Universität Bonn May 22, 2015
Physikalisches Institut
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Advanced Theoretical Condensed Matter Physics
Summer term 2015

Exercise 3: Quantum impurities

(Solutions due on June 4, 2015, 12h)

A quantum impurity is a spatially localized system with a discrete quantum degree of freedom, like a spin or atomic orbitals, embedded in a conduction electron sea. The interplay of discrete states with the continuous spectrum of conduction electrons and the Fermi edge often induces interesting, singular behavior at low temperatures. In the following we will consider some perturbative aspects of quantum impurities.

3.1 The resonant level model (15 points)

The resonant level model is comprised of a single, non-interacting atomic orbital with energy ε_d, hybridizing with the conduction band via a transition matrix element V,

$$H = \sum_{\mathbf{p}\sigma} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + \varepsilon_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + V \sum_{\mathbf{p}\sigma} \left(c^\dagger_{\mathbf{p}\sigma} d_\sigma + d^\dagger_\sigma c_{\mathbf{p}\sigma} \right) \ , \tag{1}$$

where $c_{\mathbf{p}\sigma}$, $c^\dagger_{\mathbf{p}\sigma}$ and d_σ, $d^\dagger_\sigma$ are the operators for conduction electrons (momentum $\mathbf{p}$, spin σ) and for electrons in the impurity orbital, respectively. $\varepsilon_{\mathbf{p}}$ is the conduction electron energy. The density of states (per spin) of this band is $N(\omega)$. We want to calculate the spectral density of the impurity orbital in the presence of the conduction electron sea.

a) Draw the selfenergy diagram Σ of the d-electrons due to the hybridization V with the conduction band and write down the corresponding Dyson equation for the d-electron Green's function $G_{d\sigma}(\omega)$ in diagrammatic form. Use solid lines for the d-electron and dashed lines for the c-electron Green's functions, and label all lines with the appropriate momentum, spin and energy arguments. Now write down this Dyson equation as a mathematical expression in frequency representation.

b) Calculate the imaginary part of the retarded selfenergy, $\mathrm{Im}\Sigma(\omega) =: -\Gamma(\omega)$, in terms of the conduction electron density of states [Result: $\Gamma = \pi |V|^2 N(\omega)$]. We now assume that the Fermi energy is in the center of the band ($\varepsilon_F = 0$), that the conduction band width is much larger than all other energies of the system and that the density of states is constant up to the band edges, $N(\omega) = const.$ ("wide band limit"). Show that in this case the real part of the self-energy vanishes, using the Kramers-Kroënig relation.

c) Calculate the spectral function $A_d(\omega)$ from the d-electron Green's function and draw a sketch of $A_d(\omega)$.

d) Calculate the impurity occupation number (number of electrons in the impurity level) per spin at zero temperature, $n_{d\sigma}$. Draw $n_{d\sigma}$ as a function of ε_d.

3.2 Anderson impurity model: Fermi liquid behavior

We now take into account that two electrons in the localized level ε_d of the model of problem 3.1 experience a repulsive interaction $U > 0$. This is the Anderson impurity model (P. W. Anderson, 1961),

$$H = \sum_{\mathbf{p}\sigma} \varepsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + \varepsilon_d \sum_{\sigma} d^\dagger_\sigma d_\sigma + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + V \sum_{\mathbf{p}\sigma} \left(c^\dagger_{\mathbf{p}\sigma} d_\sigma + d^\dagger_\sigma c_{\mathbf{p}\sigma} \right) \ , \tag{2}$$

with $\hat{n}_{d\sigma} = d^\dagger_\sigma d_\sigma$. The interaction U is usually large, due to the localized nature of the d-orbital.

a) Draw the d-electron selfenergy diagram due to the interaction U of 2nd order in U and label all Green's function lines with the appropriate spin and energy arguments.

b) Calculate the imaginary part of this (retarded) selfenergy, $\mathrm{Im}\Sigma^R_d(\omega)$, using the Matsubara technique, and express it in terms of the d-spectral functions of problem 3.1.
Note: It is not required to evaluate the energy integrals of the final expression.

c) Show that $\mathrm{Im}\Sigma^R_d(\omega)$ vanishes for low energies and temperatures as

$$\mathrm{Im}\Sigma^R_d(\omega) \sim \left(\omega^2 + \pi (k_B T)^2 \right) \tag{3}$$

Note: It is only required to derive the power-law dependence, not the relative prefactor π of the temperature and energy dependence.