Itinerant magnetism and the Hubbard model

In Fe, Co and Ni, magnetism comes from conduction electrons. This is what we call itinerant magnetism. The Hubbard model is the most important model in this context. It describes, besides itinerant magnetism, metal-insulator (Mott) transitions and even high temperature superconductivity.

Introduction

So far we have discussed only <u>localized</u> <u>magnetism</u>, meaning we were able to attribute a spin to each site in the lattice. This is not how things work in Fe, Ni and Co (the most important ferromagnetic elements) and many other compounds. In these cases, the magnetic electrons are actually the conduction electrons. This is what we call <u>itinerant</u> <u>magnetism</u>.

There is still a lot we don't know about itinerant magnetism. We now how to write down the Hamiltonian. We just don't know how to solve it. As always, we usually have to resort to mean field approximations (in this context they are usually called Hartree-Fock approximation, but its the same thing). For some materials mean field seems to work well. For other, it sometimes fails miserably. Systems for which mean-field fails are called <u>strongly</u> <u>correlated</u>.

The starting point is very simple. We have a system of N electrons in a box. The electrons feel a potential $U(\mathbf{r})$ due to the ions, which we assume to remain fixed. They also repel each other due to the Coulomb interaction. Thus, the first quantized Hamiltonian will be

$$H = \sum_{i=1}^{N} \left\{ \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i) \right\} + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j) \qquad (1)$$

where $V(r) = e^2/r$ is the Coulomb potential.