

---

## Examen Final – Mardi 10 Janvier 2023 à 14h00

### Topic: some effects of charged impurities in metals

---

#### Some advice and guidelines:

- You can use your manuscript notes from the lecture and the tutorial, but no book, computer, or phone
  - Address first the questions that you feel confident about
  - All questions (and sub-questions) are independent of each other, do not get stuck
  - Write clearly and highlight the important results. Only a correct argumentation will give full points
  - This 4 pages exam is too long, do not worry if you did not complete all the questions (but try your best)
  - Write your name and page number on each page, and indicate the total number of pages on page 1
  - $\hbar = 1$  is set throughout
- 

## 1 General questions

Your answers to these general questions do not require any calculations. A few sentences are enough for each question. You can add drawings to illustrate your answers.

1. Consider free electrons moving in a periodic lattice potential, without any scattering mechanism. Sketch a typical density of states (versus energy), distinguishing conducting from non-conducting regions. What is the value of the conductivity as the chemical potential moves in those different regions?
2. List three physical mechanisms that are responsible for the scattering of electrons in metals. Upon which approximation can one add up the various scattering rates  $\tau^{-1}$  associated to these different mechanisms?
3. Sketch the spectral function  $\rho(\mathbf{k}, \omega)$  in a Fermi liquid and indicate how the scattering rate  $\tau^{-1}$  appears in this curve
4. Sketch the low temperature behavior of the resistance in an interacting Fermi liquid in which static disorder is also present (we do not consider here dynamical Kondo impurities or phonons)

## 2 X-ray edge spectrum in presence of a single “core” impurity

We will derive here the orthogonality theorem proven by P. Anderson in 1967, and explore its spectacular physical consequences. The theorem states that the many-body ground state of a non-interacting fermion system becomes orthogonal in the thermodynamic limit to the modified ground state in presence of a single static impurity.

1. To put this theorem into physical context, we consider a model for a partially filled electron band with energy  $\epsilon_k \in [-D, D]$ , chemical potential  $\mu$ , and a deep atomic  $s$ -level (“core” impurity) with energy  $\epsilon_s \ll -D$ . Electrons are supposed spinless, so that the interacting Hamiltonian is simply:

$$H = \epsilon_s c_s^\dagger c_s + \sum_k \epsilon_k c_k^\dagger c_k + V(1 - c_s^\dagger c_s) \sum_{k,k'} c_k^\dagger c_{k'}, \quad (1)$$

with  $V$  the screened Coulomb interaction between the deep level and the conduction band. Assuming  $V = 0$  and that x-ray photons excite the deep core electron (in the energy level  $\epsilon_s$ ) into available states in the band, sketch the photon absorption spectrum as a function of photon frequency  $\omega$ , and write down the absorption threshold in terms of the previous electronic parameters (no calculation required).

2. We now consider finite interaction  $V$  with the core  $s$ -level. Why can one assume that the  $s$ -level is either full or empty, so that Hamiltonian (1) reduces in the case of empty core level to a non-interacting problem  $\mathcal{H}_V = \sum_k \epsilon_k c_k^\dagger c_k + V \sum_{k,k'} c_k^\dagger c_{k'}$ , with just a static potential  $V$ ? Why does physically  $V = 0$  correspond to the case of filled core level? We denote  $|\psi_k\rangle = c_k^\dagger|0\rangle$  the one-particle plane-wave eigenstates of  $\mathcal{H}_{V=0}$  at  $V = 0$  with energy  $\epsilon_k$ , and  $|\phi_l\rangle = c_l^\dagger|0\rangle = \sum_k a_{lk}|\psi_k\rangle$  the new one-particle eigenstates of  $\mathcal{H}_V$  at finite  $V$  with energy  $E_l$  (the deep level does not take part in these states). Write the many-body overlap  $\langle\Omega|\Omega_0\rangle$ , with  $|\Omega_0\rangle = \prod_{\epsilon_k < 0} c_k^\dagger|0\rangle$  (resp.  $|\Omega\rangle = \prod_{E_l < 0} c_l^\dagger|0\rangle$ ) the ground state of  $\mathcal{H}_V$  with  $V = 0$  (resp. with  $V \neq 0$ ), as a function of  $\text{Det}(\hat{a})$ , precising the conditions on  $\epsilon_k$  and  $E_l$  (note that we have set  $\mu = 0$  here).

3. Rewriting the components of  $|\phi_l\rangle$  below the chemical potential  $\mu = 0$  in terms of the “unit vectors”:

$$|\tilde{\phi}_l\rangle = \frac{1}{\sqrt{\sum_{\epsilon_k < 0} |a_{lk}|^2}} \sum_{\epsilon_k < 0} a_{lk} |\psi_k\rangle, \quad (2)$$

and using the fact that  $|\phi_l\rangle$  is normalized, show that:

$$|\langle\Omega|\Omega_0\rangle|^2 = \prod_{E_l < 0} \left( 1 - \sum_{\epsilon_k > 0} |a_{lk}|^2 \right) \times \text{Det}[\text{Matrix of unit vectors}]^2. \quad (3)$$

Show that the determinant on the right-hand side is smaller than one, and that  $1 - x < e^{-x}$  for  $x > 0$ , as to obtain the bound  $|\langle\Omega|\Omega_0\rangle|^2 \leq e^{-S}$ , with  $S = \sum_{E_l < 0} \sum_{\epsilon_k > 0} |a_{lk}|^2$ .

4. To complete the evaluation of the double sum  $S$ , solve the one-particle Schrödinger equation  $\mathcal{H}_V|\phi_l\rangle = E_l|\phi_l\rangle$  and show that  $a_{lk} = V/(E_l - \epsilon_k)$ , with the eigenenergies  $E_l$  obeying  $1 = \sum_k V/(E_l - \epsilon_k)$ . Show graphically that  $E_l$  is bracketed by two successive energies  $\epsilon_k$  and  $\epsilon_{k+1}$ , so that the spectrum  $E_l$  is mainly similar to the one of the free band, and becomes continuous in the thermodynamic limit. Deduce that  $S \simeq V^2 \int_{-D}^{-E_{\min}} dE \int_{E_{\min}}^D d\epsilon \rho_0^2 / (E - \epsilon)^2$ , with  $\rho_0$  the free density of states (assumed constant),  $D$  the half-bandwidth, and  $E_{\min} \propto 1/L$ , with  $L$  the system size. Show that  $S$  diverges like  $\rho_0^2 V^2 \log(L)$ , so that the overlap  $|\langle\Omega|\Omega_0\rangle|^2 \leq L^{-\rho_0^2 V^2}$  vanishes in a power-law fashion as  $L \rightarrow \infty$ . This is the essence of Anderson’s orthogonality theorem.

5. Argue physically why the x-ray absorption amplitude is given by  $S(\omega) = \sum_f |\langle f | \sum_k c_k^\dagger |\Omega\rangle|^2 \delta(\omega - E_f + E_g)$  (up to prefactors), with  $E_g$  the energy of the initial ground state  $|\Omega_0\rangle$ , and  $|f\rangle$  an arbitrary final state of energy  $E_f$  (here again  $\omega$  is the photon frequency). Assuming  $V = 0$ , show that  $S(\omega)$  is constant above the threshold.

6. For finite  $V$ , the fact that  $|\langle\Omega|\Omega_0\rangle|$  vanishes in the thermodynamic limit indicates that the overlap of  $|\Omega\rangle$  relative to  $|\Omega_0\rangle$  is distributed over many particle-hole excitations above  $|\Omega_0\rangle$ , which affects the shape of the x-ray absorption spectrum. Show that the Fourier transform  $\tilde{S}(t) = \int d\omega S(\omega) e^{i\omega t}$  reads  $\tilde{S}(t) = \langle\Omega_0| e^{-i\mathcal{H}_0 t} c e^{i\mathcal{H}_V t} c^\dagger |\Omega_0\rangle$ , with  $c^\dagger \equiv \sum_k c_k^\dagger$ . Some (advanced) calculation leads to the result  $\tilde{S}(t) \simeq t^{-[1+\rho_0 V]^2}$  at  $t \rightarrow \infty$  (do not attempt it). Demonstrate that the absorption spectrum is rounded at the threshold as  $S(\omega) \simeq |\omega|^{2\rho_0 V + (\rho_0 V)^2}$  for small frequency  $\omega$  relative to the threshold. This anomalous behavior is observed experimentally in the x-ray absorption for many metallic elements.

### 3 Drude transport in weakly disordered metals

We turn to the physics of disordered metals, where now a macroscopic number of impurities are affecting the electrons. We will develop here a perturbative approach (assuming disorder is weak and impurities are diluted), which will allow us to justify microscopically the Drude theory at the quantum level.

1. Assuming impurities are only charged defects, why can we consider spinless fermions to model the system? Argue why the Hamiltonian takes the form:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{k,p} V_p c_k^\dagger c_{k-p}, \quad (4)$$

with  $V_p$  the Fourier transform of the random real space potential  $V(r)$  due to disorder.

2. We want to compute the Green's function  $G(k, k', t) = -i\mathcal{T}\langle\Omega|c_k(t)c_{k'}^\dagger|\Omega\rangle$ , with  $|\Omega\rangle$  the ground state of the full Hamiltonian Eq. (4), and  $c_k(t) = e^{iHt}c_k e^{-iHt}$  ( $\mathcal{T}$  is the time-ordering operator). Without calculation, why is  $G(k, k', t)$  proportional to  $\delta_{k,k'}$  when  $V_p = 0$ , but not anymore for finite  $V_p$ ? Show that the free electron Green's function  $G^0(k, k', \omega)$  at  $V_p = 0$  obeys the equation of motion  $\partial/\partial t G^0(k, k', t) = -i\delta_{k,k'}\delta(t) - i\epsilon_k G^0(k, k', t)$ . Similarly, demonstrate that  $\partial/\partial t G(k, k', t) = -i\delta_{k,k'}\delta(t) - i\epsilon_k G(k, k', t) - i\sum_p V_p G(k-p, k', t)$ .

3. We write matrixially  $G(k, k', t) = [\hat{G}(t)]_{kk'}$  and  $G^0(k, k', t) = [\hat{G}^0(t)]_{kk'}$ . Fourier transforming to frequency  $\omega$ , show that  $\hat{G}(\omega) = [\hat{\omega} - \hat{\epsilon} - \hat{V}]^{-1}$ , with  $[\hat{\omega}]_{kk'} = \omega\delta_{kk'}$ ,  $[\hat{\epsilon}]_{kk'} = \epsilon_k\delta_{kk'}$  and  $[\hat{V}]_{kk'} = V_{k-k'}$ . Recover from this  $G^0(k, k', \omega) = \delta_{kk'}/(\omega - \epsilon_k)$ . By substitution, obtain the exact equation  $\hat{G}(\omega) = \hat{G}^0(\omega) + \hat{G}^0(\omega)\hat{V}\hat{G}(\omega)$ , noting that the last term is a matrix product and that  $\hat{G}^0(\omega)$  is a diagonal matrix. Deduce the Dyson form for the Green's function:  $G(k, k', \omega) = G^0(k, \omega)\delta_{k,k'} + G^0(k, \omega)\sum_q V_{k-q}G(q, k', \omega)$ . By iteration, obtain the perturbative series:

$$G(k, k', \omega) = G^0(k, \omega)\delta_{k,k'} + G^0(k, \omega)V_{k-k'}G^0(k', \omega) + G^0(k, \omega)\sum_{k_1} V_{k-k_1}G^0(k_1, \omega)V_{k_1-k'}G^0(k', \omega) + \mathcal{O}(V^3). \quad (5)$$

Draw these two terms as Feynman diagrams and even the general term of order  $V^n$ .

4. This exact yet formal solution is not practical as the result will depend on the specific choice of disorder  $V_p$ . We will write  $V(r) = \sum_i u(r - R_i)$ , with  $R_i$  the random position of the impurities in concentration  $n_{\text{imp}}$  and  $u(r)$  the screened Coulomb potential associated to a single impurity. Show that we get at second order:

$$G(k, k', \omega) = G^0(k, \omega)\delta_{k,k'} + G^0(k, \omega)G^0(k', \omega)\left[\sum_i u_{k-k'}e^{i(k-k')R_i} + \sum_{i,j,k_1} u_{k-k_1}G^0(k_1, \omega)u_{k_1-k'}e^{i(k-k_1)R_i + i(k_1-k')R_j}\right].$$

In the dilute impurity limit, why can we write:

$$G(k, k', \omega) = G^0(k, \omega)\delta_{k,k'} + G^0(k, \omega)G^0(k', \omega)\left[\sum_i u_{k-k'}e^{i(k-k')R_i} + \sum_{i,k_1} u_{k-k_1}G^0(k_1, \omega)u_{k_1-k'}e^{i(k-k')R_i}\right]? \quad (6)$$

Averaging over all possible (random) impurity positions  $R_i$ , argue that

$$G(k, k', \omega) = G^0(k, \omega)\delta_{k,k'} + [G^0(k, \omega)]^2 u_0 n_{\text{imp}} \delta_{k,k'} + [G^0(k, \omega)]^2 n_{\text{imp}} \sum_{k_1} |u_{k-k_1}|^2 G^0(k_1, \omega) \delta_{k,k'} = G(k, \omega) \delta_{k,k'}. \quad (7)$$

Why has become the Green's function diagonal in terms of  $k, k'$ ? We can resum these contributions to infinite order by rewriting Dyson's equation as  $G(k, k', \omega) = \delta_{kk'}/(\omega - \epsilon_k - \Sigma_k(\omega))$ . Show that the retarded self-energy is given by  $\Sigma_k(\omega) = u_0 n_{\text{imp}} + n_{\text{imp}} \sum_{k_1} |u_{k-k_1}|^2 / (\omega - \epsilon_{k_1} + i0^+)$ . Why is the first term not physically crucial? Derive the disorder-induced scattering rate as  $\tau_k^{-1} \equiv 2\text{Im}\Sigma_k = 2\pi n_{\text{imp}} \sum_{k_1} |u_{k-k_1}|^2 \delta(\epsilon_k - \epsilon_{k'})$  and sketch graphically the spectral function  $\rho(k, \omega) = -(1/\pi)\text{Im}G(k, \omega)$ . Show that the scattering rate at the Fermi level is  $\tau^{-1} \simeq 2\pi\rho_0(u_0)^2 n_{\text{imp}}$ , assuming  $u_k$  is slowly varying and the density of states  $\rho(\omega) \simeq \rho_0$ . Argue why this perturbative computation is valid provided  $k_F l_e \gg 1$ , with  $k_F$  the Fermi wavevector and  $l_e = v_F \tau$  the elastic mean-free-path, with  $v_F$  the Fermi velocity.

5. Under some hypothesis, one can obtain an approximate expression for the averaged electrical conductivity in 3d from Kubo's formula (do not attempt to derive this expression):

$$\sigma(\omega) = \frac{e^2 E_F}{3\pi m} \sum_k G(k, \omega) [G(k, 0)]^*, \quad (8)$$

with  $G(k, \omega) = 1/(\omega - \epsilon_k + i/2\tau)$ ,  $e$  the electron charge,  $m$  its mass, and  $E_F$  the Fermi energy. Using again  $\rho(\epsilon) \simeq \rho_0$  and residues theorem, recover Drude formula  $\sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau}$  and express the DC component as  $\sigma_0 = ne^2\tau/m$  using the 3d electron density  $n = 2\rho_0 E_F/3$ .

## 4 Onset of insulating regime for strong disorder

Going beyond the lowest orders in perturbation theory leads to a wealth of transport phenomena that have no classical analog due to quantum interferences, leading even to localization effects by disorder. We consider here a simplified mean-field-like treatment of the strong disorder regime, which does not account for wavefunction localization, but still correctly predicts insulating behavior.

1. We start with a simplified model of an alloy  $A_xB_{1-x}$  with two “atoms” A and B, described by Hamiltonian:

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_i v_i c_i^\dagger c_i, \quad (9)$$

with  $c_k^\dagger$  plane-wave creation operators, and  $c_i^\dagger$  real space (Wannier) operators. The alloy model assumes that  $v_i = v$  for sites  $i$  on atoms A, and  $v_i = -v$  for sites  $i$  on atoms B (atoms are placed at random on the lattice). We note  $\rho_0(\omega) = \sum_k \delta(\omega - \epsilon_k)$  the free density of states for  $v = 0$ . In the pure case of A atoms only ( $x = 1$ ), show that the local density of states at site  $i$  is constant in space and exactly given by  $\rho_0(\omega - v)$ . Why is the local Green’s function  $\sum_{k,k'} G(k, k', \omega) = G_0(\omega - v) = (-1/\pi) \int d\epsilon \rho_0(\epsilon - v)/(\omega - \epsilon + i0^+)$ ? For arbitrary  $x$ , a very crude approximation can be to replace  $v_i$  by a constant effective potential on all sites,  $v_i = v_{\text{eff}} = xv + (1-x)(-v)$ , argue why. What happens when  $x = 1/2$  (same population of A and B atoms) and why is the result not reasonable?

2. A better mean-field uses the concept of effective medium. Let us focus on a given lattice site  $j$ . If  $j$  is an A atom, we use an effective Hamiltonian of the form of Eq. (9), but with  $v_j = v$  and an effective potential  $v_i = v_{\text{eff}}$  if  $i \neq j$  (the value of  $v_{\text{eff}}$  is arbitrary for now). This basically treats exactly the potential on site  $j$  and assumes an effective potential for the rest of the lattice. Conversely, if  $j$  is a B atom, the effective potential is given by  $v_j = -v$  and  $v_i = v_{\text{eff}}$  if  $i \neq j$ . Let us consider first the effective medium for an atom of type A, assuming the local site  $j = 0$ . Why is the effective Hamiltonian for site A given by  $H_A = \sum_k (\epsilon_k + v_{\text{eff}}) c_k^\dagger c_k + (v - v_{\text{eff}}) \sum_{k,k'} c_k^\dagger c_{k'}$ ? From Dyson’s equation already derived just above Eq. (5), show that  $G(k, k', \omega) = \delta_{kk'}/(\omega - \epsilon_k - v_{\text{eff}}) + (v - v_{\text{eff}})/[(\omega - \epsilon_k - v_{\text{eff}})(\omega - \epsilon_{k'} - v_{\text{eff}})(1 - (v - v_{\text{eff}})G_0(\omega - v_{\text{eff}}))]$ , and derive the local Green’s function on site  $j = 0$  as  $G_A(\omega) = \sum_{kk'} G(k, k', \omega) = G_0(\omega - v_{\text{eff}})/[1 + (v_{\text{eff}} - v)G_0(\omega - v_{\text{eff}})]$ . Similarly for a site  $j$  on a B atom, one gets locally  $G_B(\omega) = G_0(\omega - v_{\text{eff}})/[1 + (v_{\text{eff}} + v)G_0(\omega - v_{\text{eff}})]$ .

3. Our first attempt at a mean-field treatment of the alloy problem is to assume the self-consistency equation  $G_0(\omega - v_{\text{eff}}) = xG_A(\omega) + (1-x)G_B(\omega)$ , with  $v_{\text{eff}}$  a constant effective potential. Why is it physically motivated? Simplify this equation as  $(v_{\text{eff}}^2 - v^2)G_0(\omega - v_{\text{eff}}) = x(v_{\text{eff}} - v) + (1-x)(v_{\text{eff}} + v)$ , and show that an impossibility arises unless  $x = 1$  or  $x = 0$  (pure limit), in which case one recovers the result  $v_{\text{eff}} = v$  or  $v_{\text{eff}} = -v$  respectively.

4. In order to tackle the problem with  $x \neq 0, 1$ , we replace the constant parameter  $v_{\text{eff}}$  by a frequency dependent quantity  $v_{\text{eff}}(\omega)$  that can be possibly complex, and that needs to be found self-consistently (this is called a dynamical mean-field approach). The effective Green’s function  $G(\omega)$  becomes therefore also a mean-field quantity, obtained as  $G(\omega) = \int d\epsilon \rho_0(\epsilon)/(\omega - \epsilon + v_{\text{eff}}(\omega))$ , and still obeys the previous self-consistency condition  $G(\omega) = xG_A(\omega) + (1-x)G_B(\omega)$ , with the A atoms Green’s function  $G_A(\omega) = G(\omega)/[1 + (v_{\text{eff}}(\omega) - v)G(\omega)]$  and similarly  $G_B(\omega) = G(\omega)/[1 + (v_{\text{eff}}(\omega) + v)G(\omega)]$  for B atoms. This is a complicated non-linear integral equation in terms of the unknown  $G(\omega)$  (or equivalently in terms of  $v_{\text{eff}}(\omega)$ ), which is typically solved numerically. Analytical progress can be made by taking a semi-circular density of states  $\rho_0(\omega) = (2/\pi D^2) \sqrt{D^2 - \omega^2} \theta[D^2 - \omega^2]$ , with  $D$  the half-bandwidth. We give the integral  $\int d\epsilon \rho_0(\epsilon)/(\omega - \epsilon) = (2/D^2)(\omega - \sqrt{\omega^2 - D^2})$  (do not rederive it). Show by substitution  $\omega \rightarrow \omega + v_{\text{eff}}(\omega)$  that one can express explicitly  $v_{\text{eff}}(\omega)$  in terms of  $G(\omega)$  such as  $v_{\text{eff}}(\omega) = \omega - 1/G(\omega) + (D^2/4)G(\omega)$ , and derive the now algebraic dynamical mean-field equation:

$$1 = \frac{x}{(\omega - v)G(\omega) + D^2G(\omega)^2/4} + \frac{1 - x}{(\omega + v)G(\omega) + D^2G(\omega)^2/4}. \quad (10)$$

5. Let us finally assume  $v \gg D$ , corresponding to the large disorder limit, and focus first on frequencies  $\omega \simeq v$ . In this limit, solve Eq. (10) and find the contribution to the density of states originating from the A-type atoms as  $\rho(\omega) = -(1/\pi)\text{Im}G(\omega) \simeq (2/\pi D^2) \sqrt{D^2 x - (\omega - v)^2} \theta[D^2 x - (\omega - v)^2]$ . Show that its total spectral weight is  $x$ . Similarly, show for  $\omega \simeq -v$  (contribution originating from B-type atoms) that one has  $\rho(\omega) \simeq (2/\pi D^2) \sqrt{D^2(1-x) - (\omega + v)^2} \theta[D^2(1-x) - (\omega + v)^2]$ , with total spectral weight  $1 - x$ . Sketch the resulting total density of states  $\rho(\omega)$  for small  $x$ . For  $x = 1/2$  at half-filling, why is the system insulating?