Lecture 19:

1.) **RDM Redux**

In the RDM, defects are assigned to random neighboring pairs of sites. Pairs of defects always possess a zero reflection condition and hence can avoid localization.

2.) **Semiconductors:**

In the presence of disorder some of the states become localized while the rest remain extended. Typically, it is the states in the band tails that become localized first.

![Graph showing the density of states](image)
The energy at which the extended states occur is called the mobility edge. A semiconductor is a special kind of insulator in which all the filled states lie at an energy below the conducting states.

\[ \Delta = \text{energy gap} \]

To conduct, carriers must be excited from the valence band to the conduction band. Semiconductors possess a full valence band but an empty conduction band. There are two kinds of semiconductors classified based on which states exhibit the largest gap:

For GaAs:
- **Direct Gap**
  - \[ \Delta = h\text{band} = \varepsilon_f \]

For Si:
- **Indirect Gap**
  - \[ \Delta = \varepsilon_f \]

Largest gap occurs at the center of the band:
- Excitations from \( \Gamma \rightarrow X \)
In the direct case, photon energy is sufficient to excite the carriers from the V→C transition. In the indirect case, added momentum must be supplied from the lattice, for example, to make the transition possible. \(E_g\) is typically 1-2 eV.

For holes and electrons, the effective masses are of opposite signs \(\Rightarrow\) we can treat the bond discussions as

\[ \varepsilon_k = \varepsilon_c + \frac{\hbar^2}{2} \mathbf{R}^* \mathbf{M}^{-1} \mathbf{k}^2 \]

\[ \varepsilon_k = \varepsilon_v - \frac{\hbar^2}{2} \mathbf{R}^* \mathbf{M}^{-1} \mathbf{k}^2 \]

The carrier densities are

\[ N_e = \int_{\varepsilon_c}^{\infty} d\varepsilon \cdot D(\varepsilon) \cdot f(\varepsilon) = \text{density of electrons in the conduction band} \]

\[ N_h = \int_{-\infty}^{\varepsilon_v} d\varepsilon \cdot D(\varepsilon) \cdot (1-f(\varepsilon)) = \text{density of holes in the valence band} \]

There are two key limits here:

**Non-degenerate limit:** the probability of occupying states far away from the bond center is small.
\[ \Rightarrow \epsilon_c - \mu \gg k_B T. \]

or

\[ \mu - \epsilon V \gg k_B T \]

The first inequality implies that in the expression for \( N_c \)

\[ \int_{\epsilon_c}^{\infty} D(\epsilon) \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1} \approx \int_{\epsilon_c}^{\infty} D(\epsilon) e^{-\beta(\epsilon - \epsilon_c)} d\epsilon \]

\[ = \int_{\epsilon_c}^{\infty} D(\epsilon) e^{\beta(\epsilon_c - \epsilon)} d\epsilon. \]

Let us define \( N_c = \int_{\epsilon_c}^{\infty} D(\epsilon) e^{\beta(\epsilon_c - \epsilon)} d\epsilon. \)

Similarly,

\[ N_V = \int_{-\infty}^{\epsilon V} d\epsilon D(\epsilon) e^{\beta(\epsilon - \epsilon_V)} \]

\[ \Rightarrow P_h = N_V e^{-\beta(\mu - \epsilon V)}. \]

and \( n_0 = N_c e^{-\beta(\epsilon_c - \mu)}. \)

Let's take the product

\[ n_e P_h = N_c N_V e^{-\beta(\mu - \epsilon V)} e^{-\beta(\epsilon_c - \mu)} = N_c N_V e^{-\beta(\epsilon_c - \epsilon V)}. \]
In an intrinsic semiconductor \( N = P \Rightarrow \)

\[ N_i = \# \text{of carriers} = \sqrt{N_c N_p} e^{-\beta \frac{E_g}{2}} \]

where \( \beta \) is a constant and \( E_g = E_c - E_v \).

In intrinsic semiconductors, each hole is left behind by an excited electron.

**Extrinsic Semiconductor:**

In extrinsic semiconductors, a dopant atom donates an electron to the conduction band or a hole to the valence band.

Consider the case of Si:P. Here we are adding electrons to the conduction band. \( \Rightarrow \) we obtain a partially filled band, which should normally conduct. However, what is seen experimentally is that the number of carriers has to exceed a critical value for conduction.
to obtain. Let's call this critical density $n_c$. If $n > n_c$, a transition to a metallic state obtains. This is one of the most subtle problems in physics. This is the Mott transition. Let's view the problem as a dielectric one. The extra electron on P can be viewed as part of the conduction band. Let $\epsilon$ be the dielectric constant $\Rightarrow e \rightarrow e^* = e/e_{P}^2$ and $m \rightarrow m^*$.

$\Rightarrow \quad \alpha^* = \frac{\hbar^2}{m^* e^*^2} = \frac{\hbar^2}{m e^2} = \epsilon \frac{\hbar^2}{m e^2} = \frac{m^* e^*}{m} \epsilon a_0$.

In empty space, a proton binds an electron with binding energy $E_0 = e^2/2a_0$. In Si, we obtain

$$E_0 = \frac{\epsilon e^2}{2a_0} = \frac{e^2}{2} \frac{m^*}{m} \frac{m}{m^*} \times 13.6 \text{ eV}.$$ 

Typically, $\frac{m^*}{m} \approx 0.1$ and $e^* \approx 10 \Rightarrow$ the binding energy is roughly $1 (0.1)$ or $1000$ times smaller than in empty space. $\Rightarrow$ the extra electron is bound, though to a lesser extent. So let's estimate that the binding ceases when there is sufficient overlap between P atoms.

Metal

Insulator.
there should be some critical density for
transport, namely
\[ n_{\text{cr}}^\frac{1}{3} a^* = \#. \]

Let's see if we can estimate \#. The polarizability
of a phosphorus atom is
\[ \chi = \frac{9}{2} a^*^3. \]

Let's relate this to the dielectric constant using the
Clawson - Mossoetti equation.
\[
\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi \varepsilon_0 n_p \lambda}{3}.
\]

\[ \Rightarrow 3 \varepsilon - 3 = 4\pi \varepsilon_0 n_p \lambda (\varepsilon + 2) \]

\[ \Rightarrow \varepsilon = \frac{3 + 8\pi n_p \lambda}{3 - 4\pi n_p \lambda}. \]

When the dielectric constant diverges \( a^* \rightarrow \infty \) and
the wave functions overlap.

\[ \Rightarrow 3 = 4\pi n_p \lambda \]

or
\[ n_{\text{cr}}^\frac{1}{3} a^* = 0.38. \]
This is Mott's argument and it agrees fairly well with experiment. For Si \( a^* = 4.8 a_0 \) and 
\[ n_{crit} = 2.33 \times 10^{18} \text{ cm}^{-3}. \] The experimental number is 
\[ 3.74 \times 10^{18} \text{ cm}^{-3}. \] It might not be obvious but the Mott transition is a competition between the kinetic energy and the Coulomb repulsion. Recall 
\[ E_{kin} \sim \frac{k^2}{2m} n^{2/3}. \]

\[ E_{coul} = e^2 n^{1/3}. \]

\[ \Rightarrow \quad \frac{E_{kin}}{E_{kin}} = \frac{k^2}{2m} \frac{n^{2/3}}{e^2 n^{1/3}} \Rightarrow \quad \alpha_{\text{H}} n^{1/3} > 1 \]

Note the similarity of this problem to the Wigner crystal problem.