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Advanced Condensed Matter Theory — SS10

Exercise 5

Please return your solutions during the lecture on June 9, 2010
to be discussed on June 10, 2010

1.1 The Relation between Anderson and Kondo Hamiltonian: (25 points)

In the following we consider the low energy limit of the Anderson Hamiltonian:

$$H_A = E_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k}d} c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + \text{h.c.} \right), \qquad (1)$$

where d_σ is the annihilation operator of the isolated atomic d state.

a) Restrict your considerations to the atomic part of the Hamiltonian (1), i. e.

$$H_{\text{atomic}} = E_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow},$$

and give its eigenstates. Require $E_d < 0$ and $E_d + U > 0$ and show that the ground-state of the system is a magnetic doublet.

If the ground-state configuration of the Anderson model (1) for V_{kd} is the singly occupied one, then the other configurations are higher excited states. Next we want to derive an effective Hamiltonian by taking into accound virtual excitations to these states within lowest order perturbation theory.

b) If we write the total wavefunction as

$$\Psi = \Psi_0 + \Psi_1 + \Psi_2,$$

where Ψ_n is the component in which the d-state has the occupation number n, then the Schödinger equation $H_A \Psi = E\Psi$ takes the form

$$\begin{pmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ 0 & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{pmatrix} = E \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{pmatrix} \qquad (2)$$

with $H_{nm} = P_n H_A P_m$ and P_n the projection operator on to the subspace with d occupation n. Why are H_{20} and H_{02} equal to zero?

Show that the projection operators

$$P_0 = (1 - n_{d\uparrow})(1 - n_{d\downarrow}), \quad P_1 = n_{d\uparrow}(1 - n_{d\downarrow}) + n_{d\downarrow}(1 - n_{d\uparrow}), \quad P_2 = n_{d\uparrow} n_{d\downarrow},$$

satisfy $\sum_n P_n = 1$ and $P_m P_n = \delta_{nm} P_m$.

c) Eliminate Ψ_0 and Ψ_2 from Eq. (2) to obtain

$$H_{eff}\Psi_1 \equiv \left[H_{11} + H_{12}(E-H_{22})^{-1}H_{21} + H_{10}(E-H_{00})^{-1}H_{01}\right]\Psi_1 = E\Psi_1. \quad (3)$$

d) Derive the following equations:

$$\begin{aligned} H_{12}(E-H_{22})^{-1}H_{21} &= -\sum_{\mathbf{q},\mathbf{k}}\sum_{\sigma,\tau}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{U+E_d-\epsilon_{\mathbf{k}}}\left(1-\frac{E-E_d-H_0}{U+E_d-\epsilon_{\mathbf{k}}}\right)^{-1} d_\sigma d^\dagger_\tau c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\tau} \\ H_{10}(E-H_{00})^{-1}H_{01} &= -\sum_{\mathbf{q},\mathbf{k}}\sum_{\sigma,\tau}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}\left(1-\frac{E-E_d-H_0}{\epsilon_{\mathbf{k}}-E_d}\right)^{-1} d^\dagger_\sigma c_{\mathbf{k}\sigma}c^\dagger_{\mathbf{q}\tau}d_\tau \end{aligned} \quad (4)$$

Hint: First show for the components, that $H_{00} = H_0P_0$, $H_{11} = (H_0 + E_d\mathbb{1})P_1$, $H_{22} = (H_0 + 2E_d\mathbb{1} + U\mathbb{1})P_2$, $H_{10} = \sum_{\mathbf{k}\sigma} V^*_{\mathbf{k}d} d^\dagger_\sigma c_{\mathbf{k}\sigma} P_0$, $H_{21} = \sum_{\mathbf{k}\sigma} V^*_{\mathbf{k}d} d^\dagger_\sigma c_{\mathbf{k}\sigma} P_1$, where $H_0 = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$.

e) From now on we restrict ourselves to the singly occupied subspace, i.e. lowest order in $V_{\mathbf{k}d}$, and therefore neglect the fractions of the form $\frac{E-E_d-H_0}{E_d+\ldots}$ in Eq. (4). Prove, that

$$\sum_{\tau,\sigma} c^\dagger_{\mathbf{k}\sigma}d^\dagger_\tau c_{\mathbf{q}\tau}d_\sigma = -2\left(\mathbf{S}_{\mathbf{kq}}\cdot\mathbf{S}_d + \frac{1}{4}\left(\sum_\sigma c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\sigma}\right)\left(\sum_\tau n_{d\tau}\right)\right),$$

where $S^i_{\mathbf{kq}} = \frac{1}{2}\sum_{\alpha,\beta} c^\dagger_{\mathbf{k}\alpha}\left(\sigma^i\right)_{\alpha\beta}c_{\mathbf{q}\beta}$ with σ^i the Pauli matrices. The second quatization representation of $\mathbf{S}_d$ is the same, except that the d operators appear instead of the c's.

Hint: $\sum_{i=x,y,z}\sigma^i_{\alpha\beta}\sigma^i_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}$

Finally derive

$$\begin{aligned} H_{12}(E-H_{22})^{-1}H_{21} &= 2\sum_{\mathbf{q},\mathbf{k}}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{U+E_d-\epsilon_{\mathbf{k}}}\mathbf{S}_{\mathbf{kq}}\cdot\mathbf{S}_d - \frac{1}{2}\sum_{\mathbf{q},\mathbf{k},\sigma}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{U+E_d-\epsilon_{\mathbf{k}}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\sigma} \\ H_{10}(E-H_{22})^{-1}H_{21} &= 2\sum_{\mathbf{q},\mathbf{k}}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}\mathbf{S}_{\mathbf{kq}}\cdot\mathbf{S}_d + \frac{1}{2}\sum_{\mathbf{q},\mathbf{k}}\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\sigma} - \sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}, \end{aligned}$$

where we used the relation $\sum_\sigma n_{d\sigma} = 1$.

f) Insert these results in H_{eff} to obtain

$$H_{eff} = 2\sum_{\mathbf{q},\mathbf{k}} J_{\mathbf{kq}}\mathbf{S}_{\mathbf{kq}}\cdot\mathbf{S}_d + \sum_{\mathbf{q},\mathbf{k},\sigma}\left[\epsilon_{\mathbf{k}}\delta_{\mathbf{qk}} + K_{\mathbf{kq}}\right]c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\sigma} + E_d - \sum_{\mathbf{k}}\frac{V^*_{\mathbf{k}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}, \quad (5)$$

where $J_{\mathbf{kq}} = \left[\frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{U+E_d-\epsilon_{\mathbf{k}}} + \frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}}-E_d}\right]$ and $K_{\mathbf{kq}} = \frac{V^*_{\mathbf{q}d}V_{\mathbf{k}d}}{2}\left[\frac{1}{\epsilon_{\mathbf{k}}-E_d} - \frac{1}{U+E_d-\epsilon_{\mathbf{k}}}\right]$. Moreover $K_{\mathbf{kq}}$ can be absorbed in the conduction electron dispersion as follows

$$\epsilon_{\mathbf{k}}\delta_{\mathbf{qk}} + K_{\mathbf{kq}} \longrightarrow \epsilon_{\mathbf{kq}}$$

and the energies may be measured with respect to the last two terms in H_{eff}, leading to

$$H_{\text{Kondo}} \equiv H_{eff} = 2\sum_{\mathbf{q},\mathbf{k}} J_{\mathbf{kq}}\mathbf{S}_{\mathbf{kq}}\cdot\mathbf{S}_d + \sum_{\mathbf{q},\mathbf{k},\sigma}\epsilon_{\mathbf{kq}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{q}\sigma}. \quad (6)$$

Prove that $J_{\mathbf{kq}}$ is positiv near the Fermi surface.