

## Lecture notes on probing correlation functions in experiments

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# 1 Single-particle correlation function and spectroscopic probes

In our previous lecture, we have introduced the single-particle correlation function  $G(k, \epsilon)$ , that characterises the elementary excitations of a many-body system. The role of many-body interactions is highlighted by the quasiparticle spectral function

$$A(k, \epsilon) = -\frac{1}{\pi} \text{Im}G(k, \epsilon) \quad (1)$$

characterised by a general form

$$A(k, \epsilon) = -\frac{1}{\pi} \frac{\text{Im}\Sigma(k, \epsilon)}{(\epsilon - \xi(k) - \text{Re}\Sigma(k, \epsilon))^2 + (\text{Im}\Sigma(k, \epsilon))^2} \quad (2)$$

where  $\Sigma(k, \epsilon)$  is the self-energy and  $\xi(k)$  is the electron dispersion with the chemical potential subtracted.

## 1.1 Examples of self-energy

Some of the most relevant interactions in solids are the interactions of electrons with impurities, vibrational modes of the lattice and other electrons. The calculation of the self-energy in these three cases is extremely interesting and worthwhile. Performing these calculations is beyond the scope of this course. We will take our usual pragmatic approach and take the results of these calculations and concentrate on their physical significance. We will discuss the functional form taken by the free-energy in these three cases and present the consequences for real experiments. For the case of electro-electron interactions an intuitive argument that allows us to understand the origin of its energy dependence was outlined in the previous lecture.

### 1.1.1 Electron-impurity

In a real solid, a finite concentration of impurities will always be present. Itinerant electrons will be scattered by these impurities and these processes will affect the electronic properties of the solid. One useful approximation for the potential of an impurity having a difference of valence  $Z$  in a metallic compound is the so-called Yukawa potential

$$V(q) = \frac{Ze^2}{\epsilon_0} \frac{1}{q^2 + k_{TF}^2} \quad (3)$$

The parameter  $k_{TF}$  is the Thomas-Fermi wave-vector. It accounts for the electric fields screening in metals by itinerant electrons. Assuming an isotropic, free-electron-like dispersion, the self-energy can be approximated by an almost constant real term, that results in a simple renormalization of the chemical potential, and by a constant imaginary term:

$$\Sigma_{e-i}(k, \omega) \sim -i\Gamma \quad (4)$$

As we have discussed in the previous lecture, an imaginary self-energy is related to a finite lifetime of the one-particle excitations. Equation 4 can be used to explain quantitatively the residual resistivity of metals. We will expand on this point in the following section on current-current correlation functions.

### 1.1.2 Electron-phonon

Interactions between the electrons and lattice vibrations are another source of scattering in solid state. The effect of this interaction can be described by the following self-energy:

$$\Sigma_{e-ph}(\omega, k) = \int dE' \int_0^{E_{max}} dE \alpha^2 F(E) \left( \frac{1 - f(E') + d(E)}{\omega - E' - E} + \frac{f(E') + d(E)}{\omega - E' + E} \right) \quad (5)$$

Here  $\alpha^2 F(E)$  is the Eliashberg function that contains the density of phonon states  $F(E)$  and the electron-phonon coupling constant  $\alpha$ ;  $d$  is the Bose distribution and  $f$  is the Fermi distribution. In metals this often leads to a renormalization of the electrons effective mass. This effect will be discussed in an example below.

### 1.1.3 Electron-electron

As we have seen in our previous lecture, for electron-electron interactions we can outline an intuitive (phase space) argument due to Landau, that allows us to understand the energy dependence of the scattering rate. We considered a filled Fermi sphere and an extra electron of energy  $\epsilon_1 > \epsilon_F$ . This electron interacts with the Fermi sea, being able to scatter with electrons of energy  $\epsilon_2 < \epsilon_F$ .

The scattering rate of these processes is proportional to the number of available states, bounded by conservation of momentum and energy (Fermi golden rule). The Pauli principle (no double occupation of states) and the sharp decrease of the Fermi distribution at  $\epsilon_F$  constrains the available states for scattering in two factors:

- 1) The shell of electrons within the Fermi sea available for interactions within the constraints of energy conservation and Pauli principle are limited to a top layer of the Fermi surface with energy range  $(\epsilon_1 - \epsilon_F)$ .
- 2) For the same reasons, the shell of final states available for occupation is limited also to an energy range  $(\epsilon_1 - \epsilon_F)$ .

Therefore the scattering rate is reasonably expected to show an energy dependence

$$\Gamma \propto (\epsilon_1 - \epsilon_F)^2 \propto \omega^2 \quad (6)$$

Please reflect on the meaning of this result: as we consider interacting electrons closer and closer to the Fermi surface, we expect to see an increased lifetime in the presence of electron electron scattering. The farther we move away from the Fermi surface the

faster scattering processes will manifest. More formal and rigorous approaches lead to the following form of the self-energy used to describe electron-electron scattering

$$\Sigma_{e-e}(k, \omega) = \alpha\omega + i\beta[\omega^2 + (\pi k_B T)^2] \quad (7)$$

Note that the full description also accounts for a renormalisation of the mass (real part of the self-energy), which was not present in our qualitative argument.

This relationship will be useful below, as we will illustrate the concept of quasiparticles. Using this form an important result can be derived: the resistivity of a Fermi Liquid varies as a function of temperature following a  $T^2$  law. This fact will be motivated in these notes below.

## 1.2 Angle-resolved photoemission spectroscopy (ARPES)

Angle-resolved photoemission spectroscopy (ARPES) has emerged in recent years as one of the most powerful experimental techniques for the study of the electronic structure of solids. ARPES is based on the photoelectric effect, originally observed by Hertz (1887) and subsequently explained by Einstein (1905) in terms of the quantum nature of light. When light is directed towards a material, an electron can absorb one photon and escape from the material with a maximum kinetic energy  $E_k$ .

$$E_k = h\nu - \phi \quad (8)$$

Here  $h$  is the Planck constant,  $\nu$  is the photon frequency and  $\phi$  is called the work function of the material. The work function is a measure of the potential barrier that prevents electrons from leaving a metal and escape into the vacuum.

Let's consider a concrete example. The work function of Al is  $\sim 4.1$  eV. What is the wavelength of light that an electron needs to absorb in order to escape the material (the Planck constant is  $h = 6.6 \cdot 10^{-34}$  J s =  $4.1 \cdot 10^{-15}$  eV s)? To which region of the electromagnetic spectrum does it belong? (the speed of light is  $c = 3 \cdot 10^8$  m s $^{-1}$ )

The frequency is given by

$$\nu > \phi/h = 4.1 \text{ eV} / (4.1 \cdot 10^{-15} \text{ eV s}) = 10^{15} \text{ Hz} \quad (9)$$

while the wavelength is

$$\lambda = c/\nu = 3 \cdot 10^8 \text{ m s}^{-1} / (10^{15} \text{ s}^{-1}) = 3 \cdot 10^{-7} \text{ m} = 300 \text{ nm} \quad (10)$$

The work function of metals is typically in the 4-5 eV range. Therefore, we can argue that, if we direct UV light on a metal, electrons may acquire sufficient kinetic energy to escape from it. This effect can be utilized to infer the properties that the electrons had when still inside the material, including their interactions with other elements of the solid.

In a photoemission experiment we collect the electrons that have escaped into the vacuum after UV (or X-ray) irradiation. By measuring the kinetic energy of the emitted

electrons and the angle at which they escaped the material and assuming that energy and momentum are conserved during the photoemission process, we can infer the binding energy ( $E_B$ ) and momentum that the electrons had inside the solid.

The conservation laws used for this purpose are

$$E_{k,\text{vacuum}} = h\nu - \phi - |E_B| \quad (11)$$

$$p_{\parallel,\text{vacuum}} = \hbar k_{\parallel} = \sqrt{2mE_k} \sin \theta \quad (12)$$

From these considerations it is easy to be persuaded that ARPES contains useful information on the band structure (electron dispersion) of the material. Remarkably, an ARPES experiment can also inform us on the effects of many-body interactions. Using linear-response theory and assuming that the photoemission process is instantaneous (without energy exchange during the escape from the solid, sudden approximation) it can be shown that the angle ( $\Omega$ ) and energy ( $\epsilon$ )-resolved photoemission intensity  $I$  is a measure of the Spectral function  $A(k, \epsilon)$ :

$$\frac{dI}{d\Omega d\epsilon} \propto A(k, \epsilon) f(\epsilon) \quad (13)$$

Here  $f(\epsilon)$  is the Fermi distribution and its presence accounts for the occupation of the electronic states. Thanks to this result we can apply the theoretical concepts that we have discussed to the analysis of experimental data.

Figure 1 outlines the essential features of an ARPES experiment that can be ascribed to many-body physics. In the vast majority of real experiments, the self-energy is treated as momentum independent. This approximation has solid theoretical grounds, as many relevant interactions (screened electron-electron, electron-optical phonon, etc.) exhibit a more pronounced energy than momentum dependence. This is a consequence of the local nature of interactions (momentum independent).

For a given energy  $\omega_0$  the photoemission intensity as a function of momentum is recorded. This measurement is called momentum distribution curve (MDC) and is proportional to  $A(k, \omega_0)$ . The measurement yields a peak at a momentum  $k_0$  with a line-width  $\Delta k$ . By plotting  $\omega_0$  vs  $k_0$  one obtains the quasiparticle dispersion sketched in figure 1. By subtracting the underlying non-interacting dispersion, the real part of the self energy  $\text{Re}\Sigma(\omega)$  can be obtained. The line-widths  $\Delta k$  can be used to calculate  $\text{Im}\Sigma(\omega)$ .

Let us continue discussing a real-life example, Aluminium. We take it as the prototype of a solid in which interactions are fairly weak and where the independent-electron approximation works very well. Here the main interactions at play are the electron-phonon and a weak electron-electron interaction. Figure 2 shows the ARPES data of Aluminium. On the left hand side we can observe a parabolic dispersion leading to an effective mass

$$m = \hbar^2 \left( \frac{d^2 \xi(k)}{dk^2} \right)^{-1} \simeq 1.27 m_e \quad (14)$$

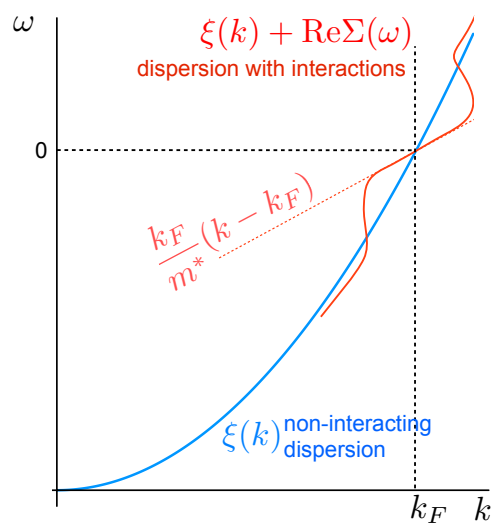


Figure 1: Essential features of an ARPES experiment.

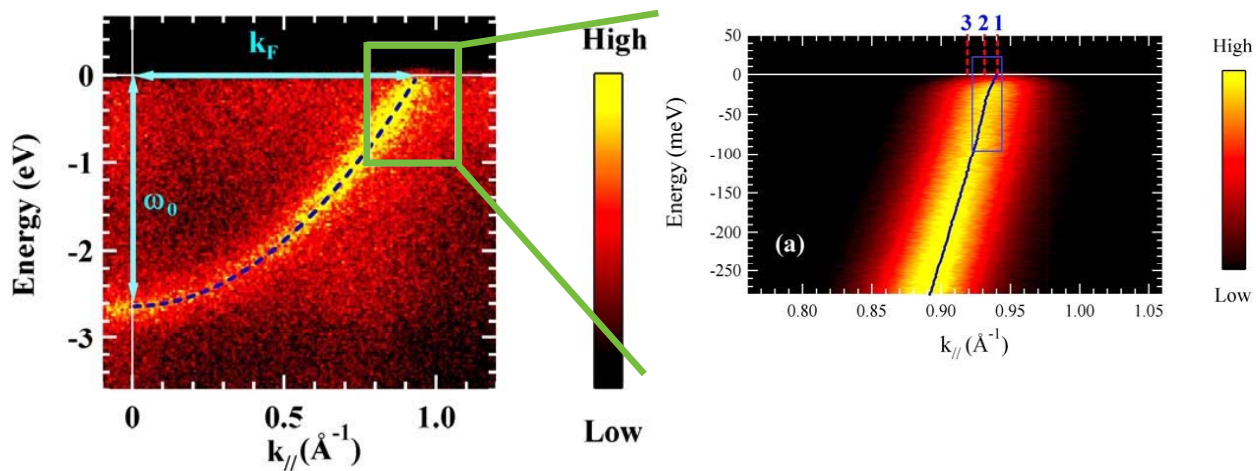


Figure 2: ARPES from Al (Jiang et al. e-J. Surf. Sci. Nanotech. 7, 57 (2009)).

This is a band structure effect, as discussed in lecture 1. In the same figure, on the right hand side, a zoom of the data in the vicinity of the Fermi energy is shown. Upon careful inspection one can notice that, in the vicinity of the Fermi energy, the effective mass is further enhanced by interactions effects. By looking at the solid line, which is a fit of the peak position of the MDC, we can appreciate a flattening of the dispersion (kink) around 40 meV. This energy scale points to an electron-phonon coupling effect. This effect could, at first sight, appear to be negligible. Yet, it leads to a significant real component of the self-energy, implying a non-negligible mass renormalization

$$m^* = \left(1 - \frac{\partial \text{Re}\Sigma}{\partial \omega} \Big|_{\omega=0}\right) m = (1 + 0.67)1.27 m_e = 2.1 m_e \quad (15)$$

## 2 Current-current correlation function and transport probes

We turn our attention to the description of transport phenomena in many-body systems. In particular we want to work our way through a quantum description of the electrical conductivity which is a widely used probe of correlation functions in experiments.

### 2.1 Current density

Our first objective is to derive a quantum mechanical description of the current density. We begin by writing the hamiltonian for charged particles in an electromagnetic field represented by a vector potential  $\mathbf{A}$ . We will use the field  $\hat{\psi}^\dagger$ ,  $\hat{\psi}$  and density  $\hat{\rho}$  operators, as introduced in the previous lectures

$$\hat{\psi}_\sigma^\dagger(\mathbf{r}) = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle^* \hat{c}_{\mathbf{k}\sigma}^\dagger \quad (16)$$

$$\hat{\psi}_\sigma(\mathbf{r}) = \sum_{\mathbf{k}} \langle \mathbf{r} | \mathbf{k} \rangle \hat{c}_{\mathbf{k}\sigma} \quad (17)$$

$$\hat{\rho}(\mathbf{r}) = \sum_{\sigma} \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_\sigma(\mathbf{r}) \quad (18)$$

We use the canonical momentum to write the hamiltonian for free particles interacting with an electromagnetic field. In this approach, the vector potential  $\mathbf{A}$  is treated as a classical field (i.e. it is not an operator with a commutation relation).

$$\hat{H} = \frac{1}{2m} \sum_{\sigma} \int \hat{\psi}_\sigma^\dagger(\mathbf{r}) [-i\hbar \nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})]^2 \hat{\psi}_\sigma(\mathbf{r}) d\mathbf{r} = \quad (19)$$

$$= \frac{1}{2m} \sum_{\sigma} \int \hat{\psi}_\sigma^\dagger(\mathbf{r}) [-i\hbar \nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})] [-i\hbar \nabla_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})] \hat{\psi}_\sigma(\mathbf{r}) d\mathbf{r} = \quad (20)$$

$$= \frac{1}{2m} \sum_{\sigma} \int \left[ -\hbar^2 \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla^2 \hat{\psi}_{\sigma}(\mathbf{r}) - i\hbar e \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) (\nabla_{\mathbf{r}} \mathbf{A}(\mathbf{r}) + \mathbf{A}(\mathbf{r}) \nabla_{\mathbf{r}}) \hat{\psi}_{\sigma}(\mathbf{r}) + e^2 \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \mathbf{A}^2(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) \right] d\mathbf{r} \quad (21)$$

We integrate by parts the term

$$\int \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla_{\mathbf{r}} \mathbf{A}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) d\mathbf{r} = \underbrace{\hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \mathbf{A}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r})}_{=0} \Big|_{-\infty}^{\infty} - \int \nabla_{\mathbf{r}} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \mathbf{A}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) d\mathbf{r} \quad (22)$$

leading to the hamiltonian

$$\hat{H} = \sum_{\sigma} \int \left[ \left( -\frac{\hbar^2}{2m} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla^2 \hat{\psi}_{\sigma}(\mathbf{r}) \right) + \frac{i\hbar e}{2m} \mathbf{A}(\mathbf{r}) \left( \nabla_{\mathbf{r}} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) - \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla_{\mathbf{r}} \hat{\psi}_{\sigma}(\mathbf{r}) \right) + \frac{e^2}{2m} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \mathbf{A}^2(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) \right] d\mathbf{r} \quad (23)$$

In this expression we recognize the familiar kinetic term

$$\hat{T} = \sum_{\sigma} \int \left( -\frac{\hbar^2}{2m} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla^2 \hat{\psi}_{\sigma}(\mathbf{r}) \right) d\mathbf{r} \quad (24)$$

and the paramagnetic

$$\hat{j}^{\text{P}} = \frac{i\hbar}{2m} \sum_{\sigma} \left( \nabla_{\mathbf{r}} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) - \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \nabla_{\mathbf{r}} \hat{\psi}_{\sigma}(\mathbf{r}) \right) \quad (25)$$

and diamagnetic

$$\hat{j}^{\text{D}} = \sum_{\sigma} \frac{e}{m} \hat{\psi}_{\sigma}^{\dagger}(\mathbf{r}) \mathbf{A}(\mathbf{r}) \hat{\psi}_{\sigma}(\mathbf{r}) = \frac{e}{m} \mathbf{A}(\mathbf{r}) \hat{\rho}(\mathbf{r}) \quad (26)$$

current densities. We note that the diamagnetic current density contains an explicit linear dependence on the vector potential, which allows us to identify a coupling at linear order of the density with the vector potential responsible for a current density. With these definitions, the hamiltonian for charged particles in an electromagnetic field can be expressed in a compact form:

$$\hat{H} = \hat{T} + \int e \mathbf{A}(\mathbf{r}) \cdot \left( \hat{j}^{\text{P}} + \frac{1}{2} \hat{j}^{\text{D}} \right) d\mathbf{r} \quad (27)$$



## 2.2 Conductivity in linear response theory: Kubo formula

We want to consider the response of a many-body system to a variation of vector potential at time  $t = t_0$  using perturbation theory.

$$\mathbf{A}(\mathbf{r}) \rightarrow \mathbf{A}(\mathbf{r}) + \Delta\mathbf{A}(\mathbf{r}, t) \quad (28)$$

A time variation of the vector potential represents an electric field, via the equation

$$\mathbf{E}(\mathbf{r}, t) = -\frac{\partial}{\partial t}\Delta\mathbf{A}(\mathbf{r}, t) \quad (29)$$

or, equivalently

$$\Delta\mathbf{A}(\mathbf{r}', \omega) = \frac{\mathbf{E}(\mathbf{r}', \omega)}{i\omega} \quad (30)$$

Our objective is to calculate the conductivity as the linear response of the current density to this electric field.

$$\begin{aligned} -e\langle \hat{J}_\mu(\mathbf{r}, t) \rangle_{\hat{H}'} &= \sum_\nu \int \sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}', t - t') \mathbf{E}_\nu(\mathbf{r}', t') d\mathbf{r}' dt' = \\ &= \int \frac{d\omega}{2\pi} e^{-i\omega t} \sum_\nu \sigma_{\mu\nu}(\mathbf{r}, \mathbf{r}', \omega) \mathbf{E}_\nu(\mathbf{r}', \omega) d\mathbf{r}' \end{aligned} \quad (31)$$

The notation  $\langle \dots \rangle_{H'}$  indicates the expectation value calculated in the presence of the perturbation  $H'$ . This form captures the characteristic non-local correlations of a quantum theory of transport. Because of these changes in vector potential (switching on the electric field), the hamiltonian will acquire a perturbation term

$$\hat{H} \rightarrow \hat{H}^0 + \hat{H}' \quad (32)$$

We will now isolate the unperturbed  $\hat{H}^0$  and perturbation  $\hat{H}'$  terms, in order to set up a linear response calculation:

$$\hat{H} = \hat{T} + \int e(\mathbf{A}(\mathbf{r}) + \Delta\mathbf{A}(\mathbf{r}, t)) \cdot \left[ \hat{J}^P + \frac{e}{2m}(\mathbf{A}(\mathbf{r}) + \Delta\mathbf{A}(\mathbf{r}, t))\hat{\rho}(\mathbf{r}) \right] d\mathbf{r} \quad (33)$$

Neglecting the quadratic term in  $\Delta\mathbf{A}(\mathbf{r})$ , we find

$$\hat{H} \approx \underbrace{\hat{T} + \int e\mathbf{A}(\mathbf{r}) \left( \hat{J}^P + \frac{1}{2}\hat{J}^D \right) d\mathbf{r}}_{\hat{H}^0} + \underbrace{\int e\Delta\mathbf{A}(\mathbf{r}, t) \left( \hat{J}^P + \hat{J}^D \right) d\mathbf{r}}_{\hat{H}'} \quad (34)$$

This analysis indicates that a variation in vector potential couples to the equilibrium current density  $\hat{J}_0$ , defined as

$$\hat{J}_0 = \hat{J}^P + \hat{J}^D \quad (35)$$

The perturbation we are looking for is therefore

$$\hat{H}' = e \int \Delta \mathbf{A}(\mathbf{r}, t) \hat{J}_0 d\mathbf{r} \quad (36)$$

and, in its presence, we describe the current as the sum of the equilibrium current and a linear coupling of density and vector potential variation (see equation 26)

$$\hat{J} = \hat{J}_0 + \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \hat{\rho}(\mathbf{r}) \quad (37)$$

We have now all the elements to calculate the linear response of the field  $\hat{J}$  to the perturbation  $\hat{H}'$ . We consider the case in which there is no electric field at equilibrium and the field is switched on at  $t = t_0$ . According to linear response theory, we have

$$\langle \hat{J}(\mathbf{r}, t) \rangle_{\hat{H}'} \approx \langle \hat{J}(\mathbf{r}, t) \rangle_{\hat{H}_0} - i \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}(\mathbf{r}, t), \hat{H}'] \rangle_{\hat{H}_0} dt' = \quad (38)$$

$$= \langle \hat{J}_0 + \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} - i \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}(\mathbf{r}, t), \hat{H}'] \rangle_{\hat{H}_0} dt' = \quad (39)$$

$$= \underbrace{\langle \hat{J}_0 \rangle_{\hat{H}_0}}_{=0 \text{ absence of current at equilibrium}} + \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} - i \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}(\mathbf{r}, t), \hat{H}'] \rangle_{\hat{H}_0} dt' = \quad (40)$$

Substituting the perturbation  $\hat{H}'$ , we find

$$= \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} - ie \int \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}(\mathbf{r}, t), \hat{J}_0(\mathbf{r}', t')] \rangle_{\hat{H}_0} \Delta \mathbf{A}(\mathbf{r}', t') d\mathbf{r}' dt' = \quad (41)$$

and substituting the expression for the current density operator, we find

$$= \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} - ie \int \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}_0(\mathbf{r}, t) + \underbrace{\frac{e}{m} \Delta \mathbf{A} \hat{\rho}}_{\text{Neglected}}, \hat{J}_0(\mathbf{r}', t')] \rangle_{\hat{H}_0} \Delta \mathbf{A}(\mathbf{r}', t') d\mathbf{r}' dt' = \quad (42)$$

Neglecting the second order term in  $\mathbf{A}$ , we find

$$= \frac{e}{m} \Delta \mathbf{A}(\mathbf{r}, t) \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} - ie \int \int_{t_0}^{\infty} \theta(t - t_0) \langle [\hat{J}_0(\mathbf{r}, t), \hat{J}_0(\mathbf{r}', t')] \rangle_{\hat{H}_0} \Delta \mathbf{A}(\mathbf{r}', t') d\mathbf{r}' dt' = \quad (43)$$

$$= \int \int_{t_0}^{\infty} \left[ \frac{e}{m} \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') - ie \theta(t - t_0) \langle [\hat{J}_0(\mathbf{r}, t), \hat{J}_0(\mathbf{r}', t')] \rangle_{\hat{H}_0} \right] \Delta \mathbf{A}(\mathbf{r}', t') d\mathbf{r}' dt' \quad (44)$$

The quantity

$$\chi_{J_0 J_0}^R(\mathbf{r}, \mathbf{r}', t, t') = -i \theta(t - t_0) \langle [\hat{J}_0(\mathbf{r}, t), \hat{J}_0(\mathbf{r}', t')] \rangle_{\hat{H}_0} \quad (45)$$

is known as the current-current correlation function. Therefore we have

$$\langle \hat{J}(\mathbf{r}, t) \rangle_{\hat{H}'} \approx \int \int_{t_0}^{\infty} \left[ \frac{e}{m} \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} \delta(\mathbf{r} - \mathbf{r}') \delta(t - t') + e \chi_{J_0 J_0}^R(\mathbf{r}, \mathbf{r}', t, t') \right] \Delta \mathbf{A}(\mathbf{r}', t') d\mathbf{r}' dt' \quad (46)$$

By Fourier transforming and remembering that  $\Delta \mathbf{A}(\mathbf{r}', \omega) = \mathbf{E}(\mathbf{r}', \omega)/(i\omega)$  we find

$$\langle \hat{J}(\mathbf{r}, \omega) \rangle_{\hat{H}'} \approx \int \left[ \frac{e}{m} \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} \delta(\mathbf{r} - \mathbf{r}') + e \chi_{J_0 J_0}^R(\mathbf{r}, \mathbf{r}', \omega) \right] \frac{\mathbf{E}(\mathbf{r}', \omega)}{i\omega} d\mathbf{r}' \quad (47)$$

$$\langle \hat{J}(\mathbf{r}, \omega) \rangle_{\hat{H}'} \approx \int \left[ -\frac{ie}{m\omega} \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} \delta(\mathbf{r} - \mathbf{r}') - \frac{ie}{\omega} \chi_{J_0 J_0}^R(\mathbf{r}, \mathbf{r}', \omega) \right] \mathbf{E}(\mathbf{r}', \omega) d\mathbf{r}' \quad (48)$$

which allows us to identify the conductivity as

$$\sigma(\mathbf{r}, \mathbf{r}', \omega) = \frac{ie^2}{m\omega} \langle \hat{\rho}(\mathbf{r}) \rangle_{\hat{H}_0} \delta(\mathbf{r} - \mathbf{r}') + \frac{ie^2}{\omega} \chi_{J_0 J_0}^R(\mathbf{r}, \mathbf{r}', \omega) \quad (49)$$

This important result is known as the Kubo formula and it is the starting point for computing the conductivity of a quantum many-body system.

The current-current correlation function calculates the average of the current-current commutator in the presence of the interactions that may be described by the hamiltonian  $\hat{H}^0$ . For example, in addition to the kinetic term  $\hat{T}$ , we may consider a one-body potential describing interactions with impurities or a two-body potential describing electron-electron interactions.

Next, in order to evaluate the conductivity for a given interacting many-body system, we need to unpack the current-current correlation function as an infinite sum of elementary contributions, using a finite-temperature diagrammatic perturbation theory. Setting up this calculation is beyond the scope of this lecture and we leave it to a more specialised advanced course. Here we want to discuss the main insights of these calculations. It turns out that the contributions to the current-current correlation function can be classified into two broad families: quasiparticle transport and vertex corrections. While the first family deals with the probability amplitude of propagating quasiparticles, the second one accounts for quantum interference, collective modes and long-range entanglement. We will show below that the first contributions can be understood as a generalisation in many-body theory of the Drude conductivity. The second contributions instead, give rise to quantum transport phenomena, such as weak localisation and weak antilocalisation, that do not have any classical interpretation.

### 2.3 Quasiparticle transport

Let's first discuss the first family of contributions to the current-current correlation function. These diagrams keep track of the electric field induced dynamics as the sum of

amplitudes of quasiparticle propagation from point  $\mathbf{r}$  to point  $\mathbf{r}'$  (alternatively, if we have translational invariance, of changing their momentum by  $\mathbf{q}$ ) considering all possible paths (alternatively, if we have translational invariance, of changing their momentum by  $\mathbf{q}$  through all possible intermediate momenta  $\mathbf{k}$  and  $\mathbf{k}'$  such that  $\mathbf{k} - \mathbf{k}' = \mathbf{q}$ ).

In this approximation, the dc limit of the conductivity, defined as

$$\sigma_{\text{dc}} = \lim_{\mathbf{q}, \epsilon \rightarrow 0} \sigma(\mathbf{q}, \epsilon) \quad (50)$$

reduces to

$$\sigma_{\text{dc}} = \frac{\pi e^2 \hbar^3}{m^2 \mathcal{V}} \sum_{k\sigma} k_\mu k_\nu \int A^2(k, \epsilon) \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) d\epsilon \quad (51)$$

We want to show that this result can be interpreted as a generalisation of the Drude formula. In order to proceed further we need to make some assumptions on the form of the self energy and electron dispersion. We will assume that the self energy has no real part and only an imaginary part with no momentum dependence. We will also assume a dispersion of the form

$$\xi(k) = \frac{\hbar^2 k^2}{2m^*} - \epsilon_{\text{F}} \quad (52)$$

and an isotropic conductivity

$$\sigma_{\text{dc}} = \frac{1}{3} \text{Re}[\sigma_{xx} + \sigma_{yy} + \sigma_{zz}] \quad (53)$$

$$\sigma_{\text{dc}} = \frac{2e^2 \hbar m^*}{3\pi m^2 \mathcal{V}} \sum_{k\sigma} (\xi_k + \epsilon_{\text{F}}) \int \frac{[\text{Im}\Sigma(\epsilon)]^2}{[(\epsilon - \xi_k)^2 + [\text{Im}\Sigma(\epsilon)]^2]} \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) d\epsilon \quad (54)$$

By operating the usual substitution

$$\frac{1}{\mathcal{V}} \sum_{k\sigma} \rightarrow \int d\xi g(\xi) \quad (55)$$

we find

$$\sigma_{\text{dc}} = \frac{2e^2 \hbar m^*}{3\pi m^2} \int d\epsilon [\text{Im}\Sigma(\epsilon)]^2 \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) \int d\xi \frac{g(\xi)(\xi_k + \epsilon_{\text{F}})}{[(\epsilon - \xi_k)^2 + [\text{Im}\Sigma(\epsilon)]^2]} = \quad (56)$$

$$\approx \frac{2e^2 \hbar m^*}{3\pi m^2} \int d\epsilon [\text{Im}\Sigma(\epsilon)]^2 \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) g(\epsilon_{\text{F}}) \epsilon_{\text{F}} \frac{\pi}{2} \frac{1}{|\text{Im}\Sigma(\epsilon)|^3} \quad (57)$$

Remembering the useful relations

$$g(\epsilon_{\text{F}}) = \frac{m^* k_{\text{F}}}{\pi^2 \hbar^2} \quad (58)$$

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m^*} \quad (59)$$

and

$$n = \frac{k_F^3}{3\pi^2} \quad (60)$$

we find

$$\sigma_{\text{dc}} = \frac{ne^2 \hbar m^*}{2m^2} \int d\epsilon \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) \frac{1}{|\text{Im}\Sigma(\epsilon)|} \quad (61)$$

We define the transport lifetime as

$$\frac{2m}{\hbar m^*} \tau(\epsilon) = \frac{1}{|\text{Im}\Sigma(\epsilon)|} \quad (62)$$

leading to our final formulation of the dc conductivity:

$$\boxed{\sigma_{\text{dc}} = \frac{ne^2}{m} \int d\epsilon \left( -\frac{d}{d\epsilon} f^{\text{FD}} \right) \tau(\epsilon)} \quad (63)$$

We find that at finite temperatures, the quasiparticle transport lifetime is determined by an average of the quasiparticle lifetime (imaginary part of the self-energy) on a region of size  $kT$  around the Fermi surface.

This establishes a correspondence between the temperature dependence of the resistivity and the energy dependence of the quasiparticle lifetime.

## 2.4 Quantum interference: weak localisation

We will now summarize the effects described by a family of vertex corrections called maximally-crossed diagrams. These contributions describe electron dynamics along the same diffusion path around impurities in opposite (time reversed) directions (illustrated in figure 3). If the temperature is cold enough to significantly reduce inelastic scattering (e.g. electron-electron and electron-phonon interactions) we can find loops that are shorter than the inelastic scattering length. In this situation, contributions following the same path in opposite directions will keep a constant phase relation and will interfere. It turns out that, disregarding spin effects, this leads to an enhancement of backscattering, and therefore to a decrease in conductance. This phenomenon is called weak localisation and it is associated with conductivity correction  $\Delta\sigma^{\text{WL}}$  that, in two-dimensions is given by

$$\Delta\sigma^{\text{WL}} = -\frac{e^2}{\pi h} \ln\left(\frac{\tau_i}{\tau}\right). \quad (64)$$

We want to underscore three notable features of this result: the magnitude of the conductivity correction is universal ( $e^2/\pi h \simeq 1.2 \cdot 10^{-5}$  S), *negative* and depends on the logarithm

of the ratio between the inelastic scattering time  $\tau_i$  and the elastic scattering time. The ratio between the Drude conductivity  $\sigma_0$  and the weak localisation correction is given by

$$\frac{\Delta\sigma^{\text{WL}}}{\sigma_0} = \frac{1}{\pi k_{\text{F}} l} \ln\left(\frac{\tau_i}{\tau}\right). \quad (65)$$

This formula highlights the importance of the product  $k_{\text{F}} l$ , for the weak localisation correction. This description breaks down for  $k_{\text{F}} l \sim 1$ , where an analysis of the effect of the disorder based on perturbation theory ceases to be appropriate. This leads us naturally to the definition of a localisation length

$$\xi_{\text{loc}} = l e^{\pi k_{\text{F}} l} \quad (66)$$

which is the phase coherence length required to observe the transition from a weak to a strong localisation regime.

We have remarked that the weak localisation correction is proportional to  $\ln(\tau_i/\tau)$ . Since we expect a growth of this ratio grows with decreasing temperature, the resistivity at low temperatures should display a logarithmic upturn. The exact temperature dependence will be set by the growth of the inelastic scattering time with decreasing temperature, as described by electron-phonon or electron-electron interactions. Therefore, we expect a temperature dependence of the conductivity of the type

$$\sigma = \sigma_0 - \frac{e^2}{\pi h} \ln T \quad (67)$$

Another useful way to probe the weak localisation correction is to observe the variation of conductance induced by a magnetic field. Since weak localisation gives a negative contribution to the conductivity, its suppression by a magnetic field leads to an increase in conductivity. The typical scale of magnetic fields is set by  $\hbar/eD\tau_i$  which corresponds to a field that couples a flux quantum  $h/2e$  through an area  $\pi D\tau_i$  over which phase coherence is established. This scale is non-universal since the diffusion coefficient depends on the electrons effective mass and on the carrier concentration.

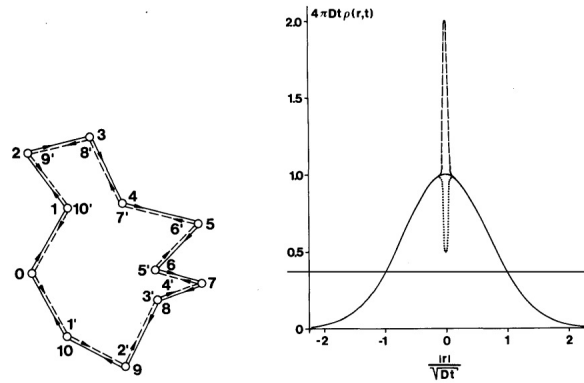


Figure 3: Weak localisation. From G. Bergmann, *Physics Reports* 107, 1—58 (1984).