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Advanced Theoretical Condensed Matter Physics — SS09

Exercise 6

(Please return your solutions before Fr. 3.7.2009, 10h)

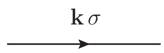
6.1. Fano resonance (10 points)

In the following we will consider a single-impurity level coupling to the conduction band electrons. As a consequence of the hybridization of the impurity level with the conduction electrons, the density of states of the conduction electrons at the impurity level will develop a pseudogap. The Hamiltonian of the model reads:

$$H = H_c + H_d + H_{hyb} \equiv \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \epsilon_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + V \sum_{\mathbf{k}\sigma} (c^\dagger_{\mathbf{k}\sigma} d_\sigma + d^\dagger_\sigma c_{\mathbf{k}\sigma}).$$

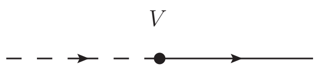
a) Show that the bare ($H_{hyb} = 0$)) single particle Green's function for the d-electron and the conduction electrons reads:

$$G^{c,0}_{\mathbf{k}\sigma}(\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}}}$$

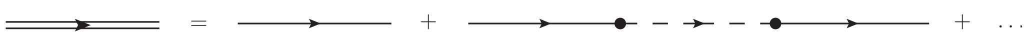


$$G^{d,0}_{\sigma}(\omega) = \frac{1}{\omega - \epsilon_d}$$

The vertex diagram is given by



and the perturbative expansion of the full conduction band electron Green's function reads



b) Show by analysing the diagrams, that the scattering matrix $T^c_\sigma(\omega)$, defined by

$$G^c_{\mathbf{k}\sigma}(\omega) = G^{c,0}_{\mathbf{k}\sigma}(\omega) + G^{c,0}_{\mathbf{k}\sigma}(\omega) T^c_\sigma(\omega) G^{c,0}_{\mathbf{k}\sigma}(\omega),$$

is given by

$$T^c_\sigma(\omega) = V^2 G^d_\sigma(\omega), \tag{1}$$

and show that the impurity self energy reads

$$\Sigma^d_\sigma(\omega) = V^2 \sum_{\mathbf{k}} G^{c,0}_{\mathbf{k}\sigma}(\omega). \tag{2}$$

By introducing the width

$$\Gamma(\epsilon) = \pi \sum_{\mathbf{k}} V^2 \delta(\epsilon_{\mathbf{k}} - \epsilon) = \pi N(\epsilon) V^2, \tag{3}$$

the sum of over $\mathbf{k}$ in (2) can be converted into an integral over frequencies. For a broad conduction band of width D one can replace the conduction band density of states (DOS), $N(\epsilon)$, by $N(\epsilon) \approx N(\epsilon_\mathrm{F}) =: N_0$ and

$$\Gamma(\epsilon) = \pi N_0 V^2 =: \Gamma \tag{4}$$

c) Use (2), (3) and (4) to calculate the retarded d-electron self energy $\Sigma^d_\sigma(\omega + \mathrm{i}0^+)$. (Hint: Use the Dirac identity). Argue why $\mathrm{Re}\Sigma^d_\sigma(\omega + \mathrm{i}0^+)$ can be neglected and show that the impurity DOS $N_d(\omega) = -\frac{1}{\pi}\mathrm{Im}G^d_\sigma(\omega + \mathrm{i}0^+)$ has a Lorentzian form. What is the width of the Lorentz peak?

d) Use (1) to calculate the retarded conduction electron Green's function $G^c_{\mathbf{k}\sigma}(\omega + \mathrm{i}0^+)$. By neglecting the real part of the bare conduction electron Green's function show that for the conduction electron DOS becomes

$$\begin{aligned} N(\omega) &= \sum_{\mathbf{k}} A_{\mathbf{k}\sigma}(\omega) = -\frac{1}{\pi}\sum_{\mathbf{k}} \mathrm{Im}G^c_{\mathbf{k}\sigma}(\epsilon + \mathrm{i}0^+) \\ &= N_0\left(1 - \frac{\Gamma^2}{(\omega - \epsilon_d)^2 + \Gamma^2}\right). \end{aligned}$$

6.2. Weakly disordered metal: Quantum transport theory (15 points)

In this exercise, we will discuss the conductivity of a weakly disordered metal on the basis of quantum transport theory and derive a basic relation between the resistivity and the single-particle scattering matrix. For that purpose, we consider the model Hamiltonian of a pure metal containing a low concentration of impurities

$$\mathcal{H} = \hat{H}_0 + \hat{V}_{imp} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}} c_{\mathbf{k}'}.$$

Within linear response theory the conductivity (for $T \to 0$) is given by (see Fig. 1)

$$\begin{aligned} \sigma &= \frac{e_0^2}{3\pi m^2}\int \frac{d^3k}{(2\pi)^3}\int \frac{d^3k'}{(2\pi)^3}\, \mathbf{k}\cdot\mathbf{k}'\, \overline{G^R(\mathbf{k},\mathbf{k}',\epsilon_\mathrm{F})\, G^A(\mathbf{k}',\mathbf{k},\epsilon_\mathrm{F})} && (5)\\ &= \frac{e_0^2}{3\pi m^2}\int \frac{d^3k}{(2\pi)^3}\, \overline{G^R(\mathbf{k},\epsilon_\mathrm{F})}\ \overline{G^A(\mathbf{k},\epsilon_\mathrm{F})}\, \mathbf{k}\cdot\mathbf{\Gamma}(\mathbf{k},\epsilon_\mathrm{F}), && (6) \end{aligned}$$

where $\overline{...}$ denotes the disorder average. The derivation of Eqs. (5) and (6) will be discussed in the tutorial. We assume the impurity concentration c_{imp} to be low and obtain

$$\overline{G^{R,A}(\mathbf{k},\epsilon_\mathrm{F})} = \frac{1}{\epsilon_\mathrm{F} - \epsilon_{\mathbf{k}} - \Sigma^{R,A}(\mathbf{k},\epsilon_\mathrm{F})} \approx \frac{1}{\epsilon_\mathrm{F} - \epsilon_{\mathbf{k}} \pm \mathrm{i}/\tau_0}.$$

a) In lowest approximation, we neglect the cross-linked diagrams and assume

$$\overline{G^R(\mathbf{k},\mathbf{k}',\epsilon_\mathrm{F})\, G^A(\mathbf{k}',\mathbf{k},\epsilon_\mathrm{F})} \approx \overline{G^R(\mathbf{k},\epsilon_\mathrm{F})}\ \overline{G^A(\mathbf{k},\epsilon_\mathrm{F})}\,\delta(\mathbf{k}-\mathbf{k}'),$$

i.e., $\mathbf{\Gamma}(\mathbf{k},\epsilon_\mathrm{F}) = \mathbf{k}$. Show that

$$\overline{G^R(\mathbf{k},\epsilon_\mathrm{F})}\ \overline{G^A(\mathbf{k},\epsilon_\mathrm{F})} \approx \pi\tau_0\delta(\epsilon_\mathrm{F} - \epsilon_{\mathbf{k}})$$

and derive ($\epsilon_{\mathbf{k}} = k^2/(2m)$)

$$\sigma \;=\; \frac{e_0^2}{3m^2} k_{\rm F}^2 \tau_0 N(\epsilon_{\rm F}) \;=\; \frac{e_0^2\, n}{m}\tau_0, \qquad n = \frac{N}{V} \;=\; \frac{1}{V}\sum_{|\mathbf{k}|\leq k_{\rm F}}, \tag{7}$$

where $N(\epsilon) = \frac{1}{V}\sum_{\mathbf{k}} \delta(\epsilon - \epsilon_{\mathbf{k}})$ is the density of states per unit volume.

b) To include the main contributions from the cross-linked diagrams, we have to find an expression for the *vertex function* $\mathbf{\Gamma}(\mathbf{k}, \epsilon_{\rm F})$. From the diagrammatic expansion (see Fig. 1(c)) we obtain ($c_{imp} \to 0$)

$$\begin{aligned} \mathbf{\Gamma}(\mathbf{k}, \epsilon_{\rm F}) \;&\approx\; \mathbf{k} + \int \frac{d^3k'}{(2\pi)^3} \overline{G^R(\mathbf{k}', \epsilon_{\rm F})}\; \overline{G^A(\mathbf{k}', \epsilon_{\rm F})}\; \left|\mathcal{T}_{\mathbf{k}\mathbf{k}'}(\epsilon_{\rm F})\right|^2 \mathbf{\Gamma}(\mathbf{k}', \epsilon_{\rm F}) \\ &\approx\; \mathbf{k} + c_{imp} \int \frac{d^3k'}{(2\pi)^3} \overline{G^R(\mathbf{k}', \epsilon_{\rm F})}\; \overline{G^A(\mathbf{k}', \epsilon_{\rm F})}\; \left|T_{\mathbf{k}\mathbf{k}'}(\epsilon_{\rm F})\right|^2 \mathbf{\Gamma}(\mathbf{k}', \epsilon_{\rm F}). \end{aligned} \tag{8}$$

$\mathcal{T}^R_{\mathbf{k}\mathbf{k}'}(\epsilon) = \langle \mathbf{k}'|\hat{\mathcal{T}}^R(\epsilon)|\mathbf{k}\rangle$ is the matrix element of the scattering matrix $\hat{\mathcal{T}}^R$, defined via (cf. exercise 6.1)

$$\overline{\hat{G}^R} \;=\; \hat{G}^{R,0} + \hat{G}^{R,0}\, \hat{\mathcal{T}}^R\, \hat{G}^{R,0}, \tag{9}$$

and $T^R_{\mathbf{k}\mathbf{k}'}(\epsilon)$ the scattering matrix of a *single impurity*. Use (cf. exercise 6.1.)

$$\mathcal{T} = \hat{V} + \hat{V}\, G^0\, \hat{V} + ...$$

and the matrix identity

$$(\mathbb{1} - \hat{A})^{-1} - (\mathbb{1} - \hat{B})^{-1} = (\mathbb{1} - \hat{B})^{-1}(\hat{A} - \hat{B})(\mathbb{1} - \hat{A})^{-1}$$

to derive from Eq. (9)

$$\begin{aligned} \langle \mathbf{k}|{\rm Im}\hat{\mathcal{T}}^R(\epsilon)|\mathbf{k}\rangle \;&\equiv\; \frac{1}{2}\langle \mathbf{k}|\hat{\mathcal{T}}^R(\epsilon) - \hat{\mathcal{T}}^A(\epsilon)|\mathbf{k}\rangle \;=\; -\pi \int \frac{d^3k'}{(2\pi)^3} \left|\hat{\mathcal{T}}^R_{\mathbf{k}\mathbf{k}'}(\epsilon)\right|^2 \delta(\epsilon - \epsilon_{\mathbf{k}'}) \\ &\approx\; -\pi c_{imp} \int \frac{d^3k'}{(2\pi)^3} \left|\hat{T}^R_{\mathbf{k}\mathbf{k}'}(\epsilon)\right|^2 \delta(\epsilon - \epsilon_{\mathbf{k}'}) \end{aligned}$$

and

$$\frac{1}{\tau_0} \;\approx\; \pi c_{imp} \int \frac{d^3k'}{(2\pi)^3} \left|\hat{T}^R_{\mathbf{k}\mathbf{k}'}(\epsilon)\right|^2 \delta(\epsilon - \epsilon_{\mathbf{k}'}). \tag{10}$$

c) Now we can include the vertex corrections into our calculation of the conductivity. From Eqs. (5), (6) and (8) we are motivated to define $\mathbf{\Gamma}(\mathbf{k}, \epsilon_{\rm F}) = \mathbf{k}\cdot\gamma(k, \epsilon_{\rm F})$. Show that this yields

$$\gamma(k, \epsilon_{\rm F}) \;=\; 1 + \tau_0 \left(\frac{1}{\tau_0} - \frac{1}{\tau_1}\right)\gamma(k, \epsilon_{\rm F}) \;=\; \frac{\tau_1}{\tau_0},$$

with

$$\frac{1}{\tau_1} \;=\; \pi c_{imp} \int \frac{d^3k'}{(2\pi)^3} \left|\hat{T}^R_{\mathbf{k}\mathbf{k}'}(\epsilon)\right|^2 (1 - \cos\Theta)\, \delta(\epsilon - \epsilon_{\mathbf{k}'}), \qquad \cos\Theta = \frac{\mathbf{k}\cdot\mathbf{k}'}{k^2}.$$

Finally, derive

$$\sigma \;=\; \frac{e_0^2}{3m^2}k_{\rm F}^2\tau_1 N(\epsilon_{\rm F}) \;=\; \frac{e_0^2\, n}{m}\tau_1 . \tag{11}$$

What is the physical meaning of the difference between Eq. (7) and Eq. (11)? What is the relation between the resistivity and the scattering matrix?

6.3. Drude conductivity (5 points)

Now we will consider the classical Drude model of a gas of noninteracting electrons. When applying an external electrical field $\mathbf{E}$ the current density is given by

$$\mathbf{j} \;=\; \sigma \cdot \mathbf{E} \;=\; -ne_0\overline{\mathbf{v}},$$

where n is conduction electron density and $\overline{\mathbf{v}}$ is the average velocity of the electrons. Let's assume that the electrons are scattered off the heavy, immobile ions of the metal. The average time between two scattering events shall be denoted by τ. Moreover, we assume that, immediately after a scattering event, the direction of motion of an electron is completely random. Between any two consecutive scattering events the electrons get accelerated by the electric force $\mathbf{F} = -e_0\mathbf{E}$. Show that the conductivity then becomes

$$\sigma \;=\; \frac{e_0^2\, n}{m}\tau.$$

This *Drude conductivity* was first obtained by P. Drude in 1900, long before the discovery of a model of the atom and the formulation of quantum theory. Remarkably, it is formally identical to the result obtained in the previous exercise by using quantum transport theory.

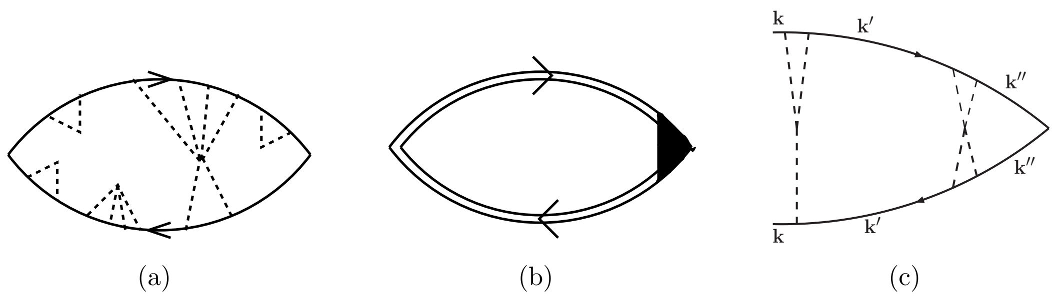


Figure 1: (a) An example of a diagram contributing to Eq. (5). Dashed lines denote scattering events. (b) Diagrammatic representation of Eq. (6). The black triangle denotes the vertex function $\Gamma(\mathbf{k}, \epsilon_{\rm F})$ containing all cross-linked parts. (c) An example of a diagram contributing to $\Gamma(\mathbf{k}, \epsilon_{\rm F})$.