Exercise for Theoretical Condensed Matter Physics

Exercise 6, June, 3rd 2024. Discussion on June, 11th 2024

Anderson impurity model

To put in practice the equation of motion method, we now turn to the Anderson impurity model, whose Hamiltonian reads

$$H = \sum_{k,\sigma} \left[(\epsilon_k - \mu) c^\dagger_{k\sigma} c_{k\sigma} + \left(t_k c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) \right] + \sum_\sigma (\epsilon_d - \mu) c^\dagger_{d\sigma} c_{d\sigma} + U n_{d\downarrow} n_{d\uparrow}. \tag{1}$$

where the operators $c^\dagger_{k\sigma}$ create itinerant electrons of spin σ and energy ϵ_k in the metallic host, while the operators $c^\dagger_{d\sigma}$ create electrons of spin σ on the local impurity. The electrons in the band are assumed to be nearly free (Fermi-liquid-like behavior), while those associated with the impurity state experience an on-site Coulomb interaction of a strength characterized by the Hubbard energy U. A hybridization term couples these two subsystems.

a) Apply the equation of motion method to derive a set of coupled equations in frequency space between G^R_{dd} and G^R_{kd} defined as

$$G^R_{dd}(\sigma, t-t') = -i\theta(t-t') \langle [c_{d\sigma}(t), c^\dagger_{d\sigma}(t')]_+ \rangle \tag{2}$$

$$G^R_{kd}(\sigma, t-t') = -i\theta(t-t') \langle [c_{k\sigma}(t), c^\dagger_{d\sigma}(t')]_+ \rangle. \tag{3}$$

Notice that all terms except the Hubbard one are bilinear in fermionic operators. make use of the fact that the interaction term depends only on the impurity operators and thus commutes with $c_{k\sigma}$.

b) Make use of the fact that the interaction term depends only on the impurity operators and thus commutes with $c_{k\sigma}$ to exclude G^R_{kd} from the equations. Show that the effect of the itinerant ("bath") electrons in the AIM is equivalent to adding a self-energy-like contribution to the isolated Hubbard site. This contribution is given by

$$\Sigma^R(\omega) = \sum_k \frac{|t_k|^2}{\omega + i\eta - \epsilon_k + \mu} \tag{4}$$

and is usually referred to as the hybridization function.

c) It is customary in such impurity problems to approximate the hybridization matrix by a constant, and consider the bath density of states $\rho(\epsilon)$ to be flat with bandwidth $2W$. This allows one to introduce the parameter Γ as $\pi\rho(\epsilon)|t_k|^2 = \Gamma\theta(W - |\epsilon|)$. Compute the hybridization function explicitly under these assumptions. Discuss the role of the imaginary part of the result.

d) In the companion notebook `Ex_06_companion.ipynb`, you will find python definitions that will help you visualize the hybridization function of a single impurity level coupled to a one-dimensional tight-binding chain. Play around with the parameters and see how the hybridization function changes.