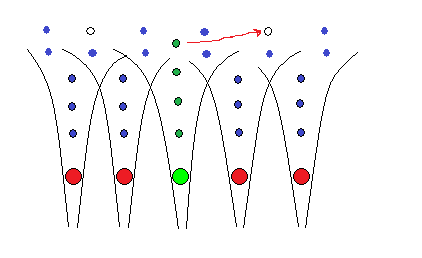
**Itinerant Exchange Interaction**

Now consider the metal has magnetic impurities in it. Magnetic impurities are those with a magnetic moment caused by partially filled d or f electron shells (see Central Field Approximation in QM notes). An example is manganese impurities in copper, or gold in copper. If we lift the same # of electrons – one I’d suspect usually – from the impurity as is done from the other lattice atoms to form the conduction band, then the impurity will exert a potential on these conduction electrons just like the other lattice atoms. But it will disrupt the periodicity and exert a slightly different potential than the other lattice atoms. I guess we’d call this difference the disorder potential Vdis(r-Rj). And so even after smearing the lattice atoms + impurity atoms into a jelly, there would remain an overall impurity potential:



That’s what we’ve done so far. But if the impurity’s valence electron is high enough, then it’s possible the conduction band electrons can screen the impurity nucleus’s influence on the valence impurity electron and it could jump into the conduction band.



If it does, then in addition to the potential it will exert on the Fermi sea of electrons, now it will contain an extra quasi-localized atomic orbital state that the conduction electrons can drop into, and pop out of. So we will attempt to include this in the analysis. Parenthetically, note that a filled band contributes no screening or anything. This is because there is no σ(ω) if the band is full, and therefore there should be no ε(ω) either, by consequence. Anyway, we will assume that the impurities at Rj contain a set, ν, of localized e- states that the mobile electrons can jump in and out of:



And they will be assumed to have energies, εν. Furthermore, since they are presumed magnetic impurity sites, we will recognize that, in accordance with the CFA discussion in the QM notes, there will form a localized magnetic moment M(Rj) on the site given by:



where the values of LT, ST, JT come from Hund’s rules, which, further note, depends on how many electrons are occupying that site’s orbital. So the e- in the gas can occupy the usual |kσ> states, and now the localized |Rjν> states as well. These states are not orthogonal to each other which violates the 2nd quantized formalism to an extent, but whatever. Our results ought to be good up to where this overlap becomes significant, like how we accommodate non-orthogonality of basis states in the tight-binding model.

For simplicity, we’ll suppose that the impurity sites can accommodate two electrons: spin up or spin down (could just be a single localized d-orbital). We’ll designate the state φσ(r-R), and the energy, εL. We’ll also presume that the concentration of such impurities is low enough that there is assured to be basically zero overlap between impurity site wavefunctions. Let V1(r) be the total potential felt by the conduction band electrons in the lattice (including the one or two impurity electrons that got promoted to the conduction band). V1(r) will include the crystal potential and the disorder potential. Extending our set of basis operators from {ckσ} → {ckσ, cRσ} (note cRσ is not the discrete FT of ckσ – unfortunate notation) we can see that we’d get something like this:



Let’s call H1Rk to be Mk. Then we’d have:



For the interaction part, there are a lot of terms. I’m probably not doing this right, but we definitely have an impurity site interaction term, and conduction band interaction term. And then we have the impurity site-conduction band interaction term. Not sure we should be using the same potential for each of these, but it doesn’t matter as we’re going to make this only phenomenological in a bit and not commit ourselves to any particular matrix elements. Apropos the impurity site-conduction band interaction term, following the general formula,



I’m leaving off any ‘three conduction band-one impurity site and vice versa’ creation/annihilation operator sets, as these are probably smaller? So maybe?



We can take away the spin index in the expectations, as it’s irrelevant. I’ll also employ the diagonality of the spin overlap in the expectations, presuming V2 to be spin-independent. Also use the fact that impurities are so widely separated that R’s must be the same to get non-zero overlap. I’ll also get rid of some of the excess primes on the k’s. Then,



where I’m taking away the spin index in the kets is just to indicate that the spin orientation is irrelevant to the expectation. I think it’s allowable to (anti)commute the site and free operators. If so, then we get:



and so we can combine some of the red terms,



It’s typical to specialize the blue term to unequal spins (well, wouldn’t we get zero otherwise?). Then we’d have:



(where we take advantage of the anti-commuting property of the c’s since their spins are unequal) Seems the green terms are ignored as not describing the spin-flip process of interest. Apropos the red terms, the two matrix elements are slightly different,



We’ll look at the Jkk´ term, while the Vkk´ term is ignored (it doesn’t describe the spin-flip process that we’re interested in). If J is greater than 0, the substance is ferromagnetic, and if less than 0 then anti-ferromagnetic. Anyway, so we’ll say:



The first term Mahan says to ignore, cause it’s basically like the Vkk´ terms we’re also ignoring. Then we have:



Introducing some definitions (these should be familiar from Schwinger’s harmonic oscillator model of angular momentum, but also simply follow from the 2nd quantized version of the spin operator – see Quantum Mechanics/Many Identical Particles/2nd Quantization-Position space):



we can write this as:



This red term is often called Vsd because it describes the magnetic impurity electron (d orbital) interacting with conduction band electrons (s orbital presumably). This term has a form which is similar (perhaps why it is important) to the Heisenberg exchange model. So this term must describe some sort of exchange process going on – itinerant exchange or something. Note that this process conserves particle number so electrons are not changing places from continuum to site or vice versa. Rather this describes a spin-flip process whereby a continuum electron in the delocalized s-orbital interacts with an d-orbital localized state, flipping spins in the process. Accordingly, this term affords a greater simplification that puts it in an ‘exchange’ format. Turns out we can write it as:



To see this, first we’ll note that:



And therefore we can write **S** the same way:



So then,



So then, using the matrix forms of σ-,+,z, we have:



So there we go! The last (purple) set of terms is the familiar e-e interaction between nearly free electrons. This is,



So altogether now we have:



And *altogether* altogether, we have:



One important subset of terms is isolated in the *Kondo model*, which keeps just the Vsd interaction:



This would seem to only describe spin flip processes, but not any other kind of impurity scattering per seʹ, like momentum changes. Another (the original) way to get this model, or a version of it, is to do this. The onsite level is replaced with a fixed site so that the core site is always occupied basically. Then we treat the impurity site as, well, an actual impurity like done before, whose interaction with the ambient electrons is modeled with an exchange interaction (just as we have above). So we have a HS for the impurity site affixed to a FS for the conduction electrons. So it’d be something like:



where is (twice) the local spin operator (see 2nd quantization files), and ψσ(r) *is* the inverse FT of ck. We could write this as:



and in momentum space as:



While this model is similar to the previous one, one difference is that we’re not implicitly restricting the local impurity site spin operator **S**R to be just a spin ½ matrix (but not calling it **J**R because, we’re already using that letter). Also, one difference between this impurity model and previous non-magnetic one is that we do have explicit R dependence in the impurity potential, thanks to **S**R.

Another important model keeps just the site-site interaction, in addition to the part of the single particle potential which would accommodate some momentum impurity scattering. This is the *Anderson model*.



Although it doesn’t look like it, the spin-flip process is also accounted for here. Mahan says that the single particle potential term allows for a transfer of a, say, spin up site electron into the continuum. And then, if unoccupied, an up continuum spin can float into the site. The onsite repulsion correlates these two processes so that they are not completely independent of one another, and so there is some accounting for the spin-flip process. I guess whether conductions electrons would prefer to drop out of the conduction band and form a spin singlet on the impurity site depends on where the impurity energy level εL is compared to the conduction band, and also on the onsite repulsion U.

We can similarly generalize this model to accommodate more than just two spins in the impurity site. So we can write:



where the indices μ,ν denote the combined orbital + spin d.o.f. of the localized electrons, or conduction electrons.

There is a canonical transformation that almost maps the Anderson model to the Kondo model. Early workers thought that the Kondo and Anderson models made very similar predictions, but it is now known that the Anderson model has a greater variety of behavior. The Kondo model treates the local spin as a separate entity. The Anderson model treates the local spin as just another electron. It can undergo exchange and other processes with the conduction electrons. In other words, instead of having the electrons interact with a fixed impurity spin, we just have an extra localized state that the electrons can pop into. The Anderson model is more realistic. We may consider the localized state/s to have oribital and spin degeneracy. Most recent applications of the Anderson model have been for heavy fermion systems, where the local orbital is one or several electrons in f-orbitals. For reviews of heavy fermions see Stewart (1984) or Lee et al. (1986). Each of these models can be solved exactly in 1D. But this isn’t useful since there is neither long range order, nor phase transitions in 1D. So the behavior in 2D and 3D must be much different.

**Feynman Diagram Rules**

So let’s go back to:



And we want to calculate the GF:



where,



and,



Further, we’re going to want to disorder average our GF, like we did in the electron-impurity file, and moreover, spin average too. Apropos the spin averages, we should find useful the following identities (taken from QM folder – Schwinger angular momentum file, and Relativistic quantum file)





We can develop a perturbative expansion of the GF from the typical diagrammatic procedure. But we have to be careful due to the presence of the spin operator. Since it doesn’t commute with itself at different times, we can’t treat it as a scalar per se´, and so we can’t straightforwardly go from the temporal domain to frequency domain, like we had before. So we just have to do the expansion term by term, and it’s hard to write any simple rules, especially because the spin averages are different at each order.