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ELECTRON LOCALIZATION IN DISORDERED SYSTEMS

(Part I)

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1. Minimum Metallic Conductivity :-

(see e.g. Mott and Davis).

$$\sigma = \frac{ne^2\tau}{m} = ne^2\frac{v_F\ell}{m v_F} = \frac{e^2}{\hbar}\left(\frac{n\ell}{k_F}\right) \quad (1\cdot1)$$

a) In three dimensions, $n = \frac{k_F^3}{3\pi^2}$ for a free electron gas, so that

$$\sigma_{3d} = \left(\frac{e^2}{\hbar\pi^2}\right)\left(\frac{k_F\ell}{3}\right)k_F \quad (1\cdot2a)$$

b) In two dimensions, $n = \frac{k_F^2}{2\pi}$, and $\sigma_{2d} = \left(\frac{e^2}{\hbar\pi^2}\right)\frac{\pi}{2}(k_F\ell)$. (1·2b)

These expressions have been derived for weak disorder, i.e. for a degenerate gas of nearly free electrons scattered occasionally by impurities or by other static disorder. One assumes large ℓ, i.e. ℓ large compared to interatomic spacing, a.

Ioffe and Regel pointed out that a the mean free path could not be smaller than interatomic spacing because the electrons have to scatter against something. Certainly for very strong disorder, this mode of description breaks down, and the limit

$$\ell \sim a \quad (1\cdot3a)$$

is the smallest ℓ for which the simple diffusive transport picture leading to (1·1) is valid. Since $a \sim k_F^{-1}$, the Ioffe Regel condition is approximately

$$k_F\ell \gtrsim 1 \quad . \quad (1\cdot3b)$$

Mott used this limit to argue that there is a minimum metallic conductivity $\sigma_{min.}$ characterized by $k_F\ell \simeq 1$. There is very extensive experimental evidence that the nature of quantum transport changes at around $\sigma_{min.}$. This evidence has been analyzed and discussed by Mott in a long series of papers and has been summarized in the book by Mott and Davis. Many experiments were stimulated by this concept.

We discuss later the question of whether $\sigma_{min.}$ marks a change of regime i.e. whether it is a quantum scale of conductivity, or whether it is actually a precise discontinuity, i.e a jump at $T=0$ in going from metal to insulator as disorder is varied.

Returning to Eq. (1·2) for σ and substituting the Ioffe-Regel condition (1·3b), we have

$$\sigma^{3d}_{min.} \simeq \frac{e^2}{3\hbar\pi^2}k_F \quad (1\cdot4a)$$

$$\simeq \frac{e^2}{\hbar\pi^2}\frac{1}{3a} \quad (1\cdot4b)$$

$$\sigma^{2d}_{min.} \simeq \frac{e^2}{2\pi\hbar} \quad (1\cdot4c).$$

Note We notice the following :-

(i) $\sigma_{min.}$ involves $\hbar$, Planck's constant.

One is talking about limits to quantum diffusion, at $T = 0$.

(ii) In 2d, $\sigma_{min.}$ has the dimensions of conductance, g, and is universal. The value mentioned above is

$$\sigma^{2d}_{min.} \simeq [30,000\,\Omega]^{-1}$$

or $$R^{2d}_{max} \simeq [30,000\,\Omega]$$

a rather small number!

The result means :- there are no thin metallic films with $R_\square$ (Resistance per square anything) $> 30,000\,\Omega$.

(iii) In 3d, $\sigma_{min.}$ depends on material parameters, i.e. inversely on interatomic spacing. To fix our ideas about numbers, consider two examples.

α) $a \sim 10^{-8}$ cm (typical for metals).

$$\rho_{max.} \simeq 3a\left(\frac{\hbar\pi^2}{e^2}\right) \simeq 3 \times 10^{-8} \times 4 \times 10^{4}$$

$$\simeq 1{,}000\ \mu\Omega\ \text{cm}.$$

β) $a \sim 50 \times 10^{-8}$ cm (e.g. P or doped Si, size of donor orbit)

$\rho_{max} \simeq 50,000\ \mu\Omega$ cm $\simeq$ 50 mΩ cm.

2. Anderson Localization :-

[P.W. Anderson, 109, 1492 (1958)

D. J. Thouless, Phys. Rep. 13C, 1974

also PWA and DJT in Ill Condensed Matter, eds. R. Balian and G. Toulouse, Gordon and Breach

Also D.J. Thouless, J. Phys. C 3, 1559 (1970)].

Anderson discussed in 1958 the nature of eigenstates for strong disorder. In the model considered by him, the Hamiltonian is of the tight binding form

$$H = \sum_i |i\rangle \epsilon_i \langle i| + \sum_{j\,i} |j\rangle V_{ji} \langle i| \qquad (2.1)$$

with the sites i located on a lattice. The site energies ϵ_i are random, e.g. independently and randomly distributed with uniform probability over the range $(-W/2)$ to $(W/2)$. [In a perfect periodic lattice ϵ_i has the same value, say zero, for all sites i]. The hopping integral V_{ji} is assumed, for simplicity, to connect nearest neighbours only, i.e. $V_{ij} = V$ for nearest neighbours and $V_{ij} = 0$ otherwise. The degree of disorder is measured by the dimensionless ratio $(W/2ZV)$. The numerator is a measure of fluctuations in the potential energy, and the denominator is the bandwidth of the perfect lattice, i.e. a measure of kinetic energy of the system. Z is the number of nearest neighbours (coordination number).

For weak disorder, i.e. $(W/2zV) \ll 1$, one has Bloch electrons weakly scattered by rather small potential fluctuations, i.e. extended states, and a conductivity going as W^{-2}. For strong disorder, the natural question to ask is :- suppose there is an electron at a particular site, say i. What is the probability that it stays there? If this probability is nonzero, the state is localized; otherwise it is extended. To estimate this probability, Anderson considered larger and larger excursions from the site i, and investigated the convergence of this sequence. For example, consider the first step. The amplitude on the nearest neighbour site j is

$$V/(\epsilon_i - \epsilon_j) \qquad \cdot (2\cdot2)$$

A typical value of the magnitude of the energy denominator is $(W/4)$. However, the site i connects to z nearest neighbours, so that the z terms $|\epsilon_i - \epsilon_j|$ are distributed uniformly in the range 0 to $\frac{W}{2}$. The smallest of them is $\sim \left(\frac{W}{2z}\right)$ th and this obviously controls the convergence of (2·2), so that very crudely, the perturbation series in hopping may be expected to converge if

$$(2zV/W) < 1$$
$$\text{or} \quad (W/2zV) > 1 \qquad (2\cdot3).$$

This is not far from the best numerical estimates, as we shall see.

Anderson's analysis is detailed and involves many subtle points, analysed and summarized very clearly by Thouless (1970). Only a very brief outline is sketched here. One problem concerns accidental degeneracies. If two states i and i' connected by hopping are close by in energy, they may contribute largely to the energy shift or self energy δ_i. However, as one knows from degenerate perturbation theory, if there is a nonvanishing matrix element λ between two such states, the new eigenstates are $\simeq 2\lambda$ apart. A similar effect arises here on resummation of perturbation terms in a particular way, so that the effective energy denominators are always of order W.

The second point concerns the meaning of perturbation series. Since the ϵ_i are random numbers with a given probability distribution, a particular term in the series is also a random number. The question to ask is :- what is the probability that say the nth order term in V has this value or that value. Anderson showed that this probability distribution was long tailed under the assumption of statistical independence of factors in the product. He established that the series converges with probability very close to one if

a condition close to Eq. (2·2) was satisfied. This is the criterion for localization, ~~derived for a state in the centre~~

The most accurate numerical estimates of localization are due to Wearie and Srivastava (1978). They find that states in the centre of the band are localized if

$$\left(W/zV\right) > 2\cdot3 \quad (3d, \text{simple cubic lattice})$$

$$\left(W/zV\right) > 1\cdot2 \quad (2d, \text{square lattice}).$$

The ~~nature of~~ eigenstates ~~has been~~ for large disorder are exponentially localized. This is most clearly seen in the graphic simulation results of Yoshino and Okazaki (J. Phys. Soc. Japan 43, 415-23 (1977)). ~~An analytical estimate of localization length~~

~~In~~ For large disorder, the localization length is small. ~~For~~ As the disorder decreases to the critical value, the localization length increases, and diverges for critical disorder. An estimate of the exponent has been obtained by Anderson and others by calculating the propagator G_{ij} in the localized regime using self avoiding walk ideas. The result is

$$G_{ij} \sim \exp\{-R_{ij}/\lambda\}$$

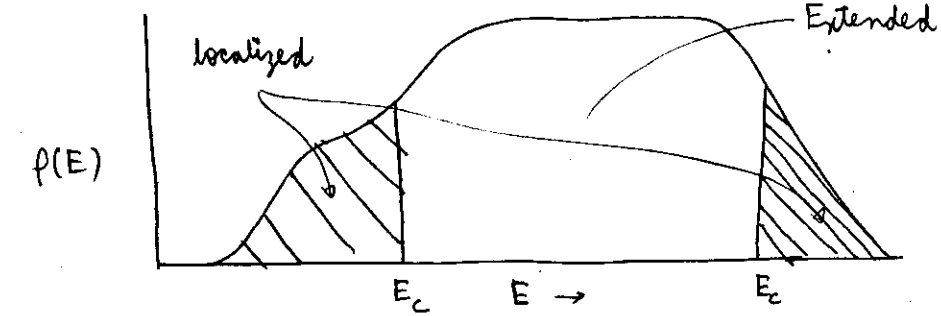
where

$$\lambda = |W - W_c|^{-3/(d+2)}$$

d being the dimensionality.

3. Mobility Edge and its consequences:-

~~For~~ for an electron of given energy, there is a well defined critical disorder. This depends on the energy of the electron, so that for a given disorder, electronic states of some energy are localized, other not. Consider then a density states curve for a given disordered system. There is a sharp energy (or energies) E_c dividing states into those which are extended and others which are Anderson localized.



This idea was introduced by Mott who called these mobility edges since they separate mobile (extended) states from immobile (localized) ones. As disorder increases, more and more states localize, or in our schematic picture above the mobility edges approach each other. For large enough disorder, all states in the band can be localized.

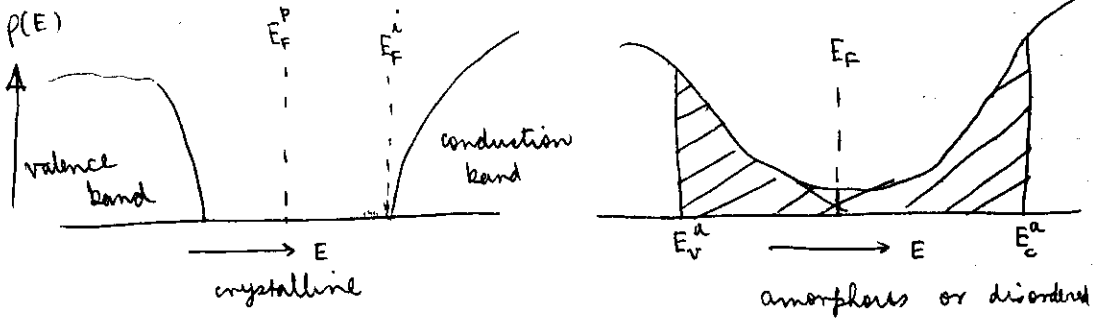
Now consider such disordered a system with say N electrons. Neglecting interaction effects, the

lowest N eigenstates will be occupied. Depending on disorder and N, the Fermi level ϵ_F can lie in the region of localized states, or in the region of extended states. The lowlying excitations are localized in the former case, so the system is an insulator. It is a new kind of insulator, due to disorder, and differs in many of its properties from crystalline semiconductors or insulators.

One can imagine either changing the disorder or the electron concentration or both, such that E_F sweeps past E_F. One then has a disorder caused metal insulator transition due to localization. This has been labelled by Mott as the Anderson transition.

We briefly discuss qualitatively some properties of the Anderson insulator.

i) Consider a disordered semiconductor.



The valence and conduction band state densities can overlap and a possible schematic form of the density of states is as shown above, with the localized states shown shaded (This is known as the Cohen Fritzsche Ovshinsky or CFO model). The Fermi level is as shown.

The most prominent optical absorption requires a minimum energy ($E_c^a - E_F$), so that there is an energy gap below which photons are not strongly absorbed. [There could be weak absorption due to transitions to unoccupied localized states]. Thus even though there are states all the way through from E_F to E_c^a, there is an effective gap.

Suppose the semiconductor is doped, i.e.g. donor electrons are added to it. They will go to the lowest unoccupied states, close to E_F. Of these there is a finite density, and these are all localized. So with small doping, there is no particular change in the nature of the insulator, i.e. in its electrical properties. Contrast this with the crystalline semiconductor, which has (when pure) Fermi energy in the middle of the gap which is entirely bereft of states. Adding a small concentration of donors therefore shifts the Fermi level immediately to near the conduction band bottom (See Figure). In an amorphous semiconductor, the Fermi level is 'pinned' by the nonzero density of states there, and this is the basic cause of its insensitivity to doping. The result is general and does not depend on a particular model for density of states.