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Physikalisches Institut
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Advanced Theoretical Condensed Matter Physics Summer term 2018

Exercise 3: Quantum impurities

(Solutions due on May 29, 2018, 12h)

A quantum impurity is a spatially localized system with a discrete quantum degree of freedom, like a spin or atomic orbital, embedded in a conduction electron sea. The interplay between discrete states and the continuous spectrum of conduction electrons with a 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 (momnetum $\mathbf{p}$, 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 self-energy 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. Choose 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 self-energy, $\text{Im}\Sigma(\omega) =: -\Gamma(\omega)$, 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 bandwidth is much larger than all other energies of the system, and that the density of states is constant ($N(\omega) = \text{const.}$) up to the band edges ("wide-band limit"). Show that in this case the real part of the self-energy vanishes, using the Kramers-Kronig relations.

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, $n_{d\sigma}$. Sketch $n_{d\sigma}$ 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),

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

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 self-energy diagram due to the interaction U up to second order in U and label all Green's function lines with the appropriate spin and energy arguments.

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

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

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