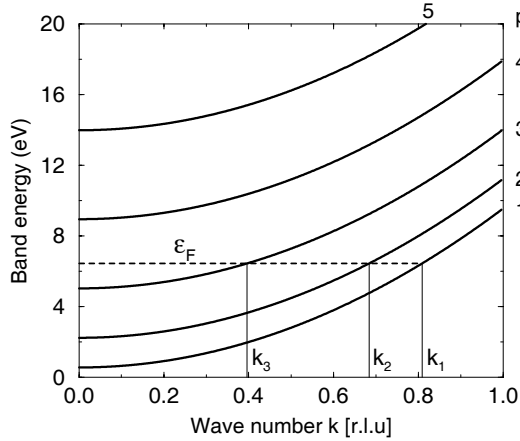
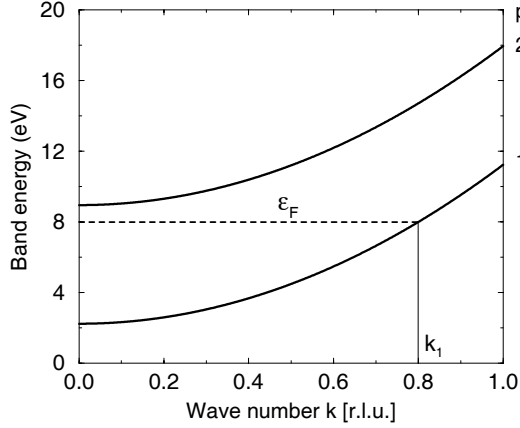
$$\varepsilon_F(\text{bulk}) = W(\text{bulk}) = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} = 5.50 \text{ eV} \quad (8)$$

(b) In the case of  $d = 8.2 \text{ \AA}$ ,  $q = \pi/d = 0.38312 \text{ \AA}^{-1}$  and  $\varepsilon_{10} = 0.5592 \text{ eV}$ . In order to determine  $\varepsilon_F$  in this case, we need to include more bands than the lowest one. The number of bands turns out to be 3, and

$$N = N_1 + N_2 + N_3 \Rightarrow 2\pi dn = q^2 \left[ \left( \frac{\varepsilon_F}{\varepsilon_{10}} - 1^2 \right) + \left( \frac{\varepsilon_F}{\varepsilon_{10}} - 2^2 \right) + \left( \frac{\varepsilon_F}{\varepsilon_{10}} - 3^2 \right) \right] \quad (9)$$

Solving this equation with respect to  $\varepsilon_F/\varepsilon_{10}$ , we get  $\varepsilon_F/\varepsilon_{10} = 11.523$ , which is larger than  $3^2$  but smaller than  $4^2$ , in accordance with the assumption that all electrons are found in the three lowest bands. Hence the results are:

$$\varepsilon_F = 6.44 \text{ eV}, \quad W = \varepsilon_F - \varepsilon_{10} = \underline{5.89 \text{ eV}} \quad (10)$$



The two first figures show the energy bands as functions of  $k$  in the cases (a) and (b), where the unit of  $k$  is the length of a reciprocal lattice vector  $2\pi/a$  [r.l.u.]. The last figure shows the Fermi energy (and the band width) as a function of the number of atomic layers of Ag. The crystal structure of Ag is fcc with the lattice parameter  $a = 4.09 \text{ \AA}$ . This is very nearly the thickness  $d$  assumed in (a), i.e. this case corresponds to a film with two atomic layers of Ag atoms.

## Solutions to the problems in Chapter 7

### 7.1 Normals to surfaces

$\vec{r} = (x_1, x_2, x_3) = \vec{s}(t)$  is the parametrization of a curve lying within the surface defined by  $f(\vec{r}) = \varepsilon$ . Since  $f(\vec{s}(t))$  is a constant  $\varepsilon$ , the derivative of this function is 0:

$$\frac{d}{dt}f(\vec{s}(t)) = \sum_{\alpha} \frac{\partial f}{\partial x_{\alpha}} \frac{ds_{\alpha}}{dt} = \nabla f \cdot \frac{d\vec{s}}{dt} = 0 \quad (1)$$

Because  $\vec{s}(t)$  may be any arbitrary curve lying within the surface, the same is true for the curve tangent  $d\vec{s}(t)/dt$ , and (1) is only generally valid if  $\nabla f$  is normal to the surface.

### 7.3 Van Hove singularities

(a) The problem becomes the same as the one considered in problem 7.1 if making the replacements  $\vec{k} \rightarrow \vec{r}$  and  $\varepsilon_{n\vec{k}} \rightarrow f(\vec{r})$ , hence  $\nabla_{\vec{k}}\varepsilon_{n\vec{k}}$  is perpendicular to the energy surface defined by  $\varepsilon_{n\vec{k}} = \varepsilon$ .

(b) The energy is assumed to be  $\varepsilon_{n\vec{k}} = \varepsilon_{\max} - k^2$ , and in the two-dimensional case

$$\begin{aligned} D(\varepsilon) &= \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{n\vec{k}}) = \frac{2}{(2\pi)^2} \int_0^{\infty} 2\pi k \delta(\varepsilon - \varepsilon_{\max} + k^2) dk \\ &= \frac{1}{2\pi} \int_0^{\infty} \delta(\varepsilon - \varepsilon_{\max} + k^2) d(k^2) = \frac{1}{2\pi} \theta(\varepsilon_{\max} - \varepsilon) \end{aligned} \quad (1)$$

The density of states is zero if  $\varepsilon > \varepsilon_{\max}$  and  $1/(2\pi)$  when  $\varepsilon < \varepsilon_{\max}$ .

(c) In the three dimensional case, the result is

$$\begin{aligned} D(\varepsilon) &= \int [d\vec{k}] \delta(\varepsilon - \varepsilon_{n\vec{k}}) = \frac{2}{(2\pi)^3} \int_0^{\infty} 4\pi k^2 \delta(\varepsilon - \varepsilon_{\max} + k^2) dk \\ &= \frac{1}{2\pi^2} \int_0^{\infty} k \delta(\varepsilon - \varepsilon_{\max} + k^2) d(k^2) = \frac{1}{2\pi^2} \sqrt{\varepsilon_{\max} - \varepsilon} \theta(\varepsilon_{\max} - \varepsilon) \end{aligned} \quad (2)$$