**Bragg-Williams MFT of Ising Model**

[might check out Condensed Matter/Metals/Interacting Electrons/Exchange/Thermal Properties file for more on these techniques applied to spins]

Let us use the Ising model as an example. Again, we’ll note that we can in principle exactly solve this model because we do know the eigenstates and energies of this system (again presuming spins are restricted to z direction, which the Ising model *is*).



So now let’s do this a different way from last time. A secret way. A dark way.

**Canonical Transformation to and calculation of f\*(T,m)**

The order parameter m = <σ> is the average spin. And we should be able to write f = u – Ts in terms of m. But m is not a parameter that naturally appears in f(T,h), well, it’s not a canonical variable. So we make a canonical transformation. f\* = f + mh. Then df\* = -sdT – mdh + mdh + hdm = -sdT + hdm. And then f\* itself is f\* = u – Ts + mh = uexchange – hm - Ts + mh = uexchange – Ts. (exchange stands for the exchange interaction). So to get a complete theory, we just need to work out the dependence of uexchange and s on T and m. This f\* is much more tractable to work with. The entropy for a given spatially uniform m can be calculated exactly. The total magnetic moment is simply the number of up spins minus the number of down spins.



where N is the total number of spins on the lattice. The energy is:



And the energy per N is:



The entropy for a given m is the logarithm of the number of configurations with a given N↑ and N↓ (setting kB = 1) (that the entropy depends only on the magnetization, and not say temperature too, follows from the work in the previous file).



and the entropy per N is:



This is what we got last time, as it turns out, though last time m was not a canonical variable like it is now. So the complete Bragg – Williams free energy is thus – no need to implicitly solve shit.



We’ll need to expand this for small m later…



Dropping the irrelevant ln2, we can write:



Note this is accurate only for small m, and so basically around the critical point. We’ll see later that this corresponds with the Landau phenomenological model really well.

**Equation of state**

The equation of state of Ising spins in an external magnetic field is … according to f\*’s differential relation in the text above …



which gives us



And so we have,



This is what we got last time of course. So this gives us an illustration of how we can have a phase transition with just a simple Hamiltonian. Note it isn’t that different interactions are present when the transitions occur. Rather it is that the temperature is small enough to allow the particles to quasi-settle into their ground state – or at least lower state. Anyway, there is an easy way to graphically ascertain the solutions to this equation when h = 0. Then we see that our equation is:



which is just the equation for a relative extremum in f\*, which is typically a relative minimum, and even an absolute minimum, in f\*. But this is for when h = 0 alone. Seems that too often texts plot f\*(T,m) and just say that m will assume the value at the relative extremum, disregarding the fact that T and m are independent variables, just as T and h were, and so in no way does T determine m. Only if you specify T *and h*, do you necessarily determine m, because then you’re exchanging one set of 2 d.o.f. for another set.

**Critical Temperature**

The critical temperature is the point at which non-zero solutions are possible for h = 0. So according to the small m, f\*, this happens when,



The only solutions would be m = 0, unless r´ < 0, and so the critical temperature is when r´ = 0 → Tc = Jz, as we found before.



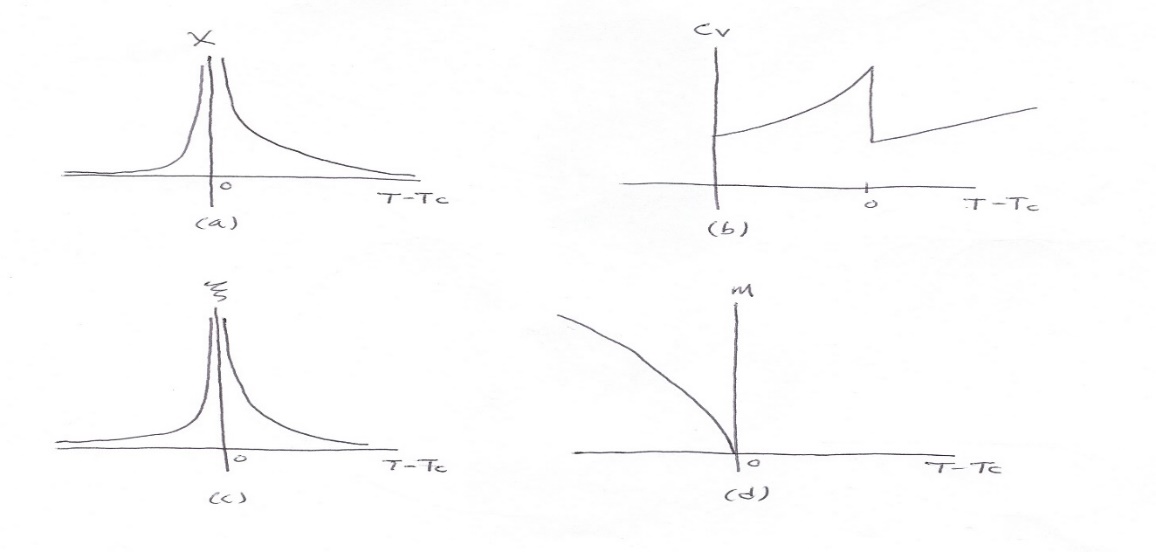
We can get the magnetization (at zero field) via the equation of state. And I’m going to write <m> here so as to make explicit that we’re finding the expectation of m as a function of T, h.



which is



Looks like this:



When critical fluctuations are important, the critical exponent β is generally less than its mean – field value, typically of order 1/3 in three dimensional systems. Says that there are two possible values for the order parameter for T < Tc and h = 0 corresponding to the two possible directions for the bulk magnetization. The sign can be fixed by allowing h to go to zero from positive or negative values. Both solutions for <m> have the same free energy so that the up and down phases coexist along the line h = 0 and T<Tc, as shown in the phase diagram elsewhere. Next,



To get ch we need f(T,h), since,



We have f\*(T,m) however. But at h = 0, we can say f = f\*. More specifically, f (T,h=0) = f\*(T,m(T,h=0)). It is clear from the free energy that the equilibrium free energy density is negative for T < Tc (assuming we take the limit h → 0+) and zero for T > Tc. By plugging in the equilibrium value of the order parameter before and after the transition, we have the equilibrium free energy. For T < Tc, it’s,



and for T > Tc, it’s 0 since m = 0. So,



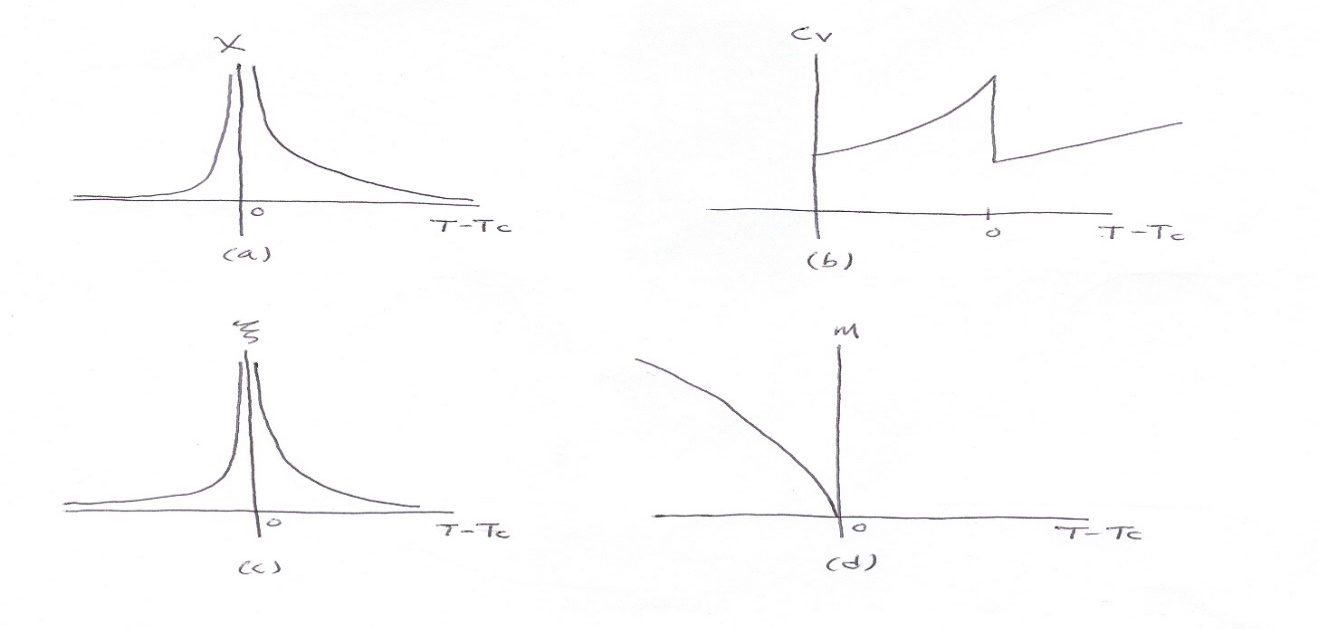
and so the heat capacity is given by:



and in the limit T → Tc, which is where our f expansion is valid anyway, we have:



So our α = 0 again. Looks like this (more generally, when go beyond MFT, but the MFT captures the discontinuity at least):



This equation gives the specific heat associated with the establishment of order. The total specific heat includes a part analytic in temperature arising from degrees of freedom not associated with ordering. Thus a smoothly varying background must be added to our expression to obtain the total specific heat. This total specific heat will have a jump discontinuity at the transition, as shown in the figure above.



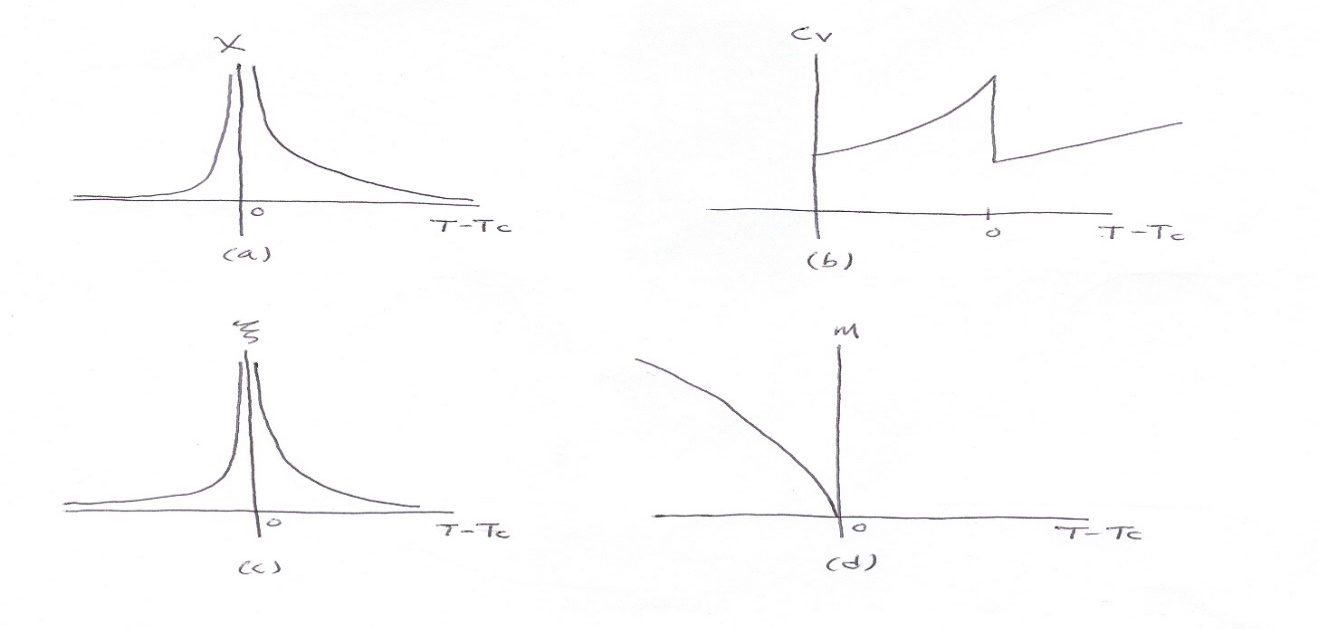
The susceptibility can be obtained by differentiating <m(T,h)> with respect to h – or just implicitly differentiate the equation of state.



Thus we have that, since r´ = T – Tc,



And so γ = 1. It is generally of order 4/3 in three dimensional systems where critical fluctuations are important. And looks like this:





(of course hc = 0 here) Finally, the dependence of <m> on h at follows from the equation of state,



and so we have, going to the limit T → Tc,



And so δ = 3 for us. The first step follows from the fact that r´ is approximately 0 near the critical temperature. Thus we have another critical exponent, δ.

**Appendix**

Let’s compare our f\* to the other free energy, f, we found in the previous file. Recall at the top of the page, we alleged f\* = f + mh. And recall we had in the previous file, and this file:



and our equation of state read:



So we should have:



So yeah that checks out.