561 Fall 2005 Lecture 13

Localized Models for Interacting Electrons

See for example Aschroft & Mermin, Ch. 32; Mahan Ch. 1; Jones & March vol. 1, p 341 ff; Most complete review to date: M. Imada, A. Fujimori, and Y. Tokura, "Metal Insulator Transitions", "Rev. Mod. Phys. 70, 1039 (1998), which reviews theory and experiment on correlated-electron systems, especially transition metal oxides.

1. Wide band vs. narrow band solids

A. Wide band: The jellium type approximation is a good starting point. More complex than Jellium, but similar physics. Example: Na. Also materials like Si, diamond carbon.

B. Narrow band: Atomic-like properties. The best example is the 4f sates of the rare earths. Also the 3d systems in some cases.

2. Hubbard Model

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.)

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 three limits:

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 $t_{ij} = 0$.

B. Others cases soluble only in special cases:

1. Exact solution by Leib and Wu in 1 dimension using "Bethe ansatz" (idea for project)
2. Hartree-Fock Approximate Solutions

Non-magnetic Band solution vs. Ferromagnetic solution

Antiferromagnetic solution (lower in energy than Ferromagnetic for this model)

C. Exact solution for 2 sites

Illustrates key features of the solution as a function of U

D. Mott metal-insulator transition

Transition as a function of the magnitude of the interaction.

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

Discussed qualitatively here - in more detail later.

Experimental examples described approximately by the Hubbard model

- Transition metal oxides

  Example of $(V_{1-x}M_x)_2O_3$, M = Ti or Cr.

  See phase diagram in a slide presented in lecture 1 and copied again in the notes

handed out in lecture 10. As a function of temperature and doping (replacing V by Cr adds and electron, Ti subtracts an electron) or pressure P (changes volume and makes the system more "band-like" and less correlated). The phase are:
Antiferromagnetic insulator at low T
Paramagnetic insulator at high T
Paramagnetic metal at high P, T

- Argued to be the model in many 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.)

3. Heisenberg Model

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

$$H = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (2)$$

where the J's are exchange constants and $\mathbf{S}_i$ 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.

Experimental examples of Heisenberg Model - Magnetic insulators

For any system with a large gap for charge excitations tends but has localized magnetic moments on atoms (partially filled shells with moments), the low energy excitations are spin excitations that are described by the Heisenberg Model.
Recent example of spin 1/2: Sr2V3O9 and Ba2V3O9: Quasi-one-dimensional spin-systems with an anomalous low temperature susceptibility (Phys. Rev. B 67, 174417 (2003))

4. Anderson Lattice Model

The Anderson Impurity Model (AIM) is a central site with strong Coulomb interactions U on the site, coupled to the sea of noninteracting electrons in a metal. In the case of large U and a localized spin (i.e., $\epsilon_L << E_F << \epsilon_L + U$ the AIM leads to "local magnetic moments" on the impurity, and interesting consequences such as the Kondo effect.

The Anderson lattice model is a generalization of impurity case in which there is a state with strong Coulomb interactions U in every cell of a crystal, weakly coupled to another band with negligible interactions. It also can be considered to be 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.

The consequences can be very anomalous properties, such as "heavy fermion" systems with electron masses at the Fermi energy thousands of times larger than expected from simple non-interacting pictures.

Experimental examples - Anderson/Kondo Lattice Model and Heavy Fermions

Ce is ideal case for large degeneracy in 4f states - $N_f = 14$. Classic examples are Ce and compounds of Ce.
A. Well-tested in impurity cases: La:Ce

- Very nearly 1 4f electron
- Example of Anderson/Kondo Impurity Model
- Application of Gunnarsson-Schonhammer large degeneracy approach
- Low energy scale: T_K observed experimentally
- Typical numbers and theory discussed in Mahan

B. See similar effects in crystals: Periodic Anderson/Kondo Models which also have low energy scale. "Heavy Fermion" materials have very low energy scale (i.e. narrow band which means heavy mass)

- CeAl Magnetic ground state below T$_c$- moments order which “freezes moments so that they cannot fluctuate and strongly affect the conduction electrons - no large renormalization effects at low temperature
- $CeAl_3$ Very low energy scale, $T_K \approx 10K \approx 10^{-3}eV$; Heavy Fermion with mass $\approx 1000m_e$.
- Effects appear to be very similar to impurity case - no magnetic order but huge renormalization effects
- $CeSn_3$ similar to $CeAl_3$ but mass not so heavy. Fermi surface observed experimentally.
- Ce: Phase transition between high volume magnetic γ phase and low volume non-magnetic α phase - proposed to be a consequence of a Anderson/Kondo type model with the energy scale very volume dependent - varying from very small in the γ phase (where the moments order) to very large (1000 0.1 eV) in the α phase (which prevebts the magnetic order and leads to a non-magnetic phase). (Predicted to lead to Volume-Collapse Transitions in the Rare Earth Metals by J. W. Allen and R. M. Martin. Coonfirmed by more recent work by A. K. McMahan, C. Huscroft, and others using dynamical mean field theory).

C. Photoemission and Inverse photoemisssion

- Observe Peaks for $f^1 \rightarrow f^0$ below E_F and $f^1 \rightarrow f^2$ above E_F
- Difficult to see anything at E_F! Corresponds to large renormalization and small Z which we have already seen always happens when the mass is increased greatly
- Examples given in notes of peaks seen in α-Ce and in $CeSn_3$