Engineering Physics (2025)
Course code 25PY101
Module 2 Unit 1: Quantum theories of solids

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Unit 2 Plan

1. Quantum Free Electron Theory
2. Fermi-Dirac distribution
3. Electronic specific heat of solids
4. Density of states (qualitative)
5. Success and Failures of quantum free electron theory of solids
6. E-k diagram
7. Classification of materials based on bands in solids
8. Fermi level in semiconductors- intrinsic and extrinsic

Unit 2 Plan

Quantum thermodynamics: Fermi–Dirac (FD) Statistics

- Describes occupancy of energy states by electrons that obey **Pauli exclusion principle**.
- The probability of occupation of an energy level E at temperature T and Fermi energy level E_F is given by

$$\boxed{P_{FD}(E) = \frac{1}{\exp\left(\frac{E-E_F}{k_B T}\right)+1}.}$$

  Here k_B is the Boltzmann constant equal to $1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$.
- To understand the FD statistics, let us analyze the probability function in two cases –
  1. $T \to 0$ limit
  2. $T \neq 0$

Key Insight

The Fermi-Dirac function is a result of Pauli exclusion principle.

Fermi–Dirac Statistics at the $T \to 0$ limit

- Take limit $T \to 0$ in definition:

$$P_{FD}(E) = \lim_{T \to 0} \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1} = \frac{1}{\exp\left(\frac{E - E_F}{0}\right) + 1}.$$

- This limit needs to analyzed for three cases –
  1. $E < E_F$
  2. $E > E_F$
  3. $E = E_F$

Fermi–Dirac Statistics at the $T \to 0$ limit

1. $E < E_F$

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{\text{-ve}}{0}\right) + 1} = \frac{1}{\exp(-\infty) + 1} = \frac{1}{0 + 1} = \frac{1}{1} = 1$$

2. $E > E_F$

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{+\text{ve}}{0}\right) + 1} = \frac{1}{\exp(\infty) + 1} = \frac{1}{\infty + 1} = \frac{1}{\infty} = 0$$

3. $E = E_F$

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{0}{0}\right) + 1}$$

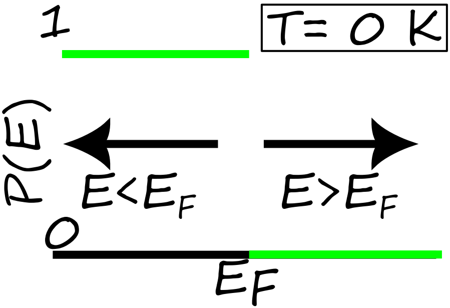
- Since $\frac{0}{0}$ is indeterminate form, $P_{FD}(E)$ is not defined at $T = 0\,\text{K}, E = E_F$.

Fermi–Dirac Statistics at the $T \to 0$ limit

- Hence, at $T = 0\,\mathrm{K}$ the distribution becomes a step function

$$P_{FD}(E) = \begin{cases} 1, & E < E_F \\ 0, & E > E_F \end{cases}$$

where E_F is the Fermi energy.



Key Insight

At $T = 0\,\mathrm{K}$, the Fermi-Dirac distribution is a step function.

Fermi–Dirac Statistics at $T \neq 0$

- At $T \neq 0$, consider $k_B T$ is a small positive quantity $+$ve.

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{E-E_F}{+\text{ve}}\right) + 1}.$$

- This limit needs to analyzed for three cases –[1]
  1. $E \ll E_F$ so that $E - E_F$ is a big negative number i.e. - -ve
  2. $E \gg E_F$ so that $E - E_F$ is a big positive number i.e. $++$ve
  3. $E = E_F$

[1] $\gg$ is symbol for very greater than and $\ll$ is symbol for very lesser than

Fermi–Dirac Statistics at $T \neq 0$

1. $E \ll E_F$ [a]

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{\text{- -ve}}{+ve}\right) + 1}$$
$$\simeq \frac{1}{\exp(-\infty) + 1}$$
$$= \frac{1}{0 + 1}$$
$$= \frac{1}{1}$$
$$= 1$$

$\therefore P_{FD}(E) \simeq 1$

2. $E \gg E_F$

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{\text{++ve}}{+ve}\right) + 1}$$
$$\simeq \frac{1}{\exp(\infty) + 1}$$
$$= \frac{1}{\infty + 1}$$
$$= \frac{1}{\infty}$$
$$= 0$$

$\therefore P_{FD}(E) \simeq 0$

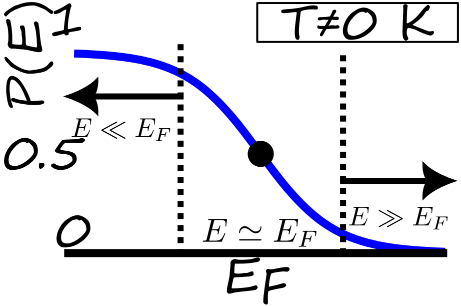
3. $E = E_F$

$$P_{FD}(E) = \frac{1}{\exp\left(\frac{0}{+ve}\right) + 1}$$
$$= \frac{1}{1 + 1}$$
$$= \frac{1}{2}$$

[a] $\simeq$ is symbol for nearly equal.

- Hence, at $T \neq 0\,\mathrm{K}$ the distribution becomes a "smeared" [2] step function

$$P_{FD}(E) = \begin{cases} \simeq 1 & E \ll E_F \\ \simeq 0 & E \gg E_F \end{cases}$$



Key Insight

At $T = 0\,\mathrm{K}$, the Fermi-Dirac distribution is a "smeared" step function.

[2] smear means smoothened.

Problems on Fermi Dirac statistics

Problem

Calculate the probability that an energy level $3k_B T$ above the Fermi energy is occupied by an electron

Problem

Calculate the probability that an energy level $3k_B T$ below the Fermi level is empty

Problem

Fermi energy of a metal is $6.25\,\mathrm{eV}$. Calculate the temperature at which there is a $1\,\%$ probability that a state $0.30\,\mathrm{eV}$ below the Fermi energy level will not contain an electron.

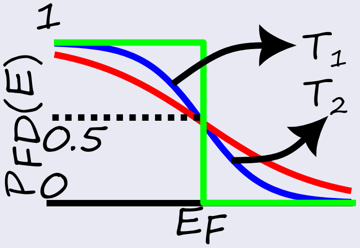
Problem

Calculate the temperature at which the probability that an energy level $0.3\,\mathrm{eV}$ below the Fermi level is occupied is 0.7.

Problem

Calculate the temperature at which the probability that an energy level $3k_B T$ above the Fermi level is occupied is 0.7. [Hint: This is a wrong question]

Problem



Statement: $T_1 > T_2$.

Is the statement true or false?

Boltzmann approximation to Fermi Dirac distribution

- In the limit of $E - E_F \gg k_B T$,

$$P_{FD}(E) \simeq \exp\left[-\frac{E - E_F}{k_B T}\right]$$

- This is called the Boltzmann approximation

Problem

Calculate the energy at which the difference between Boltzmann approximation and the Fermi-Dirac function is 5 % of the Fermi function.