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Strongly Correlated Electrons
3. Übung

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1. The non-interacting Anderson model **8 points**

We consider the Hamiltonian of the non-interacting Anderson model, or resonant level model, for spinless electrons (in absence of interactions, the spin does not play any role), which reads

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{imp}}, \tag{1}$$

$$\hat{H}_0 = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{c}_{\mathbf{k}}, \tag{2}$$

$$\hat{H}_{\mathrm{imp}} = \epsilon_f \hat{f}^\dagger \hat{f} + \sum_{\mathbf{k}} \big(V_{\mathbf{k}} \hat{f}^\dagger \hat{c}_{\mathbf{k}} + V^*_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}} \hat{f} \big). \tag{3}$$

Here, $\hat{f}^\dagger$ creates a localized electron at the impurity site $\mathbf{r} = 0$, while $\hat{c}^\dagger_{\mathbf{k}}$ crates a conduction electron with momentum $\mathbf{k}$. Using the definition for the retarded Green's function operator

$$(\epsilon + i\delta - \hat{H})\hat{G}^r(\epsilon) = \mathbb{1}, \tag{4}$$

with $\delta = 0^+$, do the following:

a) **1 point**

By taking the appropriate matrix elements, obtain from Eqn. (4) a closed set of equations for the retarded Green' s functions of f-electrons and conduction electrons,

$$\begin{aligned}
(\epsilon - \epsilon_f + i\delta) G^r_{f,f}(\epsilon) &= 1 + \sum_{\mathbf{k}} V_{\mathbf{k}} G^r_{\mathbf{k},f}(\epsilon), &(5)\\
(\epsilon - \epsilon_{\mathbf{k}} + i\delta) G^r_{\mathbf{k},f}(\epsilon) &= V^*_{\mathbf{k}} G^r_{f,f}(\epsilon), &(6)\\
(\epsilon - \epsilon_{\mathbf{k}} + i\delta) G^r_{\mathbf{k},\mathbf{k}'}(\epsilon) &= \delta_{\mathbf{k},\mathbf{k}'} + V^*_{\mathbf{k}} G^r_{f,\mathbf{k}'}(\epsilon), &(7)\\
(\epsilon - \epsilon_f + i\delta) G^r_{f,\mathbf{k}'}(\epsilon) &= \sum_{\mathbf{k}} V_{\mathbf{k}} G^r_{\mathbf{k},\mathbf{k}'}(\epsilon). &(8)
\end{aligned}$$

Here $G^r_{\alpha,\alpha'}(\epsilon) = \langle \alpha | \hat{G}^r(\epsilon) | \alpha' \rangle = \langle 0 | c_\alpha \hat{G}^r(\epsilon) c^\dagger_{\alpha'} | 0 \rangle$. Notice that the impurity breaks translation invariance. Momentum is therefore no longer a conserved quantum number.

b) **1 point**

Obtain the impurity and electron Green's functions $G^r_{f,f}(\epsilon)$ and $G^r_{\mathbf{k},\mathbf{k}'}(\epsilon)$ by solving the set of equations Eqns. (5-8).

c) **1 point**

The full Green's function operator is usually expressed in terms of the so-called $\hat{T}$ matrix which is defined as follows

$$\hat{G}^r(\epsilon) = \hat{G}^r_0(\epsilon) + \hat{G}^r_0(\epsilon)\hat{T}(\epsilon + i\delta)\hat{G}^r_0(\epsilon). \tag{9}$$

Here $\hat{G}^r_0$ indicates the Green's function operator in the absence of impurities (that is for $\hat{H} = \hat{H}_0$). Derive the following relation for the density of states $\rho(\epsilon)$

$$\Delta\rho(\epsilon) \equiv \rho(\epsilon) - \rho_0(\epsilon) = \frac{1}{\pi} \frac{\partial \eta(\epsilon)}{\partial \epsilon} \tag{10}$$

where the densities ρ and ρ_0 are related to the Green's functions G and G_0 respectively by the standard relation

$$\rho(\epsilon) = -\frac{1}{\pi} \mathrm{Im}\,(\mathrm{Tr}\,\hat{G}^r(\epsilon)), \tag{11}$$

and $\eta(\epsilon) = \arg\left(\mathrm{Det}\left(\hat{T}(\epsilon + i\delta)\right)\right)$ is the so-called phase shift. To this end, first proof the relation

$$Tr\hat{G}^r(\epsilon) = \frac{\partial}{\partial \epsilon} \ln(\mathrm{Det}\,(\hat{G}^r(\epsilon)) \tag{12}$$

for single-particle Green's functions. You may also use that the $\hat{T}$ matrix obeys

$$\hat{T}(\epsilon) = \hat{H}_{\mathrm{imp}}(\mathbb{1} + \hat{G}_0^r(\epsilon)\hat{T}(\epsilon)). \tag{13}$$

d) **2 points**

Illustrate the above results for the Hamiltonian in Eq. (2), that is using the explicit expressions obtained in items **a)** and **b)**, by (i) calculating $\langle \mathbf{k}|\hat{T}|\mathbf{k}'\rangle$, and by (ii) showing that $\eta(\epsilon)$ is described by

$$\eta(\epsilon) = \frac{\pi}{2} - \arctan\left(\frac{\epsilon_f + \Lambda(\epsilon) - \epsilon}{\Delta(\epsilon)}\right), \tag{14}$$

where $\Lambda(\epsilon) = \mathcal{P}\sum_{\mathbf{k}} |V_{\mathbf{k}}|^2/(\epsilon - \epsilon_{\mathbf{k}})$ and $\Delta(\epsilon) = \pi\sum_{\mathbf{k}} |V_{\mathbf{k}}|^2\delta(\epsilon - \epsilon_{\mathbf{k}})$. (Hint for the derivation of Eq. (14): start from the explicit expression of $\mathrm{Tr}\,\hat{G}^r(\epsilon)$).

e) **1 point**

Assume that we have a flat conduction band with

$$\rho_0(\epsilon) = \begin{cases} \rho_0, & -D < \epsilon < D, \\ 0 & \text{else}, \end{cases} \tag{15}$$

while $V_{\mathbf{k}} = V$. Determine $\eta(\epsilon)$.

f) **1 point**

In the case of $|\epsilon_f| \ll D$, show that there is a Lorentzian resonance of width $\pi\rho_0|V|^2$ in $\Delta\rho(\epsilon)$ at a renormalized impurity level $\tilde{\epsilon}_f$. What is the implicit equation determining $\tilde{\epsilon}_f$?

g) **1 point**

Calculate the impurity spectral density $\rho_{\mathrm{imp}}(\epsilon) = -\frac{1}{\pi}\mathrm{Im}\,(G^r_{f,f}(\epsilon))$. Compare this result with $\Delta\rho(\epsilon)$ obtained in item **f)**. Is this result affected when the bandwidth is decreased such that $|\epsilon_f| \not\ll D$?

2. Perturbation theory for the Kondo effect **5 points**

Experimentally, the resistivity of a metal shows a minimum at low temperatures when a finite concentration of magnetic impurities is present. Via the Drude formula $\rho = m/e^2 n\tau$ (where n is the electron density), we can characterize the resistivity ρ with the scattering time τ (defined as the time interval between two scattering events). τ can be conveniently calculated via the $\hat{T}$ matrix of a single impurity. In Matsubara frequency space the corresponding operator is

$$\hat{T}_n = \hat{H}_{\mathrm{imp}} + \hat{H}_{\mathrm{imp}} G_{0,n} \hat{H}_{\mathrm{imp}} + ..., \tag{16}$$

where the $G_{0,n}$ is the n-th Matsubara component of the local single-particle Green's function of the conduction electrons. In terms of $\hat{T}$ it is possible to show that the scattering rate is given by

$$\frac{1}{2\tau(\mathbf{k},\sigma)} = N_{\mathrm{imp}}\pi \sum_{\mathbf{k}',\sigma'} \langle |\langle \mathbf{k},\sigma|\hat{T}^r(\epsilon_{\mathbf{k}})|\mathbf{k}',\sigma'\rangle|^2\rangle_S \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}), \tag{17}$$

where we use $|\mathbf{k},\sigma\rangle = c^\dagger_{\mathbf{k}\sigma}|0\rangle$, while r indicates the retarded component, meaning the usual replacement $i\omega_n \to \omega + i\delta$. $\langle \mathbf{k},\sigma|\hat{T}^r(\epsilon_{\mathbf{k}})|\mathbf{k}',\sigma'\rangle$ is an operator in the impurity Hilbert space, and $\langle\rangle_S$ indicates the trace over the possible impurity states. Further, N_{imp} is the number of impurities. It is assumed that we are in the dilute regime where the contributions from different impurities simply add up. Notice also that

$$\mathrm{Im}\,\langle \mathbf{k},\sigma|\hat{T}^r(\epsilon)|\mathbf{k},\sigma\rangle = -\pi \sum_{\mathbf{k}',\sigma'} |\langle \mathbf{k},\sigma|\hat{T}^r(\epsilon)|\mathbf{k}',\sigma'\rangle|^2 \delta(\epsilon - \epsilon_{\mathbf{k}'}) \tag{18}$$

which is known as optical theorem. We now want to use Eq. (17) in the case of magnetic impurities. Let us consider the minimal Kondo Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \frac{J}{2L^d} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \hat{c}^\dagger_{\mathbf{k}\sigma} \vec{\tau}_{\sigma\sigma'} \hat{c}_{\mathbf{k}'\sigma'} \cdot \hat{\mathbf{S}}. \tag{19}$$

a) **2 points**

Show that, in leading order in J, the scattering rate is given by

$$\frac{1}{\tau(k_F)} = \frac{\pi}{4} C_{\text{imp}} N_0 J^2 S(S+1) \tag{20}$$

where N_0 is the density of states per volume at the Fermi energy and C_{imp} is the concentration of impurities. One relevant matrix element of $\hat{T}$ is graphically shown in Fig. 1a. Note that you have to trace over the impurity spin Hilbert space. For this purpose, you may find the identity $\langle\langle\sigma'|(\mathbf{S}\cdot\vec{\tau})(\mathbf{S}\cdot\vec{\tau})|\sigma'\rangle\rangle_S = S(S+1)$ useful.

b) **2 points**

Consider the second-order term of the perturbative expansion of the $\hat{T}$-matrix

$$T^{(2)}(\epsilon) = \hat{H}_{\text{imp}} (\epsilon^+ - \hat{H}_0)^{-1} \hat{H}_{\text{imp}}. \tag{21}$$

Show that, at zero temperature,

$$\mathrm{Re}\,\langle \mathbf{k}', \sigma' | \hat{T}^{(2)}(\epsilon_{\mathbf{k}}) | \mathbf{k}, \sigma \rangle = \frac{J^2}{4L^{2d}} \sum_{\mathbf{p}} \frac{1}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{p}}} \left[S(S+1)\delta_{\sigma\sigma'} - \hat{\mathbf{S}} \cdot \vec{\tau}_{\sigma'\sigma} (\Theta(\epsilon_{\mathbf{p}}) - \Theta(\epsilon_{-\mathbf{p}})) \right]. \tag{22}$$

Since in second order, the $\hat{T}$ matrix involves in intermediate propagator $(\epsilon^+ - \hat{H}_0)^{-1}$, one now has to go beyond the simple single particle picture with $|\mathbf{k}, \sigma\rangle = c^\dagger_{\mathbf{k}\sigma}|0\rangle$. A simple way of doing so is to replace the occupation number for electrons (or holes) in the intermediate $\mathbf{k}$ states by a Fermi factor $n_F(\epsilon_{\mathbf{k}})$ (and $1 - (\epsilon_{\mathbf{k}})$ for holes). Remember that, due to the δ-function in Eq. (17), we consider only the case $\epsilon_k = \epsilon'_k$. You may need the following suggestions:

- Taking the real part means simply omitting the infinitesimal imaginary part in the denominator.
- The vacuum contributions should be discarded. The only connected Feynman diagrams are the ones shown in Fig. 1.
- Make use of the identity $(\hat{\mathbf{S}} \cdot \vec{\tau})^2 = \hat{\mathbf{S}}^2 - \vec{\tau} \cdot \hat{\mathbf{S}}$.

c) **1 point**

In the class we will comment upon the finite temperature case. How would Eq. (22) change? If you bravely succeeded in all steps so far, you may convince yourself that the singular part of the second-order contribution at finite temperature can be reabsorbed in a new J_{eff} in Eq. (20). How does J_{eff} look like?

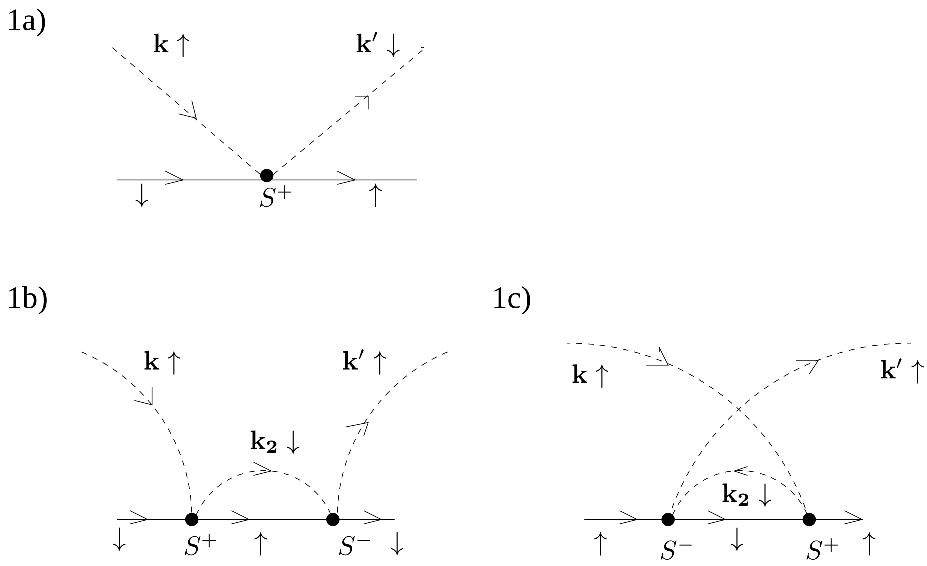

Figure 1: A first order (Fig. 1a) and two second order (Fig. 1b and 1c) diagrams contributing to the matrix element in Eq. (17). The index $\mathbf{k_2}\downarrow$ indicates an intermediate state in the conduction band.