**Thermal Equilibrium Properties**

H has several energy scales. The energy scale due to the KE and band structure is W = 2zt, where z is the # of nearest neighbors. This is called the bandwidth. Another is V0, which is the Coulomb repulsion. The behavior of the model is quite different depending on the ratio W/V0. If W >> V0, then we get the nearly free model, and if W << V0, then we get something more like the exchange model, in next folder. T is important since the magnetic phases disappear at high T. In 2D, they disappear at any nonzero T, since the Mermin-Wagner theorem (1966) states that there is never long-range order in 2D. Another important variable is the concentration, n = 0 of conduction electrons on the lattice. In the usual Hubbard model, the band is full when n = 2 (each lattice site would only then accommodate 2 electrons). The lattice has an average of one electron per site when n = 1. This case is important since AF behavior can occur when n ≈ 1. The Hubbard model has particle hole symmetry, which means that the phase diagram is symmetric about the concentration n = 1. Any phase that exists for n = a, also exists for n = 2 – a. This result is easy to prove. And one can see this result by writing the H for the holes – which is the same as the H for the particles, except with the sign switched on the KE term. A sample phase diagram is given below:

A picture containing chart

Description automatically generated

*n = 0* = N0/N is the filling of e-‘s per site. W = 2zt is called the tight binding band width. We see that if we take W → 0, which would describe exchange model best, we easily get ferromagnetism. I would say that this is because in that case, the e-‘s cannot move around, and so their diamagnetic response, which usually frustrates their paramagnetic response, cannot occur. But if we take W → ∞, which would best describe metals, then we get only a paramagnetic response. We also see that close to half-filling, we only get AF. Why? I can see that spins would prefer to half-fill all sites first, to minimize Coulomb repulsion. But why do they prefer to do so with opposite spins? Well, see that previous file where we see H reduces to the exchange model in the V0 >> W limit.

**Free-Energy**

We can get the Free Energy (L) of our model. Well – maybe check out the Interacting Electrons + Phonons/Superconducitivy/Thermal Equilibrium/LG Free Energy file for possibilities in writing up a path integral description of L, and then doing a mean field/saddle point approximation on it.

**Ferromagnetism**

So we want to see if it’s possible, at T = 0, and for a certain average site occupancy 0 = N0/N and interaction strength V0, for the spin up/down occupation numbers, N↑, N↓ to be different.

***via SCHF Green’s function***

From the single-particle excitation file, we have via the self-consistent Hartree-Fock approximation:



(bar over spin means ‘the other spin’ if I remember correctly – see earlier file) If we sum this equation over all k, and divide by N, then we’ll have:



Maybe just specialize to the onsite potential term, and we get a nicer equation:



Now at T = 0, nF is just a step function nF(x) = θ(x > μ). So we could write something like, introducing the density of states (per spin, per total lattice sites, but not per volume),



(limits of integration are just generic – actual bounds are between whatever min and max of εk is) and so,



Taking the difference,



I guess we can define magnetization, M. And I guess we have:



So let’s solve for these two in terms of M,



Filling these in,



and now we’ll expand this equation in powers of M…



Jeez. Okay now we have:



As we should have, M can be positive or negative. I understand it would choose one or the other based on internal perturbations (I suppose it could just choose neither, i.e., M = 0, but probably statistically unlikely? and could show that M = 0 corresponds to smaller free energy). And the onset of ferromagnetic behavior is given by the condition (I suspect ρ´´ is negative in 3D, like it is for free electrons??):



V0 is probably negligible compared to μ, and so I think that is why we often don’t see it in the argument of ρ. On the other hand, it could just be absorbed into the chemical potential – whatever. So we see that large repulsion favors spontaneous magnetization. This ferromagnetic phase transition is an example of a quantum phase transition – one which occurs when some control parameter (instead of Temperature) is changed past some critical value. In this case, it is the density of states which serves as the control parameter, or the e-e repulsion if you prefer.

***via MFT***

Another possible approach is to take our results from MFT,



We can calculate the thermal expectation of the occupation numbers,



If we introduce a generic density of states ρσ(ε) (per spin, per lattice number N) apropos the free band energy spectrum, we may write:



and then say,



So now we could solve for , again. And this expression is the same as what we found above, using the SCH approximation 😊, just at finite temperature. Maybe I’ll proceed a little. Can write these as:



where,



Actually, we can even eliminate the constant -V00/2 term on every one of these guys, even though it depends on N0, because it just affects the zero point energy of the particles (which we aribrarily set to 0 back in the first file, and so we can just arbitrarily set it to whatever cancels this guy now). Our ultimate results will not be in terms of μ, so it’s okay. So we can write:



*Now* we can solve for the chemical potential in the first guy, and with that, the magnetization in the second guy, using the Sommerfield expansion (see Free Day/Metals/Thermal Equilibrium/Sommerfield Expansion) to work this out. So from that file, let’s use the generic result,



So,



Now going to expand for small magnetic moment, out to 2nd oder,



Now need to solve for μ(T,M). We can expand it in a power series about T = M = 0. We’ll only go out to the lowest non-zero terms. Note that we don’t expect μ to depend on T to first order because it doesn’t for the free gas. And we don’t expect it to depend on M to first order either because the chemical potential shouldn’t depend on which way we consider ‘up’ (in other words, whether M is up or down depends on which way we hold the sample, but we shouldn’t get different μ because we flip the sample upside down). Of course we could allow such dependence, but we’ll find it’s zero. So to lowest order we can postulate.



And we’ll plug this into our N0 expression:



and expand, keeping terms only to 2nd order (and note T2M2 is 4th order), which eliminates the vast majority of them,



Now we’ll simplify,



and equate both sides, order by order



where in the first line we are defining εF as the energy up to which the free particles (with the εk = tΣδeik·δ spectrum) line up, as ρσ(ε) is the density of states (per spin, per lattice number) for the free particles. So we can say,



And now with this, we want to evaluate,



And we’ll use the result again,



So,



Now keeping in mind our expansion for μ, we’ll expand this expression out to third order in (kBT) and M.



Can write this as:



or maybe,



Let’s define,



Then we can write our M as:



So our solutions are:



Presumably M = 0 will be the equilibrium solution for T > Tc, and M = ±√[(1-a(T))/b] (one or the other) will be the solution for T < Tc, whatever Tc is. I guess we’d have to actually calculate the free energy for the magnetized solutions and verify it is indeed lower than the non-magnetized solution. But what is Tc? It’s the temperature below which a(T)-1 becomes positive, so as to make magnetized solutions possible.

**Example**

Let’s put some numbers to it. Or, let’s just use the free particle system to approximate a(T), and b. I mean, we’ll use a parabola to approximate the ε(k) = tΣδeik·δ ~ k2/2m. So, first, we have:



and so these coefficients would be something like:



and,



So the magnetized (+) solution is:



We’ll pause here to observe the Stoner criterion again [and also note that the argument of ρσ() here is εF, as opposed to εF – 0V0/2 above, but that’s because we (recall?) absorbed that extra term into our chemical potential]. Even at T = 0, we may not have a phase transition. We still need:



In normal phase transitions, it is the thermal fluctuations that wipe out an ordered phase, past a certain critical temperature. In quantum phase transitions, it is the quantum fluctuations themselves that wipe out the phase transition (well, thermal fluctuations will too). It’s notable that metals where the d-bands lie within the Fermi level would have large density of states because there are 5 such bands (as well as s-band). And so it does seem likely that these metals would be predisposed to be magnetic. But not all d-band metals exhibit magnetism. For instance, the noble metals’ Fermi surfaces lie within the s-band, and so we don’t get no magnetism.

Okay, there is a critical temperature above which the phase transition cannot happen, and this is:



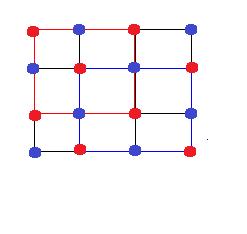
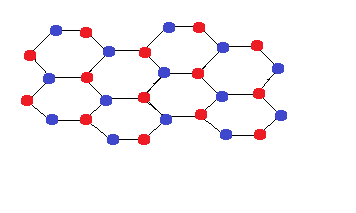
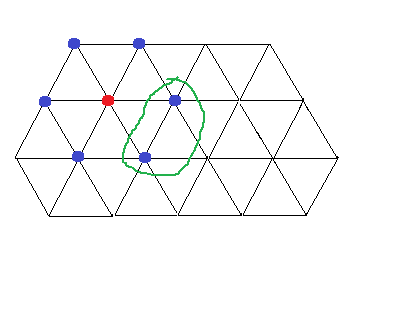
and in terms of this, we may write:



which is the familiar sqrt form of a MFT result. We could go on and calculate other thermal properties, like heat capacity, etc., but I guess I won’t.

**Antiferromagnetism**

Another important variable for magnetic ordering is the lattice type. For instance, ferromagnetism is supported for any lattice, but *antiferromagnetism* is not per seʹ. Consider the square and honey comb (graphene takes this form) lattices below. We can put one electron spin up (red), and its nearest neighbors spin down (blue).

And so these lattices can support AF. But we cannot do the same for the triangular lattice, as for instance the two circled spins are blue because they have a red as a n.n. But they should be opposite colors too, because they are n.n.’s to each other. So it is impossible to set up a conventional AF arrangement on this lattice. And the lattice is said to be frustrated. The early work on the Hubbard model concentrated on three dimensions, and most calculations were done for the simple-cubic (sc) or body centered cubic (bcc) structures. The discovery of high T superconductivity in the copper oxides, called ‘cuprates’, heightened interest in layered compounds. This focussed attention on the two dimensional lattice. Most recent work has been done on the square lattice (sq) in 2D. (So there are reasons to study 2D, if not for the purpose of magnetic ordering).