**Thermal Properties**

Now we’ll examine the thermodynamic properties of these spin systems coupled via the exchange interaction.

**Ising Model**

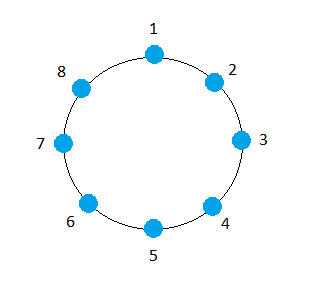
Now we’re going to add a complication to our paramagnet model by including the (electric) exchange interaction, which turns out to have a much stronger bearing on the magnetic properties of the material than the actual magnetic interactions. Recall the result we got in the QM folder/Identical Particles/Stark-Zeeman folder.



where Vinteratomic(E) and Vinteratomic(B) were internal electric and magnetic interactions between individual atoms. We have examined in the dielectric and paramagnet files the cases where the Vinteratomic guys resulted from electric and magnetic interactions between uniform bound charge and current densities. Now I think we’ll jettison the external (free) electric field, presume a uniform magnetic interaction between dipoles, fill the exchange interaction into Vinteratomic(E), and also just confine our attention to the spin part of HCFA (the part of the Hamiltonian in brackets). We can neglect all terms in HCFA not including spin because our exchange interaction model is only good within the degenerate ground state subspace of the two-body Hamiltonian of nearest neighbors, and so all the neglected terms will just amount to constants) Also just going to presume a single spin per atom. So,



The <ℓ,ℓ´> means sum over each particle’s z nearest neighbors. What z is depends on the interaction, and Jij would presumably just be a function of |i-j|. For example, if N = 8



and z = 4, then the terms we’d include in the sum are in the right column.

|  |  |
| --- | --- |
| Particle | Interactions |
| 1 | 7, 8, 2, 3 |
| 2 | 8, 1, 3, 4 |
| 3 | 1, 2, 4, 5 |
| 4 | 2, 3, 5, 6 |
| 5 | 3, 4, 6, 7 |
| 6 | 4, 5, 7, 8 |
| 7 | 5, 7, 8, 9 |
| 8 | 6, 7, 1, 2 |

And as can see this counts each interacting pair twice. So we have to multiply whole thing by that ½ in front of the sum. Now **B** = **B**f + μ0**M** is the *total* field, and **M** the magnetization density. From the general formula that **M** = -(1/ΔV)∂H/∂**B**f, we can see that:



Plugging this in, we’d have:



Now **S** = (ℏ/2)**σ** of course, and we have:



where in the last line I use g = 2, roughly. Okay now I’m going to drop the last term, which amounts to dropping **M**. Not because of mathematical complexity, since the analysis that follows would work just as well with that term as without – it’s no worse than the middle term. But it never shows up in any analysis I ever see, even though it seems kind of important, and non-negligible, since the magnetization ought to be quite high, possibly, for a ferromagnet. Well, but I think that basically Jij is much larger than μ0γ2/2ΔV (or, fairer comparison, larger than μ0γ2/2·(N/ΔV)) Also, we’re really kind of restricting our analysis to near the critical point, where **M** would be small yet. And also, it’s probably not realistic to say that M is uniform. In fact, the magnetic dipole-dipole interaction is responsible for the magnetic domains of ferromagnetics, and so **M** will be pointing up for one domain and down for the other. So yeah, just going to drop it. And now we have:



To streamline stuff, we’ll use units where ℏ = 1, and kB = 1. Also absorb the ¼ into Jij, and (1/2)gγ into Bf and call it h – my favorite letter.



And we’ll presume an isotropic medium so Jij = J. Also we’ll specialize to the Ising model whereby each of the spins is restricted to the z-direction (going to leave off the z subscript though). So now we have the Ising Model.



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.



This is practical in 1D, really really really difficult in 2D, and impossible in 3D? Let’s do 1D. We’ll presume periodic boundary conditions such that for our N spins σ1 = σN+1. Then we start by writing our Z in a more symmetric form,



Then let’s write Z as:



where we recognize the factor P can be represented as a 2×2 matrix, with row index given by σi = ±1, and column index by σi+1 = ±1. Or in other words,



where σ and σ´ can both be ±1. So then our Z can be written,



From Quantum Mechanics, or Linear Algebra, we’ll recognize this as the Trace of N, where is the matrix with the elements Pσσ´. So we have:



This can be evaluated by finding the eigenvector decomposition of . Let = UΛU-1, where Λ is the matrix of eigenvalues and U the matrix of eigenvectors. Then,



Using the cyclic property of the Tr, we can say,



where λ1,2 are the two eigenvalues of . What are these? Gotta solve,



This works out to,



Can simplify these to:



Now both eigenvalues are real, as guaranteed by the fact that is symmetric. And λ+ > λ-. This means that (λ+)N >> (λ-)N. And so the contribution of λ+ to Z will be much greater than the contribution of λ-. Thus, we may say,



and the Free energy per unit spin is F = F/N:



which is:



The average magnetic moment of each spin will be m = -∂F/∂Bf, but I’m going to calculate instead m = -∂F/∂h (recall h = 1/2·gγBf).



So we have:



From this, we can see that in the low T limit, there is no finite T transition to m → 1. Thus no spontaneous magnetization occurs, and we do not have a phase transition in 1D. But as T → 0, we do get m → 1,



So at T = 0, the spin is completely aligned with the field, as we expect. It will be of interest later to examine the behavior of F near the ‘critical point’, T = 0. So consider βF(K,j) where K = βJ and j = βh.



and in the large K (small T), small j limit we have:

