Lecture XV: Hopping Conductivity in Disordered Insulators[13]

▷ References:

Original papers:

- N. F. Mott, Philosophical Magazine **19**, 835 (1969).
- V. Ambegaokar, B. I. Halperin and J. S. Langer, Physical Review B **4**, 2612 (1971).
- A. L. Efros and B. I. Shklovskii, Journal of Physics C: Solid State Physics **8**, L49 (1975).

Reviews:

- A. L. Efros and B. I. Shklovskii in *Electron-electron interaction in disordered systems*, eds. A. L. Efros and M. Pollak. North-Holland, Amsterdam 1985.

▷ Localised states in disordered insulators

In the last lecture we studied how quantum-interference effects in disordered metals can abruptly lead to electron localisation when the Fermi level crosses the mobility edge.[14] Similarly in amorphous semiconductors, a band of localised states may exist where there are gaps in the band-structure of the ordered material.[15] [see Fig.12] In either case, if the Fermi energy falls in the localised band, the dc conductivity will vanish at zero temperature. At finite temperatures, transport in such insulators takes place by hopping between localised sites. Such transport is a very nontrivial competition of inelastic scattering with thermal activation and long-range Coulomb interaction.

▷ Activationless hopping conductivity

Denote by $\bar{N}$ the average density of states per unit volume near the Fermi energy. If the localised electron wavefunctions overlap strongly, then an inelastic collision can enable a transition between states with different energies. The distance between these states is of the order of the localisation length. Thus inelastic collisions lead to a diffusion with the coefficient

$$D \sim \frac{\xi_{\rm loc}^2}{\tau_{in}}.$$

The conductivity is proportional to the diffusion coefficient. The situation may change at lower temperatures where inelastic collisions involve very small energy changes, or when considering states with much shorter localisation lengrh. This will be the subject of the rest of the lecture.

[13]Lecture notes prepared by Vikram Tripathi

[14]Just as a reminder, the scaling theory of localisation predicts a mobility edge in three dimensions but not in one or two dimensions.

[15]The localisation length in a dirty metal would be much larger than the mean free path, while the amorphous semiconductor represents a situation where the localisation length is much smaller than the distance between the impurities.

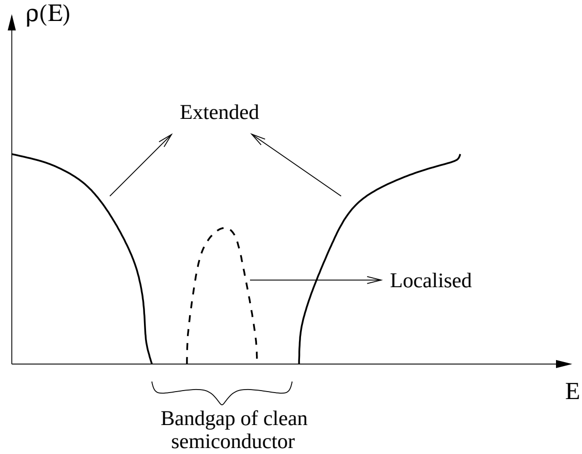

Figure 12: Extended and localised states in disordered semiconductors.

▷ Mott variable-range hopping (VRH) conductivity

DC conductivity of amorphous Ge in the temperature range $60K \leq T \leq 300K$ obeys the law

$$\sigma(T) \propto \exp[-(T_0/T)^{1/4}].$$

Similar temperature dependences are observed in many other amorphous semiconductors for a range of temperature. Mott (1969) explained this in terms of a picture where charge is transported by the thermally-excited hopping of electrons between randomly placed potential wells (impurities).

• Physical picture of Mott VRH

The number of states per unit energy range in a spherical volume of radius R is of the order of $\bar{N}R^d$. In other words, on the average, one state may be found in the energy range $\Delta E(R) = (\bar{N}R^d)^{-1}$. Therefore thermally assisted hopping of a charge over a distance R is suppressed by a Boltzmann factor $\exp[-(\Delta E(R)/k_BT)]$. Clearly this probability is larger if the hopping distance R is large. On the other hand, tunnelling in the insulator is exponentially suppressed by a factor $\exp[-(R/\xi_{\rm loc})]$, where $\xi_{\rm loc}$ is the localisation length. Combining these two factors, the probability $p(R)$ to hop a distance R is

$$p(R) = \exp\left[-\left(\frac{R}{\xi_{\rm loc}} + \frac{\Delta E(R)}{k_BT}\right)\right].$$

The dominant contribution to the conductivity comes from hops of size $R = R_*^{\rm Mott}$ for which $p(R)$ is maximised:

$$\left.\frac{dp(R)}{dR}\right|_{R=R_*^{\rm Mott}} = 0 \qquad \Rightarrow \qquad R_*^{\rm Mott} = \left(\frac{\xi_{\rm loc}\, d}{k_BT\bar{N}}\right)^{\frac{1}{d+1}}.$$

The resulting optimum hopping probability is

$$p(R_*^{\rm Mott}) = \exp\left[-\left(\frac{T_0^{\rm Mott}}{T}\right)^{\frac{1}{d+1}}\right], \text{where } \mathrm{T_0^{Mott}} = \frac{2^{\frac{1}{d+1}}\mathrm{d}}{\xi_{\rm loc}^{\rm d}\bar{\mathrm{N}}\mathrm{k_B}}.$$

The 3D case ($d = 3$) explains the experimentally observed behaviour $\sigma(T) \propto \exp[-(T_0/T)^{1/4}]$.

- What did we assume?

(a) $\bar{N}$ is constant and finite at the Fermi energy.

(b) We ignored inhomogeneities in the impurity distribution. Inhomogeneities create bottlenecks in transmission which become important in the insulating phase because charge cannot be transferred through the system if a path cannot be found between the leads. Refer to Ambegaokar *et al.* (1971) for a realistic treatment where spatial uniformity of impurities is not assumed.

More problematic is the first assumption. Following Mott's work, the understanding emerged [Ambegaokar *et al.*, 1971; Efros, Shklovskii, 1975] that the density of states at the Fermi energy in insulators will be suppressed in presence of long-range Coulomb interactions. In a metal, the electrons screen the Coulomb interaction so that the field of a charge does not extend beyond the Thomas-Fermi screening length, thus the density of states at the Fermi energy is a constant.

▷ Coulomb effects on single-particle density of states

The main effect of Coulomb interactions is already present in the static properties such as the density of states. The density of states turns out to be gapped at the Fermi energy in presence of Coulomb interactions. To obtain the conductivity, one needs to consider, besides Coulomb interaction, inter-impurity hopping.

I will show that $\bar{N}$ must vanish at the Fermi energy as a power law in presence of long-ranged Coulomb interactions,

$$\bar{N}_E \propto E^{d-1}.$$

Thus Mott's VRH behaviour will be observed in a disordered insulator only if the long-range part of Coulomb interaction is screened out.

Model Hamiltonian

$$H = \sum_i n_i \varphi_i + \frac{e^2}{2} \sum_{i \neq j} \frac{n_i n_j}{R_{ij}}.$$

The electron distribution is very nontrivial because the energy E_i of an electron on the i^{th} site depends on the electron occupation of all the other sites,

$$E_i = \varphi_i + e^2 \sum_{i \neq j} \frac{n_j}{R_{ij}}.$$

If an electron is moved from an occupied site i to an unoccupied site j, the change in energy of the system is

$$E_{ji} = E_j - E_i - \frac{e^2}{R_{ij}},$$

where e^2/R_{ij} is the Coulomb attraction of the electron-hole pair in the final configuration. These electron-hole excitations are the lowest charge-conserving excitations of the system.

Taking the ground state energy as zero, all excited states will have positive energy,[16]

$$E_{ji} > 0.$$

Our previous discussion of Mott VRH for non-interacting electrons had demonstrated that for a given hopping distance R_{ij}, one state is available with an energy separation $(E_j - E_i) = (\bar{N} R_{ij}^d)^{-1}$ on the average.

Turning the argument, given an energy separation $(E_j - E_i)$, the hopping distance for Mott VRH is $R_{ij} = [\bar{N}(E_j - E_i)]^{-1/d}$.

The Coulomb interaction energy for the electron-hole pair at this separation is

$$E_{ij}^{\text{int}} = -\frac{e^2}{R_{ij}} = -e^2 \left[\bar{N}(E_j - E_i)\right]^{\frac{1}{d}}.$$

- *The punch line*

The interaction energy cannot have a larger magnitude than $E_j - E_i$ for then we cannot satisfy the requirement that the excitation energy $E_{ji} = E_j - E_i + E_{ij}^{\text{int}} > 0$. In other words,

$$\bar{N} = \bar{N}_{E_j - E_i} < \frac{1}{e^{2d}} (E_j - E_i)^{d-1}.$$

Clearly, at the lowest energies, the density of states $\bar{N}$ must vanish at least as fast as $(E_j - E_i)^{d-1}$, else the excitation energy will not be positive.

- Density of states

So far we have found that the density of states $\bar{N}_E$ vanishes at least as fast as E^{d-1}. Now we argue that $\bar{N}_E \propto E^{d-1}$.

Suppose $\bar{N}_E$ decreases faster than E^{d-1}, say $\bar{N}_E \propto E^{d-1+\alpha}$, $\alpha > 0$. Then the interaction energy

$$E^{\text{int}} = -e^2 \left[\bar{N}_E E\right]^{1/d} \propto E^{1+(\alpha/d)} \ll E \text{as} E \to 0.$$

Thus for any finite α and small E, the interaction energy will be irrelevant compared to the non-interacting part E. In that case, we could have disregarded Coulomb interaction at the outset. The only consistent solution is therefore $\alpha = 0$, hence

$$\bar{N}_E = \frac{A}{e^{2d}} E^{d-1}, \text{where} A < 1 is a constant.$$

[16] $E_{ji} > 0$ also means that $R_{ij} > e^2/(E_j - E_i)$, thus the electron-hole "exciton" cannot collapse.

This argument for the Coulomb gap in the density of states was presented by Efros and Shklovskii in 1975.

▷ Efros-Shklovskii variable-range hopping conductivity

Following Mott's VRH argument, the probability $p(R_{ij})$ to hop a distance R_{ij} is

$$p(R_{ij}) = \exp\left[-\left(\frac{R_{ij}}{\xi_{\mathrm{loc}}} + \frac{E_{ji}}{k_B T}\right)\right],$$

where

$$E_{ji} = E_j - E_i - \frac{e^2}{R_{ij}} = (1 - A^{1/d})\frac{e^2}{R_{ij}}.$$

The dominant contribution to the conductivity comes from hops of size $R = E_*^{\mathrm{ES}}$ for which $p(R)$ is maximised,

$$R_*^{\mathrm{ES}} = \sqrt{\frac{(1 - A^{1/d})e^2\xi_{\mathrm{loc}}}{k_B T}}.$$

The resulting optimum probability is

$$p(R_*^{\mathrm{ES}}) = \exp\left[-\sqrt{T_0^{\mathrm{ES}}/T}\right], \text{where } \mathrm{T}_0^{\mathrm{ES}} = \frac{4\mathrm{e}^2(1 - \mathrm{A}^{1/\mathrm{d}})}{\xi_{\mathrm{loc}}\mathrm{k}_\mathrm{B}}.$$

Note that the Efros-Shklovskii VRH law is the same for any dimension, unlike Mott's VRH.