**Weiss MFT of Ising Model**

In general, it is too difficult to exactly solve the Ising or XY models in 3D. So we’ll turn to an approximate approach. So now we’ll explore the mean field theory approximation to analyzing the critical point. This was already done in the Stat Mech folder. But for completeness, I’m going to reproduce all the results here basically. So to employ mean field theory, you basically replace the classical, or quantum mechanical order parameter, φ, by its thermal expectation enough times to make the theory solvable, namely, to allow you to calculate Z. You thus develop a self-consistent approximation to Z. So this differs somewhat from the straight-perturbative approach to calculating Z discussed in previous files. The MF approach to calculating Z is akin to Self Consistent Hartree Fock, or saddle point evaluation of the functional integral. It should work well as long as fluctuations in this term are negligible, meaning say <φ2> ~ <φ>2. Note that often times approximations will be made in that we’ll assume <φ>2 is small, but while this may be true, it doesn’t imply that <φ2> is small – think for instance background quantum fluctuations. And this is where/why mean field theory will break down near critical points, because while the order parameter is small, its fluctuations are not. The Central Limit Theorem can still work in our favor and damp fluctuations, but this will usually require superlong range interactions and/or higher dimensions. In fact, there is usually an upper critical dimension past which mean field theory works perfectly (near critical point). But then mean field theory will definitely not work past a lower critical dimension – typically d = 1, 2. So the results we get below, like the existence of ferromagnetism, won’t actually be true in d = 1. The d = 1 case is exactly solvable, and we saw there was no phase tansition. For d ≥ 2, we do have a phase transition, but the MFT predictions vis a vis the critical exponents is pretty bad in 2D, better in 3D, and excellent in higher spatial dimensions (FWIW). Can see RG group methods for investigating when MFT works, and what to do when not.

**Ising Model**

Going to jump straight to the Ising model we’ve been using, but if you want a little more background and context, can check out the Stat Mech folder.



To streamline stuff, we’ll use units where ℏ = 1, and kB = 1. Also going to use **S** = **σ**/2. So can write:



And gonna absorb the 1/4 into the J. And absorb the (1/2)gγBf into a single term h – my favorite letter.



So now J and h both have units of energy. Okay so finally now we have (z directions implicit):



Note that we *do* know the eigenstates and energies of *this* system – as it comprises a bunch of purely independent spins, and so the eigenstates are just |ψ> = |σ1 = ±1,σ2 = ±1,σ3 = ±,…,σN = ±1>, and the eigenvalues are of course whatever you get when you plug this into HIsing. So we *could* exactly calculate the partition function.



where sum runs over all spins and their possible values. Even so, it is apparently difficult (but can be done – see internet somewhere) to do this and extract the critical information. So we employ a mean field approximation instead. In the mean-field approximation, we replace one of the spins with its mean value, since we assume fluctuations are small around the transition. So let be the average spin value (average σ value, rather, which varies between -1 and 1). I guess the probability distribution of the average spin would be something like,



and the *average* average spin would therefore be:



**Weiss Mean Field Theory of Ising Model**

OK so what follows isn’t quite the way presented in most text books, but though that way gets the job done faster, it is conceptually muddled, and doesn’t match up like one thinks it should, with other approximation methods. So going to do it this way, which is the way one typically sets up a mean field theory in other contexts too. So let’s write σi = + δσi. Then we’ll plug this into HIsing, and assume fluctuations about the average are small, which allows us to go from the second to the third line.



Then after neglecting all fluctuation2 terms, we put everything back in terms of σi, σj. So then we have:



Can do the sum now,



Combining those last guys into one term we have:



The partition function is easy to evaluate now, even though it is in terms of the unknown .



where Z1 is just any random spin’s partition function. And now we can solve, self-consistently, for the average spin by calculating the average value of any single spin – they’re all the same in our approximation of course:



If recall the Brillouin function definition,



we’ll note we can write this as, where s = ½, and s1 varies between ±1/2,



But it’s just as easy/easier to do this explicitly,



Alternatively, we can solve the model for F. We have f = F/N:



So this implicitly defines f as a function of T and h, through the equation for . And we can get m via (well m = -∂f/∂Bf, but we’ll alter the definition slightly for our present purposes):



we can implicitly differentiate the equation for to get its derivative:



So filling this in,



And so we have what we kind of already knew, m = . So we can say,



and we can write the free energy as:



Note that this f is still a function of the canonical variables T, h. And m is too, accordingly, implicitly. Turns out this can be simplified somewhat. Consider,



So,



So,



It is useful, we might find, to expand f for small m. Then we have:



Remember, we’ve implicitly written hm in terms of m here. So while h is still an independent variable, we have implicitly m(h).

**Critical Properties**

With f(T,h) in hand, at least approximately, we should be good for working out the phase boundaries and critical exponents, etc. Phase boundaries are characterized by discontinuities, generally, in the first derivatives of our potential, df = -SdT – mdh. So we’d want to consider S and m. We already did the latter.



The former would be given by (going back to unsimplified version of f):



But we know:



and for what it’s worth,



So therefore,



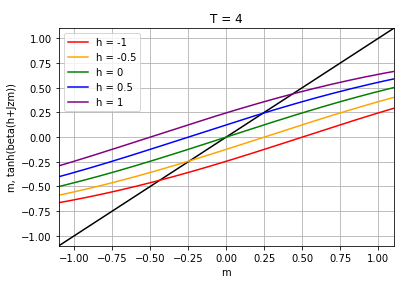
where we used the definition of tanh-1x function. So altogether, depending on preference.



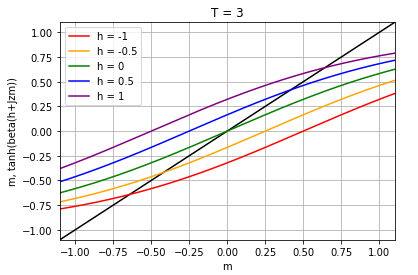
where of course m is still implicitly a function of T, h, as determined from its defining equation. Interesting that S depends on T and h only through m though. We’ll note that reassuringly, S → 0, when T → 0 (in which case m → ±1 for any field h). So all we have to do is work out m(T,h). So let’s go back to its equation:



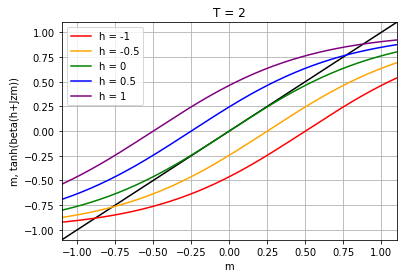
For visualization purposes, I’m going to set J = z = kB = 1, and for various T’s, plot the LHS (black line) and RHS (colored lines) as a function of ‘m’ and see where they intersect. The intersection will give us the m for that T and h.



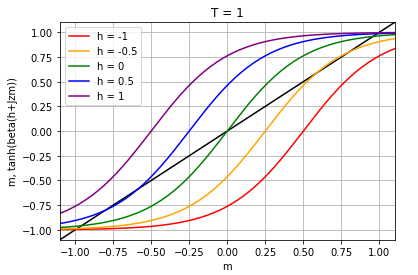
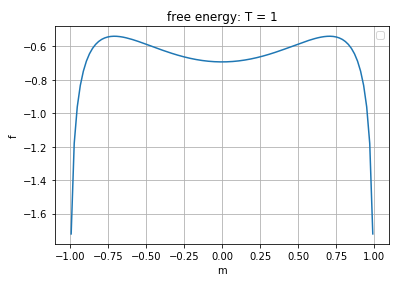
So at T = 4, as run h through values {-1, -0.5, 0, 0.5, 1}, m will go through roughly {-0.45, -0.25, 0, 0.25, 0.45}. At T = 3 we have:



So at T = 3, as run h through values {-1, -0.5, 0, 0.5, 1}, m will go through roughly {-0.65, -0.4, 0, 0.4, 0.65}. So can see at lower T, a given field is more successful at lining up the spins. At T = 2 we have:

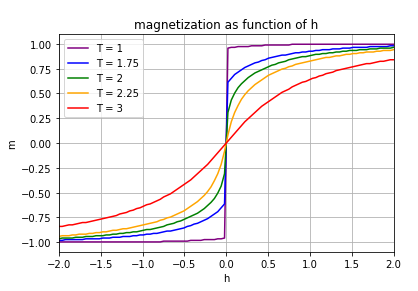
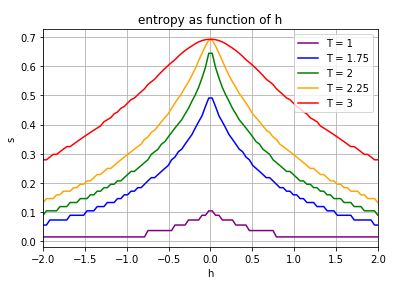


So at T = 2, as run h through values {-1, -0.5, 0, 0.5, 1}, m will go through roughly {-0.85, -0.75, 0, 0.75, 0.85}. Also the RHS and LHS slopes are lined up at the origin when h = 0. Since the RHS slope gets more vertical at the origin with lower T, we can see that for lower T there will begin to be multiple solutions to our equation, meaning multiple phases can coexist. So this T, T = 2, is the critical temperature. So now going to T = 1.

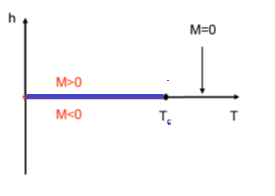
 

So at T = 1, as run h through values {-1, -0.5, 0, 0.5, 1}, m will go through roughly {-1, -0.98, ∓0.95, 0.98, 1}. There are two things of note. First, for the h = -0.5 and h = 0.5 curves, there are three solutions each, so how did we know to choose the roughly -0.98 and 0.98 roots? I believe we choose the one which has the lowest free energy. And this is the one that describes thermodynamic equilibrium. I think the other two roots represent metastable states. The other thing to notice is that at h = 0 there are also three solutions, but two of them have the same lowest free energy. So the system can choose either state to be in. Which one it chooses is somewhat random and is an example of ergodicity breaking, which means I think that the system will choose whichever one it just happens to be closer to at that time. And symmetry breaking because there is nothing in the Hamiltonian, or free energy, that prefers +m to -m, and so choosing one or the other must necessarily break that mathematical symmetry. The other solution (m = 0) when h = 0, corresponds to a metastable state again, I believe. The metastable states interpretation will gain more support when we look at the theory in the exact mean field limit.

So if we go through and calculate the m for a given T and h, we get the following rough series of plots. We can see the discontinuity in m as it crosses the h = 0 line, which persists only for 0 < T < Tc (where Tc = 2 for these chosen parameters). And the discontinuity starts out at Δm = 2 when T = 0, and gradually shrinks to 0 as T → Tc. Also made an S vs. h plot for various T’s. It doesn’t exhibit sharp features, but can see that as T → 0, S → 0. And also that it goes to 0 as |h| → ∞. This makes sense as the field tries to freeze the spins in place. Can also see that with h fixed, S grows as T grows.

So we can infer the phase diagram,



**Critical Temperature**

The critical temperature, the temperature at which phase transition occurs, is the T at which there is just barely a non-zero solution to:



when h = 0. And because tanh(x) goes as x and then increases more slowly thereafter, there will barely be a solution when the slope of the RHS = 1 at the origin,





Now working out the magnetization near the critical point, we’d want to solve:



in the limit that m = 0. Expanding the tanh for small m, we have:



which works out to, near Tc,



So the critical exponent β = ½.



Now let’s examine the magnetic susceptibility near the critical point. This is:



Heading towards Tc from higher T’s, we expect it to get larger and larger, and then finally diverge near the critical point as the system gets closer and closer to maximum sensitivity to the field. On the other side T < Tc it should decay as we go towards T = 0, since spins will be less responsive to field as their orientation is dominated by their internal interaction. So go back to:



And m is an implicit function of T and h. Since both m and h are small in our region of interest, we can do a Taylor series expansion of our equation of state.



Then we can differentiate implicitly to get the susceptibility.



Now set h = 0,



Now when T > Tc, we have m = 0, and so,



When T < Tc, we have what we found before and plugging that in,



Jeez. So then altogether,



So we have γ = 1.



Another quantity of interest is the heat capacity. This is ch = ∂<u>/∂T)h = T∂S/∂T)h. Or we can say, ch = T∂S/∂T = -T∂2f/∂T2. I think I’ll go with the former. So we have:



and near the critical point for Tc, this becomes



Then differentiating, and setting h = 0.



Now take limit that T → Tc, since this is limit where our approximation becomes valid. And for T > Tc, we just get 0. So we have:



So α = 0 for this critical exponent. Why isn’t the heat capacity sensitive to the phase transition? It *would* seem to be for non-zero h’s, as can tell if don’t set h = 0.



(of course hc = 0) Finally, we’d also like to get the critical isotherm, i.e., we want m(h) at T = Tc. So going back to:



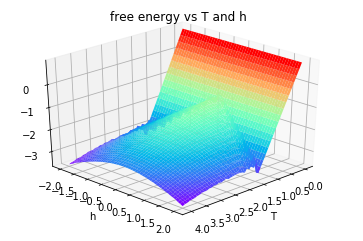
and setting T = Tc, we have:



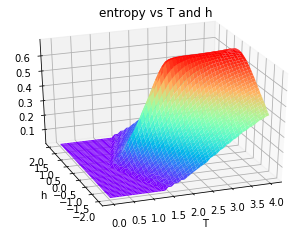
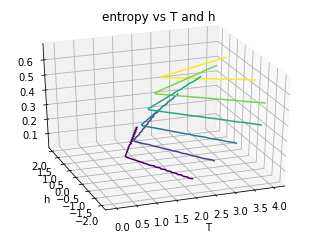
So we find δ = 3.

**Some More Graphs**

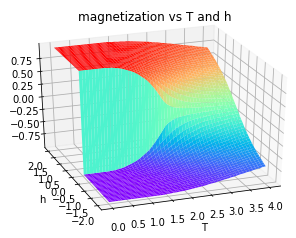
Made a few graphs. Here kB = J = 1, z = 2. First the free energy itself.



Then some entropy graphs. One on right is a contour plot, which makes clear that adiabatic demagnetization will cool the paramagnet/ferromagnet.

and magnetization.



The phase diagram presented above should make sense in the context of this graph.