**Electron-Electron Interaction**

The nearly free model applies pretty well to, well, nearly free electrons. These are the conduction band electrons found in the s and p subshells, say. In the Exchange interaction file, we’ll study electrons that are bound to their host atoms, namely those in the f-subshells. In this file we’ll look at a model where the electrons are more tightly bound than the s’s and p’s, but still mobile, unlike the f’s. Naturally I guess, this would then apply to the d’s. Recall we said that the nearly free model takes no account of the band structure of the free electrons. And so it cannot tell us what happens when our filling surpasses the point where the parabolic spectrum approximation works, and certainly not when the filling becomes nearly total. In the tight-binding model, we should see this predicts that transport coefficients approach zero (at least conductivity, etc.), a virtue the free model wouldn’t have.

This (Hubbard) tight binding model will contain basically two parameters – a ‘hopping’ term, which describes the electron KE and crystal potential, and an electrical repulsion term, which describes the electrical repulsion between electrons, obviously. When the former predominates, we get the nearly free model back again, and when the latter predominates, we get the Exchange model in the next file. We’ll be interested in intermediate cases though. I think the Hubbard → Exchange model convergence is kind of like how we in the Magnetic impurity case we have the Anderson → Kondo model convergence.

The Hubbard model has become the standard Hamiltonian for the investigation of electron behavior in metals where the electron interaction effects are quite strong – say strong enough to possibly pin electrons onto their host site. In that case, the presumption that the electrons are ‘nearly free’ is untenable. And so we resort to the tight-binding model as our basis. And presume a double occupancy (spin up/down) per site model. Refering to the 2nd Quantization folder, we have:



where nj = Σσnjα, and:



Alas, got some bad notation as the δ’s mean different things. δδ=0 is a Kronecker delta equal to 1 for δ = 0, and zero otherwise. Uδ exists for all δ values. Apparently we can get quite different material properties depending upon the number of electrons in our conduction band, N0, and the onsite repulsion V0. I presume N0 can be changed by adjusting the gate voltage on our material, basically adjusting the chemical potential.

The extended Hubbard model presumes Uδ just takes two values U0 and Uδ≠0. Then he calls these t0 and t respectively. Should note that t < 0. I guess we can choose our energy ε0 to be such as to make ε0 + t0 = 0, and then we’ll just be summing over δ ≠ 0. Then we switch δ → -δ to put everything in his form. So then:



(remember δ *cannot* be equal to 0) Note that we cannot simply write the last term as nj­nj because even though the Fermi-statistics already excludes the possibility of having two particles on the same site, the potential term written that way would give even 1 electron on the site a potential energy, which it cannot have. Thus we have to explicitly include the spin indices. Note that it is the parameter V0 which seems to determine the magnetization properties of the model. Keeping just this onsite interaction term is called the *pure/usual* Hubbard model. I think it’s also called the Stoner model. The *pure* Hubbard model does a good job of describing spin-fluctuations (itinerant exchange). Note that if V0 is large, then this will discourage having doubly occupied electron states/orbitals or whatever. And this would mean that the formation of local moments (just s = ½ though) is favored on each site – not to say these moments would necessarily be aligned. But the V0 term does a poor job with charge fluctuations, basically because it would neglect the Coulomb interaction between sites. Keeping just the off-site interaction, which is all the usual Jelly model has, therefore wouldn’t display these sort of spin-flip processes that occur in the Hubbard model, but it does do a good job with charge fluctuations. The *extended* Hubbard model includes both.

I’m going to put this in a form that is amenable to translation to Feynman diagrams. So for the position basis H, we can say,



and so,



Now let’s translate this to Fourier space as well. So we’ll introduce the Fourier space operators,



Let’s also say:



Then we have, leaving off emphasis that k sum is only over values w/in BZ, and starting from a previous line in the position space H:



and then we’ll define (R = 0) = 0, so we can extend the q term sum over all Rj and Rℓ.



and then doing the sums,



and



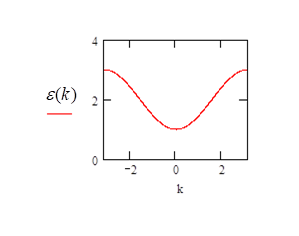
So we’ll write this as:



where we define,



The energy band is *something* like:



We’ll come back to these two expressions. But next, let’s do this…

**Spin and Charge Separation**

The Hubbard model can be written in a form which demonstrates separation of charge and spin degrees of freedom. I’m basically going to redo the translation of H from position to Fourier space, but starting from where we have it in terms of the n’s. Basically just commuting the c’s:



and then we’ll extend the j ≠ ℓ sum to include j = ℓ, and define (R=0) = 0 to allow this.



and then doing the sums,



Then we define,



via which we can write:



Now consider the following expression:



We will relate it to n↑(-q)n↓(q).



and so we can say,



Of course the LHS is the last term in our H. So now we can write our H as (he switches sign of q’s):



and finally,



So there we go. Writing it like this is useful, evidently, because, at least up to an RPA approximation, one can treat nc and ns as effectively independent operators – they say. Well when we do the Excitations, we’ll see this to be the case.

**Feynman Rules**

So back in real space we have (I know you didn’t forget that δ ≠ 0):



as the basis of our Feynman rules. And say we want to calculate:



(R and R´ are two different sites otherwise denoted Rj and say Rj´) where,



and,



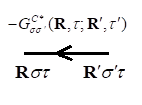
Then first we need the unperturbed GF. This is:



We can easily get this from the momentum space result below. Won’t bother here.

**Real Space Rules**

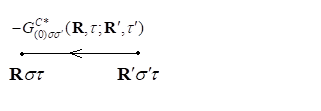
So we have just one GF now



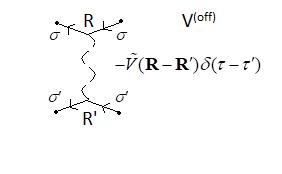
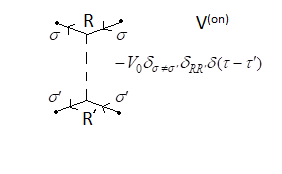
and the external points are:



which we connect with the bare GF:



via powers of our interaction vertex:

Then the general procedure is as follows…

**Topology**

Connect all topologically distinct, connected (meaning all end points must be connected to each other though not necessarily to the rest of the diagram – meaning vacuum bubbles allowed at this stage), diagrams together, associating each element in diagram with the indicated term. Note the order of indices is important, Gσσ´(xk,xj) ≠ Gσ´σ(xj,xk), so always order the positions against the directions of the arrows.

**Equal time issues**

As usual, should interpret Gσσ´(x,t;x´,t) as Gσσ´(x,t;x,t+).

**Signs/Numerical Factors**

Each diagram is associated with a numerical factor, because each topologically distinct diagram comes from a variety of contractions and because we must factor in the 1/n! term coming from the S-matrix expansion. Basically, diagrams with external legs seem to have a simple net factor of unity. Not going to worry about bubbles. We know they just end up canceling, unless we’re doing a potential or something.

(Fermion) loops have there own special sign factors. Each fermion loop get a factor of (-ε), which would be just 1 for a boson loop – this has to do with intracacies of transposing the operators to put them in proper order.

**Sum**

Then sum over all internal vertices, including spin ones. For a lot of diagrams, it looks like we can say fermion loops get a factor of two, but the V(on) diagram, wherever employed, will cut it down by an additional factor of two because of the extra restrictions it places on the spins. But this isn’t a general rule.

**Fourier Space Rules**

But let’s just go back to the simple Fourier space representation of H.



as the basis of our Feynman rules. And say we want to calculate:



where,



and,



Then first we need the unperturbed GF. This is:



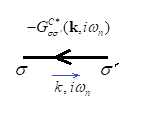
And well, we already know what this is (see stat mech folder perhaps):



and whose Fourier transform is:



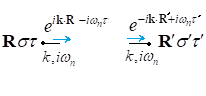
So we have our single GF again, but do note that while ξk = εk – μ, εk ≠ k2/2m any more:



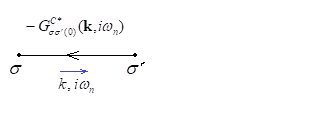
We connect the external points,



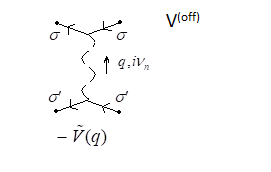
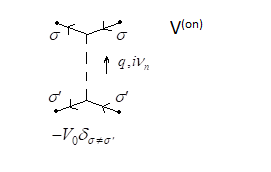
These carry the Fourier transform variable. And if we’re ultimately interested in the real space, time GF, then we must add the following factors to each:



We connect these with the bare GF:



via powers of the bare impurity vertices:

(doesn’t seem like we should have a q ≠ 0 restriction anymore) We still have iνn flowing down the line because of the artificial time-dependence brought in by the δ(t-t´) we put on each interaction potential. Note it’s a bosonic frequency, though, as energy conservation demands, because we cannot have electron lines with fermionic frequencies if we have a fermionic interaction frequency traveling into it (EM interaction is carried by bosons too – is this a coincidence?).

**Topology**

I presume we connect all topologically distinct, fully connected (meaning no vacuum bubbles), diagrams together, associating with each element in the diagram the indicated term. Remember that all energy-momentum labels **k**, ω must be going in the same way w/r to the GF arrow. They must all be going against the arrows (or with them I suppose). And then we conserve energy/momentum at each vertex.

**Equal time issues**

Apropos the equal time issue, in Fourier space this would be handled as:



So we need to include a factor of exp(iωn0+) for each bare Green’s function closed in on itself. Fundamentally, the problem occurs when the temporal argument of the bare Green’s function is zero.

**Signs/Numerical Factors**

Same as above,

**Sum**

Then sum/integrate over all independent momenta - wavenumbers/energies-frequencies/indices, and spins.



and include the external frequency/wavenumber if want the real space GF.