Weak localization: Quantitative treatment

References:


Need to bear in mind:

1. Generality of “WL” effect: localization of photons, phonons, etc. (any kind of wave in disordered medium—Bergmann’s “shouting into the forest” example.)

2. Dimensionality: Generally speaking, in any particular WL problem there will be 2 char. lengths: (i) the elastic mfp, \( l \), which is usually only weakly \( T \)-dependent and can range, typically, from a few Å to a few 1000 Å (ii) some “phase-breaking length \( L_\phi \), e.g., an inelastic length \( L_{in} \) or a “magnetic length” \( L_M \approx \sqrt{\phi_0/B} \). The phase-breaking length can be \( \gg l \). Most experiments which explicitly test theory of WL done on thin wires or films, such that the “small” dimension \( d \) is \( \ll \) phase-breaking length \( L_\phi \) but usually \( \gg l \); however, in the case of (e.g.) Si MOSFET’s, clearly \( d \ll l \).

I will go through the theory explicitly for the former case, so that “locally” (on the scale of \( l \)) the system looks 3D; the generalization to the case of a “locally 2D” (or 1D) system is straightforward and mainly affects the dimensional and numerical factors.

3. Until further notice electron-electron and electron-phonon interactions are neglected except in so far as they give rise to “dephasing” collisions (see below). The effect of e–e interactions, in particular, on WL is still highly controversial. (see Lecture 7)

4. Generally speaking, the trajectories whose interference gives rise to WL effects extend over distances \( \sim L_\phi \). However, the actual change in the nonlocal conductivity \( \sigma(r,r') \) is confined to much smaller distances, \( \lesssim l \); thus when measured over distances \( \gtrsim l \) (but \( \ll L_\phi \)) the conductance will obey Ohm’s law.

5. For a strictly translationally-invariant system (no impurities!) we can always choose the single-electron energy eigenstates to be plane waves \( \psi_k(r) \sim \exp(ikr) \), i.e. so that they are not eigenstates of the time reversal operator \( \hat{T} \), and \( \hat{T}\psi_k \) is different from \( \psi_k \) (though also an energy eigenfunction). In the presence of finite potentials
this is in general not the case, so that strictly speaking we must choose the energy eigenfunctions to be eigenstates of $\hat{T}$ (we could, but need not, do this also in the translational invariant case, e.g. $\cos kr$ and $\sin kr$). However, this effect is itself of the order of the WL effect which we should calculate, so that when calculating “to zero order in WL” it is legitimate to treat the (approximate) eigenstates $\psi_i$ and $\hat{T}\psi_i$ as different. In fact, it is legitimate to treat the $\psi_i$ as semiclassical propagating wave packets. For the moment we assume that time reversal is indeed a good symmetry of the Hamiltonian, so that if $\psi_i$ is an (approximate) energy eigenstate then so is $\hat{T}\psi_i$, with the same energy.

We start from the standard Kubo formula for the d.c. conductivity $\sigma$ (not the conductance!) of an arbitrary system:

$$\sigma = \lim_{\omega \to 0} \lim_{q \to 0} \frac{1}{i\omega} \delta j(q,\omega) = \lim_{\omega \to 0} \lim_{q \to 0} \frac{1}{i\omega} \langle [j_q(t), j_q(0)] \rangle \omega =$$

$$= \int_0^\infty dt \int \int \frac{dr dr'}{V} \langle [j_\alpha(rt), j_\alpha(r'0)] \rangle$$

where $V = \text{volume of system}$, $\alpha$ is a particular Cartesian component. In the following it must be borne in mind that $\sigma(\omega)$ is real in the limit $\omega \to 0$ (which must be true for any system which is not superconducting) only if the commutator $\langle [j_q(t), j_q(0)] \rangle$ is pure imaginary, in the limit $\omega \to 0$. The form of the current operator $j(r,t)$ in terms of the single-particle wave functions $\varphi_i(r)$ and energies $\epsilon_i$ is

$$j_\alpha(rt) = \sum_{ij} a_i^\dagger a_j \left( -\frac{i\hbar}{2m} \varphi_i^* (r) \nabla_\alpha \varphi_j (r) - \text{c.c.} \right) \exp -i(\epsilon_i - \epsilon_j)t/\hbar$$

When evaluated in thermal equilibrium, the expression for $\sigma$ thus gives

$$\sigma = \sum_{ij} f_i(1-f_j) \int_0^\infty dt \exp -i(\epsilon_i - \epsilon_j)t/\hbar \times$$

$$\int \int \frac{dr dr'}{V} \left( \frac{i\hbar}{2m} \right)^2 \left( \varphi_i^* (r) \nabla_\alpha \varphi_j (r) - \text{c.c.} \right) \left( \varphi_j^* (r') \nabla_\alpha \varphi_i (r') - \text{c.c.} \right)$$

with $f_i$ the Fermi factor.

The occurrence of the gradient operators in those formulae is awkward, and we would like to get rid of them. Consider the short-range ($|r-r'| \ll l$) contribution to the integral. The time integration projects out all states except those for which $\epsilon_i$ is very close to $\epsilon_j$. At first sight this means that $\varphi_j(r)$ is very “close” to $\varphi_i(r)$, and they are both characterized locally by some wave vector $|k| \hat{n}$ where $|k| \approx k_F$. Thus the expression $\varphi_i^* (r) \nabla_\alpha \varphi_j (r) - \text{c.c.}$ can be replaced by $2k_F \hat{n}_\alpha \varphi_i^* (r) \varphi_j (r)$, and similarly for the $r'$-dependent term. Since the
Thus, if we denote \( \nabla \) the gradient, it brings in a \(-\delta \) of the argument already used in L4.) Because the time reversal changes the sign of the \( \phi \) time-reverse is another important contribution, namely from those states for which not \( \phi \) \( i \) with energy \( \epsilon \) over \( \rho \) direction \( \hat{n} \) is random, the average of the quantity \( \hat{n}^2 \) (which, remember is \( \textit{not} \) summed over \( \alpha \)) is \( 1/3 \). Thus, the short-range part of the “classical” contribution to \( \sigma \) (i.e. that for which \( \varphi_i(r) \) and \( \varphi_j(r) \) are very close) is given by the expression (note \( \hbar k_F / m \equiv v_F \))

\[
(\sigma_{cl})_{s.r.} = \sum_{ij} f_i (1 - f_j) \int_0^\infty dt \exp -i(\epsilon_i - \epsilon_j)t / \hbar \times \]

\[
\frac{1}{3} v_F^2 \int \int _{|r-r'| \leq l} \frac{dr \; dr'}{V} \; \varphi^*_i(r) \varphi_j(r) \; \varphi^*_j(r') \; \varphi_i(r')
\]

\[
\equiv \frac{1}{3} v_F^2 \int \int _{|r-r'| \leq l} \frac{dr \; dr'}{V} \; \langle [\rho(rt), \rho(r'0)] \rangle dt \leftarrow \chi_{\rho \rho}(rr':t)
\]

It is necessary to emphasize that this is \( \textit{not} \) the main contribution to \( \sigma_{cl} \) (this would involve considering \( r - r' \gtrsim l \)); it is introduced only for pedagogic purposes.

Now comes the crunch: If we inspect the formula (3) for \( r' \rightarrow r \), we see that there is another important contribution, namely from those states for which not \( \varphi_j(r) \) but its \textit{time-reverse} \( \varphi^*_j(r) \) is very close to \( \varphi_i(r) \). (Obviously, this is just a quantitative version of the argument already used in L4.) Because the time reversal changes the sign of the gradient, it brings in a \(-\) sign in the relation between the current and density correlations. Thus, if we denote \( \varphi^*_j(r) \) by \( \varphi^-_j(r) \) (remember, this is also an eigenstate of the Hamiltonian with energy \( \epsilon^-_j = \epsilon_j \) and thus \( f^-_j = f_j \)) we get for this “interference” contribution to \( \sigma \) (call it \( \delta \sigma \))

\[
\delta \sigma = \sum_{ij} f_i (1 - f_j) \int_0^\infty dt \; \exp -i(\epsilon_i - \epsilon^-_j)t / \hbar
\]

\[
\left( -\frac{1}{3} v_F^2 \right) \int \int drdr' \; \varphi^*_i(r) \varphi^-_j(r) \varphi^-_j(r') \varphi_i(r')
\]

\[
\equiv -\frac{1}{3} v_F^2 \sum_{ij} f_i (1 - f_j) \int_0^\infty dt \exp -i(\epsilon_i - \epsilon_j)t / \hbar \times
\]

\[
\int \int drdr' \; \varphi^*_i(r) \varphi^-_j(r) \varphi_j(r') \varphi_i(r')
\]

where in the last step we used the fact that the sum over \( j \) is just a relabelling of the sum over \( j \). For convenience let us define

\[
Q(r, r') \equiv \sum_{ij} f_i (1 - f_j) \int_0^\infty dt \; \exp -i(\epsilon_i - \epsilon_j)t / \hbar \times \varphi^*_i(r) \varphi^-_j(r) \varphi_j(r') \varphi_i(r')
\]

so that

\[
\delta \sigma_{WL} = -\frac{1}{3} v_F^2 \int \int drdr' \; Q(r, r') \times e^2
\]
Now comes the crucial step. It is clear that for \( r = r' \) the quantity \( Q(r, r') \equiv Q(r, r) \) is just the classical response function \( \int_0^\infty \langle [\rho(rt), \rho(0t)] \rangle \, dt \). As we go away from coincidence, the quantity \( Q(r, r') \) undergoes rapid phase oscillations, so that we expect that the integral is equal to \( V_{\text{eff}} \langle [\rho(rt), \rho(0t)] \rangle \) where \( V_{\text{eff}} \) is the effective volume over which constructive interference is maintained. What is this volume? For any given pair \( \varphi_i, \varphi_j \) with directions \( n_i, n_j \), the phase will go through \( \sim 2\pi \) if we go a distance of the order of \( k_F^{-1} \) along either \( n_i \) or \( n_j \). On the other hand, along the direction \( \vec{n}_i \times \vec{n}_j \) the phase remains essentially constant for a much longer distance, of the order of the elastic mfp \( l \). Hence we expect

\[
V_{\text{eff}} = \alpha k_F^{-2} l \tag{8}
\]

where \( \alpha \) is some constant of order unity, and so

\[
\delta \sigma_{WL} = -\frac{1}{3} v_F^2 k_F^{-2} l \alpha \int_0^\infty \langle [\rho(rt), \rho(0t)] \rangle_{\text{cl}} \, dt \times e^2 \tag{9}
\]

where the subscript “cl” indicates that the commutator is to be evaluated in the classical approximation, i.e. neglecting the interference effects specific to WL itself.

To get a feeling for the physical significance of eqn (9), we multiply and divide the RHS by the static susceptibility \( \chi_0 \), which for a noninteracting gas is given (in 3D) by the DOS \( k_F^2/\pi^2 \hbar v_F \). Then denoting the quantity \( (\text{dim } L^{-d} T^{-1}) \chi(r = 0, t)/\chi_0 \) by \( W(t) \), we have (since \( D \sim v_F l \))

\[
\Delta \sigma_{WL} = \text{const} \frac{e^2}{\hbar} D \int_0^\infty dt \, W(t) \tag{10}
\]

The quantity \( W(t) \) is just proportional to the probability density at the origin, at time \( t \), of a particle which started at the origin at time zero. In a system described by simple classical diffusion it is simply proportional to \( (D t)^{-d/2} \); thus we see that in 1 or 2D the integral diverges at long times, whereas in 3D it is finite.

We now evaluate the expression (9) for \( \delta \sigma_{WL} \) explicitly, using the hydrodynamic (diffusive) form for the quantity \( \chi_{\rho\rho} \equiv \langle [\rho(rt), \rho(0t)] \rangle \). In Fourier transformed form we have

\[
\chi_{\rho\rho}(q, \omega) = \chi_0 \frac{D q^2}{D q^2 - i\omega}, \quad \chi_0 = \text{static susceptibility} \quad D = \text{classical diffusion coeff.} \tag{11}
\]

and we remember that, since we know that the RHS of eqn. (9) is nil, we are allowed to
take the imaginary part $\chi_{\rho\rho}(q,\omega)$ only. Thus we have

$$\int_0^\infty \langle\rho(r_0),\rho(r_0)\rangle dt = \lim_{\omega \to 0} L^{-d} \frac{1}{i\omega} \text{Im} \sum_Q \chi_0 DQ^2 \frac{\omega}{DQ^2 - i\omega} = \chi_0 L^{-d} \sum_Q (DQ^2)^{-1}$$

where the upper cutoff in the $\sum_Q$ should be at $\sim l^{-1}$, beyond which the diffusive expressions no longer hold. Hence

$$\delta\sigma_{WL} = -\alpha \frac{1}{3} v_F^2 k_F^{-2} l \chi_0 L^{-d} D^{-1} \sum_Q Q^{-2} e^2$$

At this point we recall that whatever the overall dimensionality of the system, “at short distances” ($\lesssim \ell$) it behaves essentially 3-dimensionally, so that on the RHS of eqn. (13) we can use the 3D expressions for $\chi_0$ (namely $k_F^2/\pi^2 h v_F$) and for the (classical) diffusion coefficient $D$ (namely $1/3 \cdot v_F \ell$). Hence the dimensional factors reduce to $-(\alpha/\pi^2)(e^2/h)$. A quantitative calculation gives $\alpha = 2\pi$, and thus we finally get

$$\delta\sigma_{WL} = -\frac{2}{\pi} \frac{e^2}{h} L^{-d} \sum_Q Q^{-2}$$

This is the general formula for the weak-localization correction to the conductivity for a system with unbroken time-reversal invariance; it can be derived more quickly (but perhaps less intuitively) by summing the so-called Langer-Neal (or “maximally crossed”) diagrams in the Kubo formula for the conductivity.

It is remarkable that in the result (14) all the microscopic properties of the system ($k_F$, $l$, etc.) have fallen out (as has the temperature): in fact, apart from a numerical constant the correction to the dimensionless conductance $g$ is simply $\sum_Q (QL)^{-2}$, which depends only on the dimensionality of the system! In detail:

(a) in 3D the WL correction to $\sigma$ is

$$\delta\sigma_{WL} \sim -\frac{e^2}{h} \int_0^{l^{-1}} \frac{d^3q}{q^2} \sim -\frac{e^2}{h} (l^{-1} - L^{-1}) \sim \frac{e^2}{h} l^{-1}$$

(actually $\times \pi^{-3}$)
Comparing this with the Drude conductivity $\sigma_{cl} \sim (e^2/\hbar)k_F^2l$, we see that the relative correction $\delta\sigma/\sigma_{cl}$ is of order $(k_F l)^{-2}$ and is independent of the sample dimensions.

(b) In 2D we have

$$\delta\sigma_{WL} \sim -\frac{e^2}{\hbar} \int_{l^{-1}}^{l^{-1}} \frac{dq}{q^2}$$

(16)

There is now formally a divergence for small $q$, which must be cut off at $q \sim L^{-1}$ where $L$ is the sample dimension. Thus, $\delta\sigma_{WL} \sim (e^2/\hbar) \ln(L/l)$, or putting in the correct numerical factors

$$\delta\sigma_{WL} = -\frac{e^2}{\hbar \pi^2} \ln(L/l)$$

(17)

(c) Finally, in 1D we get

$$\delta\sigma_{WL} \sim -\frac{e^2}{\hbar} \int_{L^{-1}}^{L^{-1}} \frac{dq}{q^2} = -\frac{e^2}{\hbar \pi} (L-l)$$

(18)

so that in this case the correction is no longer small as soon as $L$ becomes comparable to the elastic mfp $l$ (as indeed we found earlier from the scaling analysis). [Note if we define the dimensionless conductance $g$ as that of a cube of side $\pi L$ rather than $L$, the prefactor is $-e^2/\pi^2 \hbar$ in any dimension.]

There is one tricky point about the above argument. We started off by considering the behavior of the correlations entering the conductivity for short distances, $|\mathbf{r} - \mathbf{r}'| \lesssim \ell$. Yet in evaluating the sum in eqn. (12) we limited ourselves to values of $Q \lesssim \ell^{-1}$, i.e. in effect to long distances! The logic behind this procedure may be seen by inspection of the figure on page 7: the time-reversed paths which interfere must return to a point within (at most) $\sim \ell$ of their origin, but in the process may travel distances $\gg \ell$ (and it is these “long” paths which give rise to the divergences).

We now consider effects which may limit WL, and in particular may cut off the divergences in 1 and 2D. At first sight, it is tempting to think that any effect which breaks TRI will “spoil” the interference which leads to WL. However, this is not true when the spin degree of freedom is involved, since TR reverses the spin whereas, to get interference, the final spin of the electron must be independent of which of the two paths it travelled. Let us for the moment assume there are no spin-dependent forces in the problem (these will be taken up in the next lecture), and consider the effects which break the orbital TR symmetry; i.e., destroy the possibility of constructing a linear combination of states $\psi_i$ and $\psi_i^*$, which have exactly the same energy. There are two main classes of such effects:

(a) the (orbital effects of a) magnetic field, which has to be handled separately (see below)

(b) inelastic or “phase-breaking” collisions.
The reason why the latter tend to destroy WL is that they tend to correlate the states of the electron to (mutually orthogonal) states of "something else" (phonons, other electrons, ...), so that a linear combination of $\varphi_i$ and $\varphi_i^*$ becomes

$$\alpha \varphi_i(r) + \beta \varphi_i(r) \Rightarrow \alpha \varphi_i(r) \chi_i(\xi) + \beta \varphi_i^*(r) \overline{\chi}_i(\xi),$$

$$\left(\chi_i(\xi), \overline{\chi}_i(\xi)\right) \approx 0. \quad (19)$$

Once this has happened irreversibly, the return probability density no longer contains an interference term.

To estimate the order of magnitude of effect (b), it is sufficient simply to cut off the time integral at an "inelastic (dephasing) time" $\tau_\varphi$ which is the characteristic time for inelastic collisions. Somewhat more accurately, one can assume that the classical return probability $W(t)$ is replaced by $W(t)^\ast \tau_\varphi$ so that the corrected probability satisfies the modified diffusion equation

$$\frac{\partial \tilde{W}}{\partial t} = D \nabla^2 \tilde{W} - \tilde{W} / \tau_\Phi \quad (20)$$

(\text{where } \nabla^2 \text{ denotes the } d\text{-dimensional Laplacian). Taking the Fourier transforms as above, we find that the effect is to replace the quantity } DQ^2 \text{ by } DQ^2 + 1 / \tau_\Phi \text{ thus, eqn. (14) is replaced by}

$$\delta \sigma_{WL} = -\frac{2}{\pi} \frac{e^2}{\hbar} L^{-d} \sum_Q \frac{1}{Q^2 + L_\Phi^{-2}}$$

(21)

where the "phase-breaking length" $L_\Phi$ is defined by $L_\Phi \equiv \sqrt{D \tau_\Phi}$, i.e., it is the characteristic distance that an electron diffuses in the time $\tau_\Phi$. This then leads (up to a possible numerical factor) to the replacement of the sample dimension $L$ in the above expressions by $L_\Phi$; e.g. for 2D

$$\delta \sigma_{WL} = -\frac{e^2}{\hbar \pi^2} \ln(L_\Phi/l) \quad (22)$$
In general, we expect $\tau^{-1}_\phi$ (and thus $L_{\phi}^{-1}$, since D is usually not strongly $T$-dependent) to depend on temperature \textit{and to vanish as $T \to 0$}. This statement is rather generic, and depends only on the statement (a version of the 3rd law of thermodynamics) that the available density of states for inelastic collisions tends to zero as $T \to 0$. Suppose that $\tau^{-1}_\phi$ vanishes as $T^{p}$, $p > 0$. Then in 1D we find

$$\delta \sigma_{WL} \simeq -\frac{e^2}{\hbar \pi} L_{\phi}(T) \sim T^{-p/2}$$

and in 2D\(^1\)

$$\delta \sigma_{WL} = -\frac{e^2}{\pi^2 \hbar} \ln(L_{\phi}(T)/l) \sim -\frac{e^2}{\pi^2 \hbar} p \ln \frac{T_0}{T}$$

(where $T_0$ is defined by $\ln L_{\phi}(T) \sim l$). Thus we expect a \textit{universal} behavior $\delta \sigma \sim -\ln(T_0/T)$ in 2D, i.e. the system tends continuously to insulating behavior as $T \to 0$. The details of the dephasing mechanism affect only the prefactor of the logarithm.

In general, we expect the phase-breaking rate $\tau^{-1}_\phi$ due to electron-phonon collisions to vary as $T^3$ for $T \ll \theta_D$ (remember that the $T^5$ in the Bloch-Gr"uneisen law has an extra power of $T^2$ because it is weighted by the directional factor $(1-\cos \theta)$ which expresses the effectiveness of the collision in destroying the electric current: no such factor enters $\tau^{-1}_\phi$, since correlation of the electron state to that of any phonon, whatever its wavelength, is effective in destroying phase coherence). Actually, the $T^3$-dependence is valid only down to $k_B T \sim \hbar c/\ell$, i.e. in the regime where the relevant phonon wavelengths are much smaller than the electron mfp: for still lower temperatures there is a crossover to a $T^4$ dependence.

If we think about inelastic collision processes in a fairly pure metal, then in addition to el-phonon collision we have electron-electron collisions; these are usually not very effective in degrading the electric current (because of the conservation of quasimomentum), but they are perfectly effective in destroying the phase coherence of either of the electrons involved\(^2\).

In a pure metal the rate of such collisions is proportional to $T^2$, so at sufficiently low $T$ they would be more effective than the e-ph collisions. In fact, since we can estimate:

$$\tau^{-1}_{\text{el-ph}} \sim \theta_D(T/\theta_D)^3, \quad \tau^{-1}_{\text{el-el (pure)}} \sim \epsilon_F(T/\epsilon_F)^2$$

we get a crossover at a temperature $\sim \theta_D^2/\epsilon_F$, which is typically of the order of a few degrees. Actually, it turns out that there is a complication: For a dirty metal the inelastic electron-electron collision rate is \textit{not} given by the standard $T^2$ dependence of FL theory,$^3$ because $L_{\phi}^{-1} \sim \sqrt{3 \tau\sigma/\pi}$, one often ignores the 3 and replaces $\ln L_{\phi}/l$ by $\frac{1}{2} \ln (\tau_{\sigma}/\pi)$.\(^3\)

\(^{1}\)We could, of course, take the view that the coherence has merely been shifted to the entangled state of the two electrons, which exists in a configuration space of dimension $2d$. However, for $d > 1$ the probability of return in such a space is nondivergent and we would get at best a small finite correction to $\sigma$.

\(^{2}\)These estimates are essentially dimensional in nature; in the case of the el – ph interaction we use the fact that for $T \gtrsim \theta_D$, $\tau^{-1} \sim k_B T/\hbar \times$ a coupling constant which is generally $O(1)$.

\(^{3}\)Since $L_{\phi}/l = \sqrt{\tau_{\phi}/3 \tau}$ elastic scattering rate, i.e., $\sqrt{\tau_{\phi}/3 \tau}$, one often ignores the 3 and replaces $\ln L_{\phi}/l$ by $\frac{1}{2} \ln (\tau_{\sigma}/\pi)$.\(^3\)
but is enhanced: in fact in $d$ dimensions $\tau_{el-el}^{-1} = T^{d/2}$ (with logarithmic connections in 2D). This enhancement comes about, crudely speaking, because the electrons travel diffusively rather than ballistically and hence can spend longer close together (cf. lecture 7). Thus we expect that at sufficiently low temperatures $\tau_\phi$ is proportional to $T^{d/2}$ (and hence $L_\phi$ to $T^{d/4}$). The same result follows from a calculation of the phase-breaking due to Nyquist noise (which of course is in the last resort due to the other electrons of the system). In any case, the crucial point is that the generic structure of the relation $\delta \sigma \sim -\ln(T_0/T)$ is preserved in 2D in the face of electron-electron collisions, and thus the system cannot be a metal in the limit $T \to 0$. 