Theoretische Festkörperphysik – Herbstsemester 2010 **Exercise series 11**
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Perturbation theory for the Kondo model

Motivation The Kondo model is one of the prototype models for strong electron correlation physics. This means, that even if it looks very simple, it leads to very complex ground states and system properties that cannot be explained in a simple single-particle picture. Instead, the physics at low temperatures is described by states that involve a macroscopic fraction of the electronic collective.

The model was designed to explain the experimental observation of an unexpected logarithmic increase of the resistivity in metals with magnetic impurities upon cooling down the sample below a certain, very low, temperature. This was unexpected in the sense that electrical resistivity originates from a delay (in a quasi-classical picture) of the electron motion through the conductor by repeated scattering processes with other constituents of the solid state environment, such as impurities or lattice vibrations (phonons). The increase of resistivity thus indicated that at very low temperatures another scattering channels opens, and the fact that it occurs only at very low temperatures means that it cannot be a simple first-order effect (such as banging only once against an impurity), but that it requires a coherent repetition of scattering events. Such an effect is destroyed at higher temperatures because temperature fluctuations destroy the memory of the system wave function to the last scattering event, mainly its phase (known as dephasing). Kondo's insight was that not only this effect is due to scattering on the localized magnetic moments formed by the impurities, but that it was necessary to push the calculation to second order in perturbation theory to see the effect at all. In fact, the first order perturbative result is discouragingly uninteresting such that it is rather surprising that Kondo went to second order.

In this exercise set you will follow Kondo's calculation and determine the logarithmic increase of the resistivity. The Kondo model is a model designed to capture the essential physics for the increased scattering rate, leaving aside any other processes that do not contribute. It consists of a single localized magnetic moment, the Kondo spin, $\mathbf{S}$ at position $x = 0$ (assuming the dilute limit in which other impurities are far away; the final result then includes a final summation over all impurities, mainly, the multiplication by their number), and a single-band metal of noninteracting electrons, described by operators $c_{\mathbf{k}\sigma}$, with momentum $\mathbf{k}$ and spin $\sigma =\uparrow,\downarrow$,

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - J\mathbf{S}\cdot\mathbf{s} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - JS^z s^z - \frac{J}{2}\left[S^+ s^- + S^- s^+\right], \tag{1}$$

where $\mathbf{s} = \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} \frac{1}{2} c^\dagger_{\mathbf{k}\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{\mathbf{k}'\sigma'}$ is the (dimensionless) electron spin density at position $x = 0$, where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector formed by the Pauli matrices, and $S^\pm = S^x \pm iS^y$, $s^\pm = s^x \pm is^y$ are the spin raising and lowering operators. The quantity $H' = -J\mathbf{S}\cdot\mathbf{s}$ describes the important exchange coupling between the localized Kondo spin and the electron spin. The direct charge interaction is left aside, because it is known that pure potential scattering adds only a temperature-independent term to the resistivity (what we know as the resistance of Ohm's law).

The quantity to calculate is the average rate $\Gamma(T)$ that an electron is scattered per unit time at temperature T. This quantity is directly proportional to the resistivity $\rho(T)$, and is given by the Golden Rule expression

$$\Gamma = \sum_i \rho_i(T)\,\Gamma_i \tag{2}$$

with (we set $\hbar = 1$ everywhere and measure energy in frequency units)

$$\Gamma_i = 2\pi \sum_f |\langle f|\,\mathcal{T}(\omega = E_i)\,|i\rangle|^2\,\delta(E_i - E_f), \tag{3}$$

where i, f are initial and final states of the scattering process with eigenenergies $E_{i,f}$, and ρ_i is the density matrix (thermal distribution) of the initial states. The scattering amplitude is given by the scattering matrix (T-matrix) satisfying the Dyson equation

$$\mathcal{T}(\omega) = H' + H'G^r(\omega)\mathcal{T}(\omega), \tag{4}$$

where $G^r(\omega) = [\omega + i\eta - H_0]^{-1}$ is the retarded *many-body* Green's function, also known as *resolvent* (the so far used single-particle Green's function is obtained by taking matrix elements between states with a single-particle excitation).

Exercise 1: First order perturbation (2 points) The problem in doing perturbation theory with spin operators is that they are neither fermions nor bosons and so they do not obey the Wick theorem. This means, we cannot do perturbation theory by the diagrammatic rules we know. There are (at least) two ways out of this misery: First, for a Kondo spin 1/2, we can use a fermionic representation $\mathbf{S} = \frac{1}{2}\sum_{\sigma\sigma'} d^\dagger_\sigma \boldsymbol{\sigma}_{\sigma\sigma'} d_{\sigma'}$. Second, we can work with the matrix elements over the eigenstates $|m_S\rangle$ of S^z (such that $S^z|m_S\rangle = m_S|m_S\rangle$, $m_S = -S, -S+1, \ldots, +S$), and keep explicitly track of all time ordering of the operators.

Here, we suggest to use the matrix element approach (which is more general). The first order contribution to Γ_i is then given by

$$\Gamma_i^{(1)} = 2\pi \sum_f \left|\langle f| H' |i\rangle\right|^2 \delta(E_i - E_f). \tag{5}$$

Use initial and final states $|i\rangle = |\mathbf{k}, \sigma =\uparrow; m_S\rangle$ and $|f\rangle = |\mathbf{k}', \sigma'; m_S'\rangle$, with energies $E_i = \epsilon_k$ and $E_f = \epsilon_{k'}$, and show that

$$\begin{aligned}\Gamma_i^{(1)} &= 2\pi J^2 \Big\{ \underbrace{\left[\langle m_S| S^z |m_S\rangle\right]^2}_{=m_S^2} + \underbrace{\left[\langle m_S+1| S^- |m_S\rangle\right]^2}_{=S(S+1)-m_S(m_S-1)} \Big\} \sum_{k'} \delta(\epsilon_k - \epsilon_k') \\ &= 2\pi\nu(\epsilon_k) J^2 \left[S(S+1) - m_S\right].\end{aligned} \tag{6}$$

with $S^\pm = S^x \pm iS^y$ raising or lowering $|m_S\rangle$ by 1. In the thermal averaging, the term proportional to m_S drops out because S^z and $-S^z$ values are identically occupied (there is no other field favoring a direction, and no spontaneously broken symmetry in the unperturbed system). Hence

$$\Gamma = 2\pi J^2 \nu S(S+1). \tag{7}$$

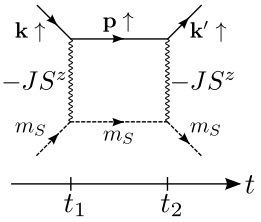
with $\bar{\nu} \approx \nu(\epsilon_F)$ the density of the states over which the thermal average extends (involving energies in the vicinity of ϵ_F only). This result is not very appealing because it is small and essentially temperature independent (a bit is hidden in ν but there is certainly no logarithm).

Exercise 2: Second order perturbation (8 points) At second order perturbation theory things become more interesting. Consider

$$\Gamma_i^{(2)} = 2\pi \sum_f \left|\langle f| H' + H'G^r(E_i)H' |i\rangle\right|^2 \delta(E_i - E_f). \tag{8}$$

with again initial and final states $|i\rangle = |\mathbf{k}, \sigma =\uparrow; m_S\rangle$ and $|f\rangle = |\mathbf{k}', \sigma'; m_S'\rangle$, with energies $E_i = \epsilon_k$ and $E_f = \epsilon_{k'}$. For the evaluation of the amplitude $\langle f| H'G^r(E_i)H' |i\rangle$, it is most convenient to work in time space. Recall that we need to write down the time ordering explicitly and to evaluate the contractions (there is no help from time-ordering operators). The results can still be represented in diagrams.

a) We consider here only those where $m_S = m'_S$ and $\sigma = \sigma' = \uparrow$ (the others give equivalent results). There are in total 4 diagrams, 2 involving the twice the operator S^z and 2 involving S^+ and S^-. For convenience, the first diagram is drawn here:



Draw the remaining 3 diagrams.

b) In the following, we will focus on the case of the displayed diagram only, since all other diagrams give more or less identical results. Since we have taken matrix elements between single-particle states, the propagator line is the retarded single-particle Green's function of the free electron gas (for the $\mathbf{p}$ momentum, the $\mathbf{k}, \mathbf{k}'$ lines indicate only the entry and exit points of the scattering vertex but are no propagators themselves). Give the diagram the name $\gamma(t_2 - t_1)$ and write down the corresponding formula.

c) Assume now that $\epsilon_k, \epsilon_{k'} > \epsilon_F$. This implies necessarily that also $\epsilon_p > \epsilon_F$. Show then that the diagram in momentum space reads

$$\begin{aligned}\gamma(\omega = \epsilon_k) &= +J^2 m_S^2 \sum_{\mathbf{p}} \frac{1 - f(\epsilon_p)}{\epsilon_k - \epsilon_p + i\eta} = J^2 m_S^2 \int \mathrm{d}\epsilon \frac{\nu(\epsilon)[1 - f(\epsilon)]}{\epsilon_k - \epsilon + i\eta} \\ &= J^2 m_S^2 \left[\fint \mathrm{d}\epsilon \frac{\nu(\epsilon)[1 - f(\epsilon)]}{\epsilon_k - \epsilon} + i\pi\nu(\epsilon_k)[1 - f(\epsilon_k)] \right],\end{aligned} \tag{9}$$

with $\nu(\epsilon)$ the electron density of states and $f(\epsilon)$ the Fermi function.

d) At very low temperatures, the Fermi function provides a sharp cutoff at ϵ_F, which dominates the value of the integral. The upper integral boundary cannot affect the result. Indeed, first the density of states vanishes for high energies (it is limited to a final bandwidth) and so the integrand is there zero, second the low-energy physics cannot be influenced by the high energy sector, which can therefore only contribute with at most a constant shift in energy (a so-called ultraviolet cutoff scale). Close to ϵ_F we can then approximate $\nu(\epsilon) \approx \nu(\epsilon_F)$ and write

$$\fint \mathrm{d}\epsilon \frac{\nu(\epsilon)[1 - f(\epsilon)]}{\epsilon_k - \epsilon} \approx \nu(\epsilon_F) \int_{\text{unimportant}}^{\epsilon_F} \frac{\mathrm{d}\epsilon}{\epsilon_k - \epsilon} = -\nu(\epsilon_F) \ln \left| \frac{\epsilon_k - \epsilon_F}{\epsilon_F} \right|. \tag{10}$$

Here is the logarithm (note that it must be dimensionless and the only available energy scale for the normalization is ϵ_F).

e) Now we need to average over the temperature distribution of the initial states ϵ_k. This is to bring back the Fermi function: Only ϵ_k within an interval $k_B T$ about ϵ_F are thermally excited. The major insight is now that if $k_B T$ sets the largest low-energy scale (there is, for instance, no larger voltage) then any averaging over temperature fluctuations will lead to replacing the fluctuating energy $\epsilon_k - \epsilon_F$ by something proportional to $k_B T$ (plus higher order corrections on the order of $k_B T / \epsilon_F \ll 1$). This means the thermal average leads (without doing any calculation here!) to

$$\ln \left| \frac{\epsilon_k - \epsilon_F}{\epsilon_F} \right| \to \ln \left(\frac{c k_B T}{\epsilon_F} \right), \tag{11}$$

with c some proportionality constant. Since $\ln(ck_BT/\epsilon_F) = \ln(k_BT/\epsilon_F) + \ln(c)$ and $\ln(c)$ is a small constant in comparison with the diverging temperature dependent logarithm, we can neglect $\ln(c)$. The result is then correct to what is known as *logarithmic accuracy*. Setting then $T_F = \epsilon_F/k_B$ we find for the thermally averaged γ

$$\gamma \approx -\nu J^2 m_S^2 \ln\left(\frac{T}{T_F}\right), \tag{12}$$

with $\nu \approx \nu(\epsilon_F)$. Explain why the imaginary part $\propto \nu(\epsilon_k)[1 - f(\epsilon_k)]$ can be neglected.

f) All the other diagrams and also the processes where the electron and Kondo spins flip (e.g., $(\uparrow, m_S) \to (\downarrow, m_S + 1)$) lead to identical expressions (up to some prefactors arising from the matrix elements of the Kondo spin). Show then that we have found

$$\Gamma_i^{(2)} = \Gamma_i^{(1)}\left[1 - \alpha J\nu \ln\left(\frac{T}{T_F}\right) + \dots\right], \tag{13}$$

with α a constant covering all the matrix elements over S (don't calculate it!). Note that the logarithmic correction depends on the sign of J. Observe also that the logarithm diverges as $T \to 0$. Give an argument until which temperature we can trust the perturbation theory, and show that the so-called *Kondo temperature*

$$T_K \sim T_F \mathrm{e}^{\frac{1}{\nu J}} \tag{14}$$

gives a good idea when this happens. The fact that perturbation theory breaks down is an excellent indicator that the system is no longer described by simple elementary excitations of the noninteracting type but enters a phase formed by a strong coupling between all constituent particles in the system (or at least a large fraction of them); here electrons and the Kondo spin. This is what we know as *strong correlation physics*. Experimentally this phase is seen because for $T < T_K$, the temperature dependence of any response function is replaced by the larger, temperature independent many-body correlation scale T_K.