**Electron-Electron Interaction**

So going back to the pure Hubbard model,



(remember δ *cannot* be equal to 0) Would like to look at excitations in the limit V0 >> t. In this limit, to zeroth order, the eigenstates are just the position space occupation numbers. And the energy is just V0 × the number of doubly occupied orbitals. So, repeating myself.



Here’s a couple states,

A screenshot of a computer screen

Description automatically generated

The unperturbed GS would be where we have no doubly occupied orbitals – all orbitals are singly occupied. And the energy would be 0.



The first excited state(s) would be all states with just one doubly occupied orbital, and the energy would be V0. And similarly the second excited state(s) would be constructed. We’ll observe the GS is 2N-fold degenerate, because we can point our spins in any direction. We’d like to see how the addition of the orbital and hopping terms lifts this degeneracy. So according to PT, we need to diagonalize the perturbation within the subspace of our degenerate GS.



The perturbation is the blue stuff, and, well, turns out the perturbation already is diagonal in our subspace, because tcj+δ,σ†cjσ is zero. This is because this term will create a doubly-occupied orbital, which is automatically orthogonal to our subspace which has only singly-occupied orbitals. So we go to 2nd order PT,



And focusing on the GS, or rather, one of the GS’s.



Let’s say we’re interested in this result, to first order in t/V0. Then we need only concern ourselves with Ei(0) which are first excited states. And then EGS(0) – Ei(0) = -V0. So can say,



Let’s suppose that δ just runs over nearest neighbors. The blue operator takes a spin at j and moves it to j±1, unless the Pauli Exclusion principle forbids it, in which case we just get zero. So in fact, it creates 1st excited states. If we think about it, we can see that a |ψGS(0)> with all spins up or all spins down will just return zero when operator on by the blue guy. And in fact the |ψGS(0)> with alternating spins will always return something non-zero when acted on by the blue operator. And so, thanks to the minus sign, it will be the lowest energy state. So let’s focus on *that*.



Looks like with N sites, there are about 2N first excited states that one can create by moving a spin into an adjacent site to the right, or to the left, like this (assuming line geometry now):



and for every excited state, the blue operator acting on the GS,



should eventually generate it. And when it does,



will give us 1. Otherwise 0. So ultimately, we should get:



So,



And FWIW, we can see that the GS would be anti-ferromagnetic, since the spins are all anti-aligned. Now we’d like to relate our Hubbard model to the exchange interaction Hamiltonian. To do that we’ll focus on the low-lying energy states. We’ll work out H in the basis of the |ψGS(0)> wavefunctions. Well, actually, since the KE perturbation is zero in this basis, we’ll work out H in the basis |ψGS(1)>, i.e., the potential energy ground states perturbed out to first order. So 1st order perturbation theory says:



where n ∈ GS. Taking expectation, where m, n ∈ GS(0), and i, j, k can be any state,



In the last line we restrict the sum over i and k to exclude all|ψGS(0)>’s, as the perturbation gives zero there anyway. If we want to keep things to first order in 1/V0, then can restrict the i,j,k states to first excited states ∈ FES(0). We can simplify a bit, given that the |ψGS(0)>’s are diagonal in the t-term, and also have energy 0 in the V0 term. This eliminates the <ψm(0)|H|ψn(0)> guy. And also eliminates the 1/(Em(0) – Ei(0))·1/(En(0) – Ek(0)) term, as it will be 2nd order in 1/V0. So now we have:



Well, the V0-term acting on <ψm(0)| and |ψn(0)> gives zero. So we have:



Rearranging terms a bit,



All first excited states have energy V0 above the ground state, so we can say,



and now switching summation index i → k, we can say,



Going to write this way now,



Going to actually look at H itself,



Now let’s consider some particular |ψk(0)>. It will have random spin configurations at each site, except for two. One at say j, where it will be empty, and another at j+δ, where it will be doubly occupied. For that given |ψk(0)>, can see that the perturbation (in blue), operating on |ψm(0)> must deliver us |ψk(0)>, and the same must happen for |ψn(0)>. Since the perturbation generates all the states obtained from a GS(0) by transfering a spin from one lattice site to a nearest neighbor, we can see the perturbation will generate |ψk(0)> iff |ψm(0)> and |ψn(0)> are identical in all respects to |ψk(0)> except at j and j+δ. Looks like this:

A screenshot of a computer

Description automatically generated

Let’s denote the FES(0)’s and GS(0)’s by:



where apropos |ψk(0)>, j identifies the empty site, j+δ identifies the doubly occupied site, and *else* refers to all the other spin d.o.f. on the other sites. And apropos |ψm(0)>, mj is the spin on site j, mj+δ denotes the spin on site j+δ, and *else* refers to the other spin d.o.f. which must match those of |ψk(0)>. Similarly for |ψn(0)>. So now we can collapse the H sum over m and n, and write something like,



Now we need to evaluate the matrix elements. First note that if mj = mj+δ, or m´j = m´j+δ, then we must get 0, as the blue perturbation will atempt to put these same spins on the same site. So we only have four non-zero combinations. Now our four matrix elements are:



and,



and,



and finally,



The outer (first and last) matrix elements should be the same (just stand upside down and the last becomes the first). The inner (second and third) matrix elements should be the same for the same reason. But the inners are not quite equal to the outers. They are actually negatives of each other. Can see this by comparing the two terms where they differ. For instance, consider the third and fourth terms, with the difference highlighted in red,



Let j+δ be denoted 2, and j be denoted 1, then:



So there. And now we’ll say:



So this brings our H to:



Insofar as the ‘else’ part of |ψ> just gives us the identity matrix, I think we can leave it off, to write:



Definitely fudged that. Now recall how a generic 2-body interaction 1st quantized operator,



(quantum numbers read inside out, from | to >) can be written in 2nd quantized notation as:



Comparing, we see we can write H as:



So this is an effective low-energy Hamiltonian. Now we can put this in terms of the on-site spin operator. Recall how in the QM/Identical Particles/2nd quantization position space file, we found the spin density operator was:



In our case, this would translate to:



And the now let’s form the exchange Hamiltonian operator,



Since the subspace for which are H is operative, there is a single spin on each site, the number operator will always give us 1. And we’ll add a constant to our exchange expression,



Let’s choose K = ¼. Then,



Now let’s rearrange these terms in proper 2nd operator form. Since we’re transposing groups of two operators, we get no negative signs from the anti-commutation relations.



Comparing to our H,



we see we can write,



Ignoring the irrelevant constant, we end up with:



which we recognize as a version of the exchange Hamiltonian. Exchange arising from electron hopping from site to site is called ‘*superexchange*’. The effective coupling constant is positive, which tells us that (see Exchange H folder) the spins will prefer to settle into an anti-ferromagnetic state at low T, as we know from our analysis of the GS above. The coupling constant is apparently sensitive to the filling. When filling is close to half-full (here we assumed it was *exactly* half-full), the coupling constant is positive. But when filling is much less, or much greater than half-full, the coupling constant turns negative, and we see ferromagnetic behavior.