598SCM Fall 2004 Lecture 23

Localized Models for Interacting Electrons

See for example Aschroft & Mermin, Ch. 32; Mahan Ch. 1; Jones & March vol. 1, p 341 ff; Review by Imada, et al.

- **Hubbard Model and Mott metal-insulator transition**

Described in a set of papers by J. Hubbard, Proc. Roy. Soc. A276, 238 (1963); A281, 401 (1964); A285, 542 (1964). (Also independent papers at the same time by Gutzwiller and by Kanimori.)

The central model in present theories of Hi-Tc superconductors: Hubbard Model on 2-d square lattice. (P. W. Anderson, Science 256, 1526 (1992); E. Fradkin, "Field Theories of Condensed Matter Systems", Ch. 2 and following.)

One-band Hubbard Hamiltonian:

$$H = \sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \tag{1}$$

where i, j label the sites in the lattice. The electrons are assumed to be restricted to one band which is not degenerate except for spin. The interaction U is only between electrons on the same site. The "hopping" terms t_{ij} give dispersion to the electron states. The simplest model assumes the $t's$ are zero except for nearest neighbor hopping terms.

A. Soluble in four cases:

1. The non-interacting case $U = 0$

2. The ferromagnetic state with all spins parallel

3. Small systems (1, 2, 3 , ... sites) For example, the one-site atomic limit is just $t_{ij} = 0$.

4. Exact solution by Leib and Wu in 1 dimension using "Bethe Ansatz" (special method that works in 1D only - idea for project)

B. Exact solution for 2 sites (Exercise in homework.)

Illustrates key features of the solution as a function of U

Small U - described by perturbation theory in U about the $U = 0$ soltution
Large U - described by perturbation theory in t^2/U – but note that the model is degenerate for $t^2/U = 0$ – an indication of the special features of strongly correlated systems.

C. Hartree-Fock Approximate Solutions

Non-magnetic Band solution vs. Ferromagnetic solution

Basic idea - transition from band metal to magnetic insulator, but wrong in many ways

Example of two site model in Hartree-Fock approximation

D. Mott metal-insulator transition

Transition as a function of the magnitude of the interaction.

Transition as a function of "doping" or band-filling.

- **Heisenberg Spin Model - low energy magnetic excitations of system with localized moments**

  Low energy excitations in the magnetic limit of the Hubbard model; i.e., $U >> t$ limit where the spins on each site which are coupled because of small hopping t, leading to spin excitations described by

$$H = \sum_{ij} J_{ij} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j \tag{2}$$

  where the J's are exchange constants and $\vec{\mathbf{S}}_i$ is a spin vector on lattice site i.

  Example of 1 electron per site, with $U >> t$. Illustrated by two-site example. Generalizable to higher spins.

- **Anderson Impurity Model and the Kondo Effect: Effects of localized magnetic moments Metals:**

  See for example Mahan p. 57-59, 977 ff; Doniach p 186 ff; Harrison Cp. V, Sect. 7; P. W. Anderson, Phys. Rev. 124, 41 (1961).

  1. Impurity in 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

$$\sigma(E) = \frac{4\pi}{k^2} \sum_l (2l+1) sin^2(\delta_l(E)) \tag{3}$$

  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. Friedel Sum Rule

  For an impurity of charge ΔZ (relative to the host metal, i.e., the number of added protons on impurity) one can prove that the sum of accumulated extra electrons around impurity (which is Z by charge neutrality) is directly related to phase shift at the Fermi energy:

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

Proved by Friedel for non-interacting electrons. Formal proof by Dewitt, Phys. Rev 103, 1565 (1956).

Consequences: there is a direct relation of resistance of impurity to 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

$$\delta_0 = \frac{\pi}{2}\Delta Z \tag{5}$$

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.

2. Anderson Impurity Model

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

Simplest model with the key effects. Assume electrons interact on the impurity site (like a Hubbard Model on this one site) but that they are non-interacting on all other sites in the surrounding metal. An example would be a transition metal impurity (strong e-e interactions for electrons in the 3d state) in a metal like Cu where the electrons have only weak interactions. The Anderson impurity hamiltonian is

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

A. Solution for $U = 0$ in terms of Greens Functions (Mahan 272 ff; Doniach 176 ff) Leads to coupled equations:

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

which leads to

$$G_{LL\sigma}(\omega) = \frac{1}{\omega - \epsilon_L - \Sigma^*_\sigma(\omega)} \tag{8}$$

with

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

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

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

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

$$\rho_{L\sigma}(\omega) = -\frac{1}{\pi} ImG_{LL\sigma}(\omega) = \frac{1}{\pi} \frac{\Delta(\omega)}{(\omega - \epsilon_L - Re\Sigma^*_\sigma(\omega))^2 + \Delta^2(\omega)} \tag{11}$$

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 $\omega = \epsilon_L - Re\Sigma^*_\sigma(\omega)$.

B. Relation to the phase shift

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

$$\delta\rho(E) = \frac{1}{\pi} \frac{d\delta_0(E)}{dE}, \tag{12}$$

where $\delta_0(E)$ is the phase shift at energy E. This leads to

$$\int_{-\infty}^{E} dE \rho(E) = \frac{1}{\pi} \delta_0(E), \tag{13}$$

If we choose $E = E_F$ this leads to a different version of the Friedel sum rule, relating the integrated number of added electrons to the phase shift.

Result: Maximum scattering for the "magnetic" case where there is one extra electron, $\Delta Z = 1$.

3. 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.

4. 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.**

5. Kondo Effect

Increase of resistance at low T.

Solved by K. G. Wilson, for which he got the Nobel prize.

The characteristic Kondo Temperature can be very low, which leads to enormous effects (per impurity) at low temperatures.

- **Anderson Lattice Model**

  The Anderson lattice model is a generalization of impurity case, to a lattice with strong interactions in a state on each site. There is also a sate on each site with no electron interactions. This defines a two-band Hubbard model with one wide band with no Coulomb interactions which hybridizes with a narrow band that has a Coulomb interaction. In the "local moment" magnetic case, this leads to spins on each site coupled to band electrons; Kondo-like effects; "Heavy Fermion" systems.

- **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. 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. Other possible ideas related to this problem.

  Dynamical mean field theory (next lectures) maps lattice problems (like the Hubbard model) onto self-consistent single-site problems much like the impurity problem, but with the requirement that the surrounding medium be consistent with the properties of the central site. Good recent references by G. Kotliar and co-workers.