Chapter 4

*4.6 Density of states for a two-dimensional electron gas

Consider a two-dimensional electron gas in which the electrons are restricted to move freely within a square area $a^2$ in the $xy$ plane. Following the procedure in Section 4.5 (in the textbook), show that the density of states $g(E)$ is constant (independent of energy).

Solution

For a two dimensional electron gas confined within a square region of sides $a$ we have:

$$ E = \frac{\hbar^2}{8m_e a^2} \left( n_1^2 + n_2^2 \right) $$

Only positive $n_1$ and $n_2$ are allowed. Each $n_1$ and $n_2$ combination is an orbital state. Define a new variable $n$ as:

$$ n^2 = n_1^2 + n_2^2 $$

substitute:

$$ E = \frac{\hbar^2}{8m_e a^2} n^2 $$

Let us consider how many states there are with energies less than $E'$. $E'$ corresponds to $n \leq n'$.

$$ E' = \frac{\hbar^2}{8m_e a^2} n'^2 $$

$$ \therefore n' = \sqrt{\frac{8a^2 m_e E'}{\hbar^2}} $$

![Figure 4Q6-1](image)

Each state, or electron wavefunction in the crystal, can be represented by a box at $n_1, n_2$. 

4.1
Consider Figure 4Q6-1. All states within the quarter arc defined by \( n' \) have \( E < E' \). The area of this quarter arc is the total number of orbital states. The total number of states, \( S \), including spin is twice as many,

\[
S = 2 \left( \frac{1}{4} \pi n'^2 \right) = 2 \left( \frac{1}{4} \pi \left[ \sqrt{\frac{8a^2 m_e E'}{\hbar^2}} \right]^2 \right)
\]

\[
\therefore \quad S = \frac{4\pi a^2 m_e E'}{\hbar^2}
\]

The density of states \( g \) is defined as the number of states per unit area per unit energy. Therefore,

\[
g = \frac{1}{a^2} \frac{dS}{dE'} = \frac{1}{a^2} \frac{4\pi a^2 m_e}{\hbar^2} = \frac{4\pi m_e}{\hbar^2}
\]

Thus, for a two dimensional gas, the density of states is constant.

### 4.8 Fermi energy and electron concentration

Consider the metals in Table 4Q8-1 from groups I, II and III in the Periodic Table. Calculate the Fermi energies at absolute zero, and compare the values with the experimental values. What is your conclusion?

<table>
<thead>
<tr>
<th>Metal</th>
<th>Group</th>
<th>( M_{at} ) (g/mol)</th>
<th>Density (g cm(^{-3}))</th>
<th>( E_F ) (eV) [Calculated]</th>
<th>( E_F ) (eV) [Experiment]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>I</td>
<td>63.55</td>
<td>8.96</td>
<td>-</td>
<td>6.5</td>
</tr>
<tr>
<td>Zn</td>
<td>II</td>
<td>65.38</td>
<td>7.14</td>
<td>-</td>
<td>11.0</td>
</tr>
<tr>
<td>Al</td>
<td>III</td>
<td>27</td>
<td>2.70</td>
<td>-</td>
<td>11.8</td>
</tr>
</tbody>
</table>

**Solution**

Since Cu is in group I, its valency is also 1. The electron concentration \( n \) is then the atomic concentration multiplied by the group number, or:

\[
n = \text{(Valency)} \frac{N_A D}{M_{at}} = (1) \left( \frac{6.022 \times 10^{23} \text{ mol}^{-1}}{63.55 \times 10^{-3} \text{ kg/mol}} \right) = 8.490 \times 10^{28} \text{ m}^{-3}
\]

Using Equation 4.22 in the text:

\[
E_{FO} = \frac{\hbar^2}{8 m_e} \left( \frac{3 n}{\pi} \right)^{2/3} \left( \frac{1}{q} \right)
\]

\[
\therefore \quad E_{FO} = \frac{6.626 \times 10^{-34} \text{ J s}}{8(9.109 \times 10^{-31} \text{ kg})} \left( \frac{3(8.490 \times 10^{28} \text{ m}^{-3})}{\pi} \right)^{2/3} \left( \frac{1}{1.602 \times 10^{-19} \text{ J/eV}} \right)
\]

\[
\therefore \quad E_{FO} = 7.04 \text{ eV}
\]
Comparing with the experimental value:

\[
% \text{ difference} = \left| \frac{7.04 \text{ eV} - 6.5 \text{ eV}}{6.5 \text{ eV}} \right| \times 100\% = 8.31\%
\]

\( E_{FO} \) can be calculated for Zn and Al in the same way (remember to take into account the different valencies). The values are summarized in the following table and it can be seen that calculated values are close to experimental values:

Table Q4.8-2  Summarized values for Fermi energy at absolute zero temperature.

<table>
<thead>
<tr>
<th>Metal</th>
<th>( n (\text{m}^{-3}) \times 10^{28} )</th>
<th>( E_{FO} ) (eV) ( \text{(calculated)} )</th>
<th>( E_{FO} ) (eV) ( \text{(experimental)} )</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>8.490</td>
<td>7.04</td>
<td>6.5</td>
<td>8.31</td>
</tr>
<tr>
<td>Zn</td>
<td>13.15</td>
<td>9.43</td>
<td>11.0</td>
<td>14.3</td>
</tr>
<tr>
<td>Al</td>
<td>18.07</td>
<td>11.7</td>
<td>11.8</td>
<td>0.847</td>
</tr>
</tbody>
</table>

4.9 Temperature dependence of the Fermi energy

a. Given that the Fermi energy for Cu is 7.0 eV at absolute zero, calculate the \( E_F \) at 300 K. What is the percentage change in \( E_F \) and what is your conclusion?

b. Given the Fermi energy for Cu at absolute zero, calculate the average energy and mean speed per conduction electron at absolute zero and 300 K, and comment.

Solution

a. The Fermi energy in eV at 0 K is given as 7.0 eV. The temperature dependence of \( E_F \) is given by Equation 4.23 in the textbook. Remember that \( E_{FO} \) is given in eV.

\[
E_{F} = E_{FO} \left( 1 - \frac{\pi^2}{12} \left( \frac{kT}{E_{FO}} \right)^2 \right)
\]

\[
\therefore \quad E_{F} = (7.0 \text{ eV}) \left( 1 - \frac{\pi^2}{12} \left( \frac{1.381 \times 10^{-23} \text{ J/K}}{7.0 \text{ eV}} \right) \left( 1.602 \times 10^{-19} \text{ J/eV} \right) \right) = 6.999921 \text{ eV}
\]

\[
\therefore \quad \% \text{ difference} = \left| \frac{6.999921 \text{ eV} - 7.0 \text{ eV}}{7.0 \text{ eV}} \right| \times 100\% = 0.00129\%
\]

This is a very small change. The Fermi energy appears to be almost unaffected by temperature.

b. The average energy per electron at 0 K is:

\[
E_{av}(0 \text{ K}) = \frac{3}{5} (E_{FO}) = 4.2 \text{ eV}
\]

The average energy at 300 K can be calculated from Equation 4.26 (in the textbook):

\[
E_{av}(T) = \frac{3}{5} E_{FO} \left( 1 + \frac{5\pi^2}{12} \left( \frac{kT}{E_{FO}} \right)^2 \right)
\]
\[
E_{\text{av}}(300 \text{ K}) = \frac{3}{5} (7.0 \text{ eV}) \left( 1 + \frac{5\pi^2}{12} \left[ \left( \frac{1.381 \times 10^{-23} \text{ J/K}}{300 \text{ K}} \right) \left( \frac{1.602 \times 10^{-19} \text{ J/eV}}{7.0 \text{ eV}} \right) \right]^2 \right)
\]

\[\therefore\]

\[E_{\text{av}}(300 \text{ K}) = 4.200236 \text{ eV}\]

This is a very small change.

Assume that the mean speed will be close to the effective speed \(v_e\). Effective speed at absolute zero is denoted as \(v_{eo}\), and is given by:

\[E_{\text{av}}(0 \text{ K}) \times q = \frac{1}{2} m_e v_{eo}^2\]

\[\therefore\]

\[v_{eo} = \sqrt{\frac{2qE_{\text{av}}(0 \text{ K})}{m_e}} = \sqrt{\frac{2 \left( 1.602 \times 10^{-19} \text{ J/eV} \right) \left( 4.2 \text{ eV} \right)}{9.109 \times 10^{-31} \text{ kg}}} = 1215446 \text{ m/s}\]

At 300 K, the effective speed is \(v_e\):

\[v_e = \sqrt{\frac{2qE_{\text{av}}(300 \text{ K})}{m_e}} = \sqrt{\frac{2 \left( 1.602 \times 10^{-19} \text{ J/eV} \right) \left( 4.200236 \text{ eV} \right)}{9.109 \times 10^{-31} \text{ kg}}} = 1215480 \text{ m/s}\]

Comparing the values:

\[\% \text{ difference} = \left| \frac{1215480 \text{ m/s} - 1215446 \text{ m/s}}{1215446 \text{ m/s}} \right| \times 100\% = 0.002797\%\]

The mean speed has increased by a negligible amount (0.003%) from 0 K to 300 K.

Note: For thermal conduction this tiny increase in the velocity is sufficient to transport energy from hot regions to cold regions. This very small increase in the velocity also allows the electrons to diffuse from hot to cold regions giving rise to the Seebeck effect.

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\*4.17 Overlapping bands

Consider Cu and Ni with their density of states as schematically sketched in Figure 4Q17-1. Both have overlapping 3d and 4s bands, but the 3d band is very narrow compared to the 4s band. In the case of Cu the band is full, whereas in Ni, it is only partially filled.

a. In Cu, do the electrons in the 3d band contribute to electrical conduction? Explain.

b. In Ni, do electrons in both bands contribute to conduction? Explain.

c. Do electrons have the same effective mass in the two bands? Explain.

d. Can an electron in the 4s band with energy around \(E_F\) become scattered into the 3d band as a result of a scattering process? Consider both metals.

e. Scattering of electrons from the 4s band to the 3d band and vice versa can be viewed as an additional scattering process. How would you expect the resistivity of Ni to compare with that of Cu, even though Ni has 2 valence electrons and nearly the same density as Cu? In which case would you expect a stronger temperature dependence for the resistivity?
**Solution**

a. In Cu the $3d$ band is full so the electrons in this band do not contribute to conduction.

b. In Ni both the $3d$ and $4s$ bands are partially filled so electrons in both bands can gain energy from the field and move to higher energy levels. Thus both contribute to electrical conductivity.

c. No, because the effective mass depends on how easily the electron can gain energy from the field and accelerate or move to higher energy levels. The energy distributions in the two bands are different. In the $4s$ band, the concentration of states is increasing with energy whereas in the $3d$ band, it is decreasing with energy. One would therefore expect different inertial resistances to acceleration, different effective mass and hence different drift mobility for electrons in these bands.

d. Not in copper because the $3d$ band is full and cannot take electrons. In Ni the electrons can indeed be scattered from one band to the other, e.g. an electron in the $4s$ band can be scattered into the $3d$ band. Its mobility will then change. Electrons in the $3d$ band are very sluggish (low drift mobility) and contribute less to the conductivity.

e. Ni should be more resistive because of the additional scattering mechanism from the $4s$ to the $3d$ band (Matthiessen's rule). This scattering is called $s$-$d$ scattering. One may at first think that this $s$-$d$ scattering de-emphasizes the importance of scattering from lattice vibrations and hence, overall, the resistivity should be less temperature dependent. In reality, electrons in Ni also get scattered by magnetic interactions with Ni ion magnetic moments (Nickel is ferromagnetic; Ch. 8 in the textbook) which has a stronger temperature dependence than $\rho \sim T$. 

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**Figure 4Q17-1** Density of states and electron filling in Cu and Ni.