Class 19: Features of the Fermi Dirac Distribution Function

In the last couple of classes we have derived the Fermi-Dirac distribution function. In this class we will take a look at some of the features of the Fermi-Dirac distribution and the implications of these features.

The Fermi-Dirac distribution function is as follows:

\[
f(\varepsilon_i) = \frac{1}{1 + e^{\frac{\varepsilon_i - E_f}{k_b T}}}
\]

In the above expression, \(\varepsilon_i\) is a variable, and we wish to evaluate \(f(\varepsilon_i)\) for various values of \(\varepsilon_i\). This evaluation can be carried out at various temperatures, so \(T\) is the other variable. \(k_b\) is Boltzmann’s constant, and \(E_f\) is a particular value of the energy level and is a constant for a given system. We will look at the significance of \(E_f\), a little later in this class.

On examining the expression for \(f(\varepsilon_i)\), we notice that there are three different regimes of values of \(\varepsilon_i\) over which the response of the function can vary significantly. The regimes are as follows:

\[
\varepsilon_i < E_f
\]

\[
\varepsilon_i = E_f
\]

\[
\varepsilon_i > E_f
\]

Let us first consider these three regimes when the temperature tends to absolute zero Kelvin. For all \(\varepsilon_i < E_f\), \(\frac{\varepsilon_i - E_f}{k_b T}\) tends towards \(-\infty\), and hence \(f(\varepsilon_i)\) tends to 1. In the limiting case of \(T = 0\) Kelvin, \(f(\varepsilon_i) = 1\)

Similarly, when the temperature tends to absolute zero Kelvin, for all \(\varepsilon_i > E_f\), \(\frac{\varepsilon_i - E_f}{k_b T}\) tends towards \(+\infty\), and hence \(f(\varepsilon_i)\) tends to 0. In the limiting case of \(T = 0\) Kelvin, \(f(\varepsilon_i) = 0\).

When \(\varepsilon_i = E_f\), in the limiting case of \(T = 0\) Kelvin, \(f(\varepsilon_i)\) is undefined and varies between the two limits 1 and 0.

Figure 19.1 below shows the behavior of \(f(\varepsilon_i)\) as a function of energy at \(T = 0\) Kelvin.
Let us now consider the Fermi-Dirac distribution at temperatures greater than absolute zero.

The effect of increasing temperature on the Fermi-Dirac distribution is such that as the temperature increases, the change in \( f(\varepsilon_i) \) from 1 to 0, occurs over a larger range of temperatures.

When \( \varepsilon_i = E_f \), and the temperature \( T > 0 \text{ Kelvin} \), \( \frac{\varepsilon_i - E_f}{k_b T} = 0 \), and \( f(\varepsilon_i) = 0.5 \) regardless of the actual value of the temperature.

When the temperature is greater than 0 Kelvin, for all \( \varepsilon_i < E_f \), \( \frac{\varepsilon_i - E_f}{k_b T} \) is a negative number which becomes a larger negative number as \( \varepsilon_i \) decreases. Hence \( f(\varepsilon_i) \) starts from a value of 0.5 at \( \varepsilon_i = E_f \) and tends towards 1 as \( \varepsilon_i \) decreases.

Similarly, when the temperature greater than 0 Kelvin, for all \( \varepsilon_i > E_f \), \( \frac{\varepsilon_i - E_f}{k_b T} \) is a positive number which increases as \( \varepsilon_i \) increases. Hence \( f(\varepsilon_i) \) starts from a value of 0.5 at \( \varepsilon_i = E_f \) and tends towards 0 as \( \varepsilon_i \) increases.

This behavior of \( f(\varepsilon_i) \) is summarized in Figure 19.2 below.

Figure 19.1: Variation of \( f(\varepsilon_i) \) as a function of energy at \( T = 0 \text{ Kelvin} \)
Figure 19.2: Variation of $f(\varepsilon_i)$ as a function of energy at various temperatures.

While we have looked at the Fermi-Dirac distribution in a mathematical sense above, let us now consider the impact of this distribution in a descriptive sense.

We have noted earlier that there are a fixed and finite number of states at any given energy level, in the framework within which we derived the Fermi-Dirac distribution. Therefore, because of Pauli’s exclusion principle, there is a limit on the number of particles we can place on these states. At T= 0 Kelvin, if we arrange the energy levels of the system in order of increasing energy, nature will choose to fill the lowest energy level first. When all the states at the lowest energy level are full, if there are still particles that remain, they will start filling the states at the next higher energy level. This process will continue till we run out of particles to place in the energy levels. Therefore, even at absolute zero temperature, we are forced to fill energy levels that are higher than the lowest energy level available in the system – which is directly a result of the fact that the electrons are behaving in a manner consistent with the restrictions on Fermions. The number of electrons available in the system is a large value but a finite value, therefore as we continue the process of filling up states at increasing energy levels, we will eventually run out of electrons to fill further states with. Even higher energy levels may be defined for the system, but will remain unfilled. In other words, as we fill the states, at $E_0$, we run out of states, then at $E_1$, we run out states…and then at some higher energy level $E_f$, we run out of electrons. This $E_f$, at T=0 Kelvin, is called the Fermi energy and is identified in the figures 19.1 and 19.2 above. Since all states are getting filled up for all $E < E_f$, $f(\varepsilon_i) = 1$ for all energy levels less than the Fermi Energy. At $E = E_f$, the $f(\varepsilon_i)$...
transitions from 1 to 0 and then stays at 0 for all values of $E > E_f$. We are therefore able to see why the Fermi-Dirac distribution function looks the way it does at 0 Kelvin.

The Fermi energy is therefore defined as the highest energy level that is occupied at 0 Kelvin and it is of the order of 2.5 eV for a typical metal. There is an alternate definition for the Fermi energy, for temperature greater than 0 Kelvin, which we will describe shortly.

It is important to note that $f(\epsilon_i)$ is only the probability of occupancy of a state at a given energy level $\epsilon_i$. It does not give any information on the number of states actually available at that energy level. The number of available states will typically vary from energy level to energy level. There is another function which will give us that information, which we will develop in a later class. The $f(\epsilon_i)$ merely tells us the probability of occupancy of states at a given energy level, regardless of the actual number of states at that energy level.

Purely for illustrative purposes let us use some hypothetical numbers of states at various energy levels, in order to understand the significance of $f(\epsilon_i)$.

<table>
<thead>
<tr>
<th>Energy level</th>
<th>Number of states</th>
<th>$f(\epsilon_i)$</th>
<th>Number of occupied states</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon_1$</td>
<td>50</td>
<td>1.0</td>
<td>50</td>
</tr>
<tr>
<td>$\epsilon_2$</td>
<td>70</td>
<td>1.0</td>
<td>70</td>
</tr>
<tr>
<td>$\epsilon_3$</td>
<td>100</td>
<td>0.0</td>
<td>0</td>
</tr>
</tbody>
</table>

It is evident from the discussion above that there is an additional and important piece of information that is not captured in the plots of the Fermi-Dirac distribution function that we have seen so far. So, for example, if there are some 3500 states at $E = E_{F+1}$, all of these states will be empty at T=0 Kelvin. We will look at this complete information in a later class, you are merely being alerted to it at this point. The Fermi-Dirac distribution is itself an important piece of information and hence we are focusing on it at this time.

As indicated above, when the temperature is greater than 0 Kelvin, some energy levels close to but below $E_f$ have $f(\epsilon_i) < 1$, and some energy levels close to but higher than $E_f$ have $f(\epsilon_i) > 1$. At higher and higher temperatures, the range of energy values over which the $f(\epsilon_i)$ varies from 1 to 0 increases, as shown in the Figure 19.2 above. Using Figures 19.1 and 19.2 above, we are therefore able to understand the variation of $f(\epsilon_i)$ as a function of energy as well as temperature.

From the equation for $f(\epsilon_i)$, we find that when $T \neq 0 \text{ Kelvin}$, at $\epsilon_i = E_f$, $f(\epsilon_i) = 0.5$. This is then the other definition for the Fermi energy – it is the energy level at which the probability of occupancy is $\frac{1}{2}$, when the temperature is greater than absolute zero.

To understand the concept of states and filling up of states consistent with the Fermi-Dirac statistics, we can draw an analogy to a vessel being filled with water or sand. The vessel will fill from bottom upwards till we run out of water or sand. This analogy creates
an energy level similar to \( E_f \) – assuming that we are drawing this analogy at 0 Kelvin. The information that the Fermi-Dirac distribution has captured is that the probability of occupancy is 100% for energy levels below \( E_f \), and 0% for energy levels above \( E_f \). The information that has not been captured by the Fermi-Dirac distribution is the shape of the vessel, and therefore the number of states at each of those energy levels. As can be seen from Figure 19.3 below the shapes of the vessels can be significantly different, and hence they can get filled to significantly different levels with the same amount of sand or water.

**Figure 19.3:** Analogy of sand or water being used to fill vessels of different shapes. The probability of occupancy of the container at any given height merely indicates whether or not sand or water is available at that height. To know the actual amount of sand or water held in the containers we also need to know detailed information about the shape of the containers, an aspect that is not captured by the Fermi-Dirac distribution.

The significance of the Fermi energy level is that it is the energy level at which the electrons are in a position to interact with energy levels above them. Therefore only energy values close to \( E_f \) participate in the process of gain in temperature. Greater the change in temperature, more the number of states on either side of \( E_f \) that participate in the change in temperature. Much further away from \( E_f \), the states are oblivious to the change in the temperature.

In summary, in this class we have looked at the plot of the Fermi-Dirac distribution, and examined how the distribution function varies as a function of energy, and how it varies as a function of temperature. We have also looked at the Fermi energy, which is the border across which all transactions with respect to energy occur. These are the major
features of the Fermi-Dirac distribution. We have also noted that the important information which we have not addressed is the actual number of states at each energy level, or the shape of the container in our analogy.

In the next class we will compare the Fermi-Dirac distribution to the Maxwell-Boltzmann distribution, and examine how the Drude-Sommerfeld model is better than the classical Drude model.