

561 Fall 2005 Lecture 11**Effects of Electron Interactions in Metals: Anderson Impurity Model and the Kondo Effect**

See Phillips, Ch. 6 and 7. Also Mahan, Sec. 1.4, Ch. 11; P. W. Anderson, Phys. Rev. 124, 41 (1961).

1. Kondo Effect

Increase of resistance at low T - very hard to understand on simple physical grounds. Why?

Occurs for impurities with “localized” magnetic states. We will discuss what “localized” means.

See figure in Phillips for Fe in Mo-Nb alloys.

Characteristic temperature T_K varied wildly - from 300 K for V in Au (even higher but hard to observe at high T where many other effects obscure the Kondo effect) to 10^{-4} K for Mn in Au.

Specific heat per impurity: $C = \gamma T$, $\gamma \propto 1/T_K$.

Becomes non-magnetic” for low T.

Solved by K. G. Wilson, using numerical renormalization group, for which he got the Nobel prize.

Exact solutions later using the “Bethe Ansatz”.

2. Impurity in a metal with no electron-electron interactions**A. Resistance due to scattering**

Treat as scattering due to localized potential in isotropic medium. Same as well-known quantum mechanical expressions for scattering in vacuum in terms of phase shifts $\delta_l(E)$ for angular momentum l . (See Ziman; Mahan, p. 249; Doniach, 81 ff)

Crosssection σ for scattering of plane wave at energy E

$$\sigma(E) = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2(\delta_l(E)) \quad (1)$$

which leads to resistivity. Note that the maximum possible resistivity in an angular momentum channel is given by the “unitarity limit” $\sin(\delta_l) = 1$ or $\delta_l = \pm \frac{\pi}{2}$.

B. Relation of phase shift to added density of states due to impurity

The change in the density of states of the system (for each spin and angular momentum l) is given by

$$\delta\rho_l(E) = \frac{1}{\pi} \frac{d\delta_l(E)}{dE}, \quad (2)$$

where $\delta_l(E)$ is the phase shift at energy E . This leads to

$$\sum_l \int_{-\infty}^E dE \rho_l(E) = \frac{1}{\pi} \sum_l \delta_l(E), \quad (3)$$

C. Friedel Sum Rule

If we choose $E = E_F$ this leads to the result that the integrated number of added electrons of spin σ is equal to the phase shift for spin σ at the Fermi energy, i.e. the phase shift that determines the resistivity.

The Friedel sum rule follows from the simple fact that the charge of an impurity is screened in a metal. For an impurity of charge ΔZ (relative to the host metal, i.e., the number of added protons on impurity) the number of extra electrons that accumulate around impurity must equal Z by charge neutrality, from which it follows that the sum of phase shifts at the Fermi energy must obey the condition:

$$\Delta Z = \frac{1}{\pi} \sum_{l,m,\sigma} \delta_{l,m,\sigma}(E_{Fermi}) \quad (4)$$

This was derived by Friedel for non-interacting electrons. A formal proof by was given by Dewitt, Phys. Rev 103, 1565 (1956).

Consequences: there is a direct relation of resistance of impurity to the nuclear charge. With some simplifications it provides very useful rules. In particular if we assume scattering is restricted to only $l = 0$ and is spin independent, then the sum rule is simply

$$\delta_0 = \frac{\pi}{2} \Delta Z \quad (5)$$

i.e., the resistance is given by the charge. If ΔZ is odd, maximum resistance; if ΔZ is even, no resistance! This is actually a good approximation for an impurity in simple metals. This is because scattering is large only for small angular momenta if the impurity potential is short range, since higher $l > 0$ have small amplitude at the impurity site.

3. Anderson Impurity Model

Described in P. W. Anderson, Phys. Rev. 124, 41 (1961) and many texts.

Simplest model with the key effects. Assume electrons in metal are non-interacting; interactions only on impurity (like a Hubbard Model on this one site).

$$\begin{aligned} H &= H_{band} + H_{impurity} + H_{hybridization} \\ &= \sum_{k\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} + \epsilon_L c_{L\sigma}^+ c_{L\sigma} + U n_{L\uparrow} n_{L\downarrow} + \sum_{k\sigma} V_{kL} [c_{k\sigma}^+ c_{L\sigma} + c_{L\sigma}^+ c_{k\sigma}] \end{aligned} \quad (6)$$

A. Solution for $U = 0$ in terms of Greens Functions (Phillips; Mahan; Doniach 176 ff) Leads to coupled equations:

$$\begin{aligned} (\omega - \epsilon_L) G_{LL\sigma}(\omega) &= 1 + \sum_{k\sigma} V_{kL} G_{kL\sigma}(\omega) \\ (\omega - \epsilon_k) G_{kL\sigma}(\omega) &= 0 + \sum_{k\sigma} V_{kL} G_{LL\sigma}(\omega) \end{aligned} \quad (7)$$

which leads to

$$G_{LL\sigma}(\omega) = \frac{1}{\omega - \epsilon_L - \Sigma_{\sigma}^*(\omega)} \quad (8)$$

with

$$\Sigma^*(\omega) = \sum_k \frac{V_{kL}^2}{\omega - \epsilon_k + i\eta} \quad (9)$$

which is independent of σ and is here given for the retarded form.

Now we can find $\Sigma^*(\omega)$ explicitly in simple cases. If we assume $V_{kL} = V$ (as Anderson did) then

$$\text{Im}\Sigma^*(\omega) = -\pi V^2 \rho^0(\omega) \equiv -\Delta(\omega) \quad (10)$$

where $\rho^0(\omega)$ is the unperturbed density of states of in the metal.

Now the added density of states due to the impurity is

$$\rho_{L\sigma}(\omega) = -\frac{1}{\pi} \text{Im}G_{LL\sigma}(\omega) = \frac{1}{\pi} \frac{\Delta(\omega)}{(\omega - \epsilon_L - \text{Re}\Sigma_{\sigma}^*(\omega))^2 + \Delta^2(\omega)} \quad (11)$$

Finally if we approximate the metal density of states as constant (usually good approximation for energies near E_F) this leads to $\Delta(\omega) = \Delta$ and a Lorentzian shape for density of states. This is a "resonant level" in the continuum with maximum scattering at the resonance at $\omega = \epsilon_L - \text{Re}\Sigma_{\sigma}^*(\omega)$.

B. The phase shift and Friedel sum rule again

The Friedel sum rule, relating the integrated number of added electrons to the phase shift, leads to the remarkable conclusion that scattering is controlled by the charge independent of the size of the local interactions.

Result for the Anderson model which has only s-states: The phase shift is give by Eq. 5. For a non-magnetic solution, there is maximum scattering for the case where there is one extra electron, $\Delta Z = 1$. This follows even though there would appear to be a magnetic moment.

4. Anderson's Hartree-Fock Solution for $U \neq 0$

You are asked in a homework problem to verify Anderson's solution for the case of $Z = 1$ that if U exceeds a critical value, then the Hartree-Fock solution has a broken symmetry (unrestricted Hartree-Fock) with different energies for up and down spins.

5. Relation of Anderson Impurity Problem and Kondo Effect

For the strongly magnetic case, the H-F solution is a degenerate ground state (spin \uparrow and \downarrow) with very little effect at the Fermi energy (just the tail of the Lorentzian). This is the formation of a "localized magnetic moment".

But the mean-field broken-symmetry H-F solution misses a key point. The spin is still coupled to the electrons in the metal which have low energy excitations (arbitrarily low energy near the Fermi energy). No matter how small is the coupling it is sufficient to couple the low energy metal excitations and the zero-energy spin excitation of the localized spin, to form a qualitatively new state. **There is still the maximum possible scattering at the Fermi energy at $T = 0$ At higher T the effect goes away. This is the Kondo effect.**

Schrieffer-Wolfe transformation establishes relation.

6. Possible Projects

There are several suggested projects associated with this problem.

1. The reason why the Friedel sum rule still holds in the interacting system.
 - 1a. The relation of the Friedel sum rule for an impurity to the Luttinger sum rule on the volume enclosed by the Fermi surface in a crystalline metal.
2. The nature of the Kondo effect - relation to other problems.

3. The Schrieffer-Wolfe transformation of the Anderson model with large U , to the Kondo model in which the low energy excitations are the electrons near the Fermi energy, and the localized spin.
4. The analytic solution of this problem in the large degeneracy case.
5. The Anderson lattice model, which is a generalization of the impurity case, which leads to a lattice problem related to the Kondo problem. In the "local moment" magnetic case, this leads to spins on each site coupled to band electrons; Kondo-like effects; "Heavy Fermion" systems.
6. Observation of Kondo effects on crystal surfaces using STM
7. Other possible ideas related to this problem.