Localization I: General considerations, one-parameter scaling

Traditionally, two mechanisms for localization of electron states in solids:

(a) Mott mechanism, interactions: believed to work even in pure crystalline lattice: many-electron effect. Typically sets in *abruptly* (first order phase transition)

(b) Anderson mechanism, disorder, believed to exist even in absence of interactions. Typically sets in smoothly (second order phase transition in 3D)

In real life, both effects may be simultaneously present, and more generally there is an important question about effects of interactions on mechanism (b) [cf. L. 7]. Here will discuss only (b), for *noninteracting* electron system. We will consider $T = 0$ until further notice.

Preliminaries

Random walk in d dimensions. Consider first a simple drunkard's walk: At each step the drunkard takes one step along each axis, positive or negative at random (and uncorrelated). Consider motion along one ($z-$) axis. After an (even) number N of steps, the probability of being back at $z = 0$ is $2^{-N}N!/[(N/2)!]^2 \approx (2/\pi)^{1/2}N^{-1/2}$. So in d dimensions the probability of returning to the origin after N steps is approximately $(2/\pi)^{d/2}N^{-d/2}$. Hence, average number of returns to the origin made (say) between N and $2N$ steps is $\sim N^{-1/2}$ in 3D, constant in 2D and $\sim N^{1/2}$ in 1D. I.e. in 1D or 2D, but not in 3D, "return to the origin" is virtually certain if we wait long enough.

This result is not confined to the special model: Generally, for a model of classical diffusion in d dimensions starting from a δ-function distribution, the probability density $P(0,t)$ at the origin after time t is proportional to $(Dt)^{-d/2}$ (D = diffusion coefficient), so the quantity $\int_0^\infty P(0,t)\,dt$ is infinite in 1 or 2D (but finite in 3D).

However, in classical diffusion the *average* probability of being at the origin in the limit of infinite time, that is $\lim_{T\to\infty} T^{-1}\int_0^T P(0,t)\,dt$, is zero for all d, i.e. there is no localization (but the above remark is still important, cf. below). In QM things are rather different ...

A rather more general result follows from a consideration (á la Landauer) of a succession of partially reflecting barriers in 1D (Imry, §5.3.1).

In general, if we have in series two barriers with reflectances R_1, R_2 and transmittances T_1, T_2, then the overall reflectances and transmittances R_{12}, T_{12} are given by (L. 3)

$$T_{12} = \frac{T_1 T_2}{1 + R_1 R_2 - 2\sqrt{R_1 R_2}\cos\theta} \tag{1}$$

$$R_{12} = 1 - T_{12} \tag{2}$$

and so

$$\frac{R_{12}}{T_{12}} = \frac{R_1 + R_2 - 2\sqrt{R_1 R_2}\,\cos\theta}{T_1 T_2} \tag{3}$$

where the angle θ is given (L. 3) by $2\phi + \arg(r_2 r_1')$ where ϕ is the phase difference accumulated between 1 and 2 and r_2, r_1' the appropriate (complex) reflection coefficients. The result (3) is exact.

Suppose now that we naively average over the "random" quantity $\cos\theta$. Then on average we will have

$$\overline{\left(\frac{R_{12}}{T_{12}}\right)} = \frac{R_1 + R_2}{T_1 T_2} \equiv \frac{R_1 + R_2}{(1-R_1)(1-R_2)} \tag{4}$$

Now it is clear that for any given barrier the quantity R/T is some measure of the resistance (inverse conductance) associated with the barrier: indeed, in the Landauer approach we have exactly for resistance $\equiv G^{-1}$, (*provided* $L_{\rm in} \gg$ distance between the barriers!)

$$G^{-1} = \frac{\pi\hbar}{e^2}\left(\frac{R}{T}\right) \tag{5}$$

If now we add the resistances of the two junctions 1 and 2, we find

$$(G^{-1})_{\rm add} = \frac{\pi\hbar}{e^2}\left(\frac{R_1}{T_1} + \frac{R_2}{T_2}\right) = \frac{\pi\hbar}{e^2}\frac{R_1 + R_2 - 2R_1R_2}{(1-R_1)(1-R_2)} \tag{6}$$

On the other hand (4) gives

$$(G^{-1})_{\rm tot} = \frac{\pi\hbar}{e^2}\frac{R_1 + R_2}{(1-R_1)(1-R_2)} > (G^{-1})_{\rm add} \tag{7}$$

In other words, when averaged in this way the total resistance due to two barriers is *greater* that the resistances of each separately!

Suppose now we have a whole series of barriers in series. However small the R of each, eventually, n becomes large enough that the total R_n is ~ 1. Now suppose we add one more barrier of reflectance $R \ll 1$. Neglecting the R in the denominator, we find from (4)

$$\overline{\left(\frac{R_{n+1}}{T_{n+1}}\right)} = \frac{R_n + R}{T_n} \tag{8}$$

or in terms of the dimensionless resistance $g^{-1} \equiv G^{-1}/\frac{\pi\hbar}{e^2}$,

$$\overline{g_{n+1}^{-1}} = g_n^{-1} + R/T_n \tag{9}$$

or since $T_n^{-1} = g_n^{-1} + 1$,

$$\frac{d\overline{g_n^{-1}}}{dn} = R(g_n^{-1} + 1) \tag{10}$$

so that the dimensionless resistance increases linearly while it is $\lesssim 1$ but thereafter *exponentially*, indicating localization.

Actually the above result is a bit too naive, in fact one should average not g_n^{-1} itself but rather $\ln(1 + g_n^{-1})$ (see Imry, p. 102). The result is that one finds

$$\langle \ln(1 + g_n^{-1}) \rangle = p_1 n \tag{11}$$

where p_1 is the dimensionless resistance (R/T) for a single barrier. To the extent that one can identify $\langle \ln g^{-1} \rangle$ with $\ln \langle g^{-1} \rangle$, the above result is recovered.

$\star$ PP "pair" exception

Classical (Drude) conductivity: Dimensional considerations.

Reduce the true d-dimensional quantum transport problem to a *Boltzmann equation*, in which any effects of interference between scattering by different impurities is neglected. If cross-section for a single impurity is $\sigma_{\rm imp}$, introduce mean free path $l \equiv 1/n_{\rm imp}\sigma_{\rm imp}$; this is then only length scale in problem (other than ${k_{\rm F}}^{-1}$, cf. below).

For a degenerate Fermi system the Drude expression for the *conductivity* σ is

$$\sigma_{\rm Dr} = ne^2\tau/m \qquad (\sim \frac{e^2}{\hbar}{k_{\rm F}}^2 l \ \text{ in 3D}) \tag{12}$$

Useful to introduce *conductance* G of a specified (e.g. hypercubic) shape of linear dimension L. Note that the dimensions G are $I/V = QT^{-1}/EQ^{-1} \sim Q^2/ET \sim e^2/\hbar$, so useful to introduce dimensionless conductance $g(L) \equiv G(L)/(e^2/\hbar)$ (nb. $e^2/\hbar \approx 2.5 \cdot 10^{-4}\,\Omega^{-1}$(S)). In Drude theory we have

$$g(L) = \sigma_{\rm Dr} L^{d-2}/(e^2/\hbar) \tag{13}$$

Note that in 2D, where $\sigma_{\rm Dr} = n_a e^2\tau/m$, we have $n_a = {k_{\rm F}}^2/2\pi$, so since $\tau = l/v_{\rm F} = lm/\hbar k_{\rm F}$ we have $\sigma_{\rm Dr} = (e^2/2\pi\hbar)(k_{\rm F} l)$ or

$$\boxed{g^{\rm 2D}_{\rm Dr} = \frac{1}{2\pi}\, k_{\rm F} l} \qquad \text{also} \qquad \boxed{g^{\rm 1D}_{\rm Dr} = \frac{1}{\pi}\,\frac{l}{L}} \qquad \begin{matrix}\text{for two}\\ \text{spin species}\end{matrix} \tag{14}$$

We will see that, crudely speaking, the criterion for localization effects to be important is $g(L) \lesssim 1$. In 3D, since $g_{\rm Dr}(L) \sim L$, if this criterion is not met at short distances it is unlikely to be met at larger ones. In 1D ($g \sim L^{-1}$) however, even the Drude conductance satisfies the criterion for sufficiently large L. In 2D it is not immediately clear what is going to happen.

Note that in Drude theory the quantity τ, and thus the conductance, almost invariably *decreases* with increasing temperature. In particular, for a textbook (3D) metal the standard formula at low T ($\ll \theta_{\rm D}$) is

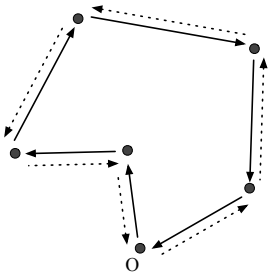
$$\tau^{-1} \ \propto \ \underset{\text{static imps}}{A} \ + \ \underset{\text{el-el}}{BT^2} \ + \ \underset{\text{phonos}}{CT^5} \tag{15}$$

Note that the sense of "3D" metal for this formula to hold may be much weaker than the one used below (i.e. (15) may hold even for metals which are 2 or 1D from the localization point of view).

Weak localization - the basic physical idea.

Let's assume that the single-particle Hamiltonian is closed (e.g. no phonons, no el-el interaction ...) and *invariant under time reversal (this is crucial)*. Then consider those paths which start and finish at some point (arbitrary chosen as origin). Classically, the *probability* of returning to the origin is just the sum of the probabilities of propagating along each path separately. In QM, on the other hand, the *amplitude* of return is the sum of amplitudes to do so by different paths (and the total return probability is the square of the total amplitude), so we may get interference effects. In fact,

$$P_{\rm tot} = |A_{\rm tot}|^2 = |\sum_i A_i|^2 = \sum_i P_i + 2\,{\rm Re}\sum_{ij} A_i^* A_j \qquad (16)$$



For a couple of randomly selected paths i, j there is no special phase relation between A_i and A_j, so the cross-term averages to zero. However, for pairs of *time-reversed* states as shown, $A_i = A_j$ in the absence of T-violating effects and thus the summed (interference) term contributes equally to the first. Thus the total return probability is exactly twice its classical value and the conductivity σ (and conductance G or g) is *less* than its classical value. Since the *classical* probability of return is higher in 2D than in 3D (and even more in 1D) one might expect intuitively the the weak-localization effect should be stronger in 2D and even more in 1D. Moreover, the probability of return should be larger for smaller diffusivity, i.e. larger resistivity.

Scaling theory: The Thouless argument. (Nb: $L_{\rm in} \to \infty$!)

Imagine combining large blocks of side L to make super-blocks. Will the single electron states tend to localize within the original blocks, or will they extend over the super-blocks? According to Thouless, this depends on the ratio of two energies, δW and ΔE. δW is simply the level spacing within the original block and is of order $(N_0 L^d)^{-1})$ where N_0 is the single-electron DoS. ΔE is essentially defined as the "sensitivity of a typical energy level to the boundary conditions" (e.g. antiperiodic vs. periodic) but may be more useful to think of it as an effective "hopping matrix element" from one block to the next. In that case it should be of order $\hbar/\tau(L)$ where $\tau(L)$ is the time taken to traverse the block. If the motion on scale L is diffusive (true if $L \gg l$, elastic mean free path) than for any dimension $\tau(L) \sim L^2/D$, so the "Thouless energy" ΔE is $\sim \hbar D/L^2$. Thouless argued that when $\Delta E \gg \delta W$, the states would be extended whereas when $\Delta E \ll \delta W$, they should be localized within a single block (cf. the impurity problem with $\langle V^2\rangle^{1/2} \gg t$). More generally, the rate at which the conductance changes as a function of L should depend, apart from dimensionality and L itself, only on the ratio $\Delta E/\delta W$. Now according to the above, we have

$$\Delta E/\delta W \sim (\hbar D/L^2)/(N_0 L^d)^{-1} = \hbar D N_0 L^{d-2} \qquad (17)$$

But N_0 is of the order[1] of the static "neutral compressibility" χ_0, and $D\chi_0$ is simply e^{-2} times the electrical conductivity σ. Moreover, the conductance $G(L)$ is (independently of Drude theory, provided σ is implicitly a function of L) just σL^{d-2}. Hence

$$\Delta E/\delta W(L) \sim (\hbar/e^2)\sigma L^{d-2} \equiv G(L)/(e^2/\hbar) \equiv g(L) \tag{18}$$

Thus, apart for a factor ~ 1, the Thouless ratio is simply the dimensionless conductance!

One-parameter scaling.

It is convenient at this point to introduce the quantity

$$\beta(g) \equiv d(\ln g)/d(\ln L) \tag{19}$$

and moreover to redefine (for subsequent convenience) the quantity $G(L)$ to be the conductance of a hypercube (block) of side πL rather than L (clearly this does not affect the above order-of-magnitude estimates). Then the one-parameter scaling hypothesis is, following Thouless, that for given spatial dimension d,

$$\boxed{\beta(g) = \begin{array}{c}\text{function of } g \\ \text{only}\end{array}} \tag{20}$$

What do we know about the dependence of $\beta(g)$ on g? Suppose, first, that in a given system we know that as $L \to \infty$ we iterate to the Drude form, i.e. $g(L) \sim \sigma L^{d-2}$ where σ is independent of L. Then from the explicit definition of $\beta(g)$ above we have $\beta(g) = d - 2$ in this limit. On the other hand, if the electron states in a block of side $\sim L$ are localized on a scale of some length ξ, then we expect that $g(L) \sim L^{d-2} \exp -L/\xi$, and so within logarithmic accuracy $\beta(\xi) = -L/\xi = -\ln(g_0/g)$ (< 0), where g_0 is the dimensionless conductance at scale ξ. (The exact result is $\beta(g) = (d-2) - \ln g_0/g$). We expect this result to be generic in the limit $g \to 0$ ($g \ll 1$). We will furthermore see below that for *large* g ("weak localization" limit) the form of the scaling function is (with the above choice of definition for $G(L)$) simply

$$\beta(g) = (d-2) - \alpha/g \tag{21}$$

where $\alpha = 1/\pi^2$ for any dimension g.

Quite generally, by the Thouless argument, one would expect that the β-function has the form

$$\beta(g) \equiv \frac{d\ln g}{d\ln L} = (d-2) + f_L(g) \tag{22}$$

where the "localization" correction $f_L(g)$ is *always negative* (or at best zero). Hence, in 1D, the conductance tends to zero with increasing L farther than the Drude result ($g \propto L^{-1}$), in agreement with what we found by the Landauer approach for a *strictly* 1D system. On the basis of the above argument, we should expect that when L reaches a

[1] This relation might fail e.g. very close to a CDW transition.

value ξ such that $g(\xi) \sim \epsilon$ (where ϵ is some number $\lesssim 1$), then localization should set in so that for $L \gg \xi$ we have $g(L) \sim \exp -L/\xi$. To estimate ξ we simply approximate g by its Drude form (thereby obtaining an upper limit); since $g_{\rm Dr}(l) = l/(\pi L)$, it immediately follows that $\xi \sim l$, i.e. for a 1D system the localization length is just of the order of the elastic mean free path.

In 2D we see that $\beta(g)$ is again always < 0, and hence we expect g to decrease with L and eventually reach a point where localization will set in. However, if we insert the weak-localization form for g the decrease is very slow ($g \sim g_0 - \ln L/l$). Since in this result g_0 is $g(l)$, which again we approximate by its Drude value $k_{\rm F} l$, the resulting estimate for ξ is exponentially large:

$$\xi_{\rm 2D} \sim l \exp(\text{const } k_{\rm F} l) \tag{23}$$

(where a more detailed consideration shows that the constant is $\pi/2$). Nevertheless, it is always finite, so we reach the generic conclusion that in the one-parameter scaling theory *all electron states are localized in 2D.*[2] This conclusion may be seen to be insensitive to the details of the behavior of the scaling function $\beta(g)$, provided that the latter is bounded above by some negative constant.

In conclusion, it should be emphasized that by its nature the one-parameter scaling argument assumes

(a) that the electrons are completely noninteracting (not only with one another but with phonons, etc.) and

(b) that there are no characteristic lengths in the problem larger than the elastic mean free path l (other than the localization length ξ itself).

[2] *But*, even if states localized, finite σ at finite T, because of variable range hopping.