

The single-impurity Anderson model

The fundamental model to theoretically describe local moments in metals is the single-impurity Anderson model¹ Its Hamiltonian reads

$$\hat{H}_{\text{SIAM}} = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} \hat{c}_{\vec{k}\sigma}^\dagger \hat{c}_{\vec{k}\sigma} + \sum_{\sigma} \left(\epsilon_f + \frac{U}{2} \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} \right) \hat{f}_{\sigma}^\dagger \hat{f}_{\sigma} + \frac{1}{\sqrt{N}} \sum_{\vec{k}\sigma} \left[V_{\vec{k}} \hat{c}_{\vec{k}\sigma}^\dagger \hat{f}_{\sigma} + \text{h.c.} \right]$$

The operators $\hat{c}_{\vec{k}\sigma}^{(\dagger)}$ annihilate (create) states in a conduction band with dispersion $\epsilon_{\vec{k}}$, and $\hat{f}_{\sigma}^{(\dagger)}$ annihilates (creates) a fermionic state localized at lattice site $\vec{R} = 0$. The local level has an on-site energy ϵ_f and if two particles with opposite spin are present one has to pay the Coulomb energy U . Both subsystem talk to each other through a hybridization with strength $V_{\vec{k}}$. Usually one assumes $V_{\vec{k}} \equiv V$ independent of \vec{k} .

- (a) Solve the SIAM in Hartree approximation for $\langle \hat{n}_f \rangle = \langle \hat{n}_{f,\uparrow} + \hat{n}_{f,\downarrow} \rangle = 1$, i.e. factorize

$$\hat{n}_{f,\uparrow} \hat{n}_{f,\downarrow} \rightarrow \hat{n}_{f,\uparrow} \langle \hat{n}_{f,\downarrow} \rangle + \langle \hat{n}_{f,\uparrow} \rangle \hat{n}_{f,\downarrow}$$

Allow for solutions $\langle \hat{n}_{f,\uparrow} \rangle \neq \langle \hat{n}_{f,\downarrow} \rangle$. When do these occur as function of the model parameters? Does the precise value and phase of the hybridization V play a role?

Hint: The solution is very easy when one uses Green's function methods.

- (b) Discuss the physical relevance of the polarized Hartree solution. Do you expect it to be realized in impurity systems? What do you believe the system will do?
- c) A very simplified version of the SIAM is the two-site model, i.e. we replace the band states by one level, too. Solve the resulting Hamiltonian in the limit $U = \infty$. What is the ground state and how does it depend on the model parameters?

¹P.W. Anderson, Phys. Rev. **124**, 41 (1961).