8.512 Theory of Solids II
Spring 2009

8.512 Theory of Solids **Problem Set 10** **Due May 6, 2004**

Consider the non-interacting problem of an impurity d orbital at energy ϵ_d hybridizing with matrix element V_k with a conduction band. In class we showed the relation

$$\langle n_d \rangle = \delta(\epsilon_F)/\pi \tag{1}$$

where

$$\delta(E) = \tan^{-1} \frac{\Delta}{\epsilon'_d - E} \quad , \tag{2}$$

$$\epsilon'_d = \epsilon_d + \Sigma'(E) \quad , \quad \Delta = -\Sigma''(E) \quad and$$

$$\Sigma(E) = \sum_k \frac{|V_k|^2}{E - \epsilon_k + i\eta} \quad . \tag{3}$$

You should have complained that Eq.(1) cannot be correct, because according to Friedel sum rule, the phase shift at the Fermi energy is related to the total charge accumulation around the impurity site, not just the charge $\langle n_d \rangle$ which sits on the impurity site. The conduction electron charge accumulated around the impurity is missing in Eq.(1). The goal of this problem is to account for this missing charge.

1. Show that

$$\delta(E) = Im\{\ln G_d(E)\}$$

where $G_d(E) = \langle d|(E - H + i\eta)^{-1}|d\rangle$.

2. Show that

$$\int_{-\infty}^{\epsilon_F} dE \frac{\partial}{\partial E} \ln G_d(E) = -\int_{-\infty}^{\epsilon_F} dE G_d(E) \left(1 - \frac{d\Sigma}{\partial E}\right) \tag{4}$$

Hint: Start with the identity $\frac{\partial}{\partial E} \ln G_d^{-1} \frac{\partial G_d^{-1}}{\partial E}$

3. By taking the imaginary part of both sides of Eq.(4), show that

$$\delta(\epsilon_F) = \pi\langle n_d\rangle - Im\int_{-\infty}^{\epsilon_F} dE G_d \frac{\partial\Sigma}{\partial E} \tag{5}$$

   The second term on the right hand side is the correction of Eq.(1). Note that in class we have assumed Δ and Σ' to be constant, which explains why this term was missing in Eq.(1).

4. Show that the conduction electron charge accumulated in the vicinity of the impurity is given by

$$\delta\rho_c = Im\sum_{\boldsymbol{k}}\int_{-\infty}^{\epsilon_F} dE\left(G_{\boldsymbol{k}}(E) - G^0_{\boldsymbol{k}}(E)\right) \tag{6}$$

   where $G_{\boldsymbol{k}} = \langle\boldsymbol{k}|(E - H + i\eta)^{-1}|\boldsymbol{k}\rangle$ and $G^0_{\boldsymbol{k}} = (E - \epsilon_k + i\eta)^{-1}$ is the conduction band Green function in the absence of the impurity orbital.

5. Show that the second term on the R.H.S. of Eq.(5) is just $\pi(\delta\rho_c)$ so that the Friedel sum rule is satisfied. **Hint:** Write down an equation for G_k following the method we used to derive the G_d equation.

6. Estimate the energy dependence of Σ and argue that the correction to Eq.(1) is small when $\Delta \ll \epsilon_F$, i.e., when the resonance is narrow.