Asssignment 1

Physics 451

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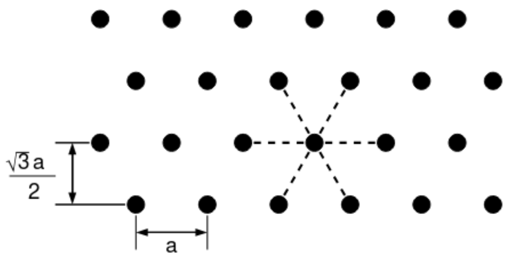


Figure 5.11: Each spin has six nearest neighbors on a hexagonal lattice. This lattice structure is sometimes called a triangular lattice.

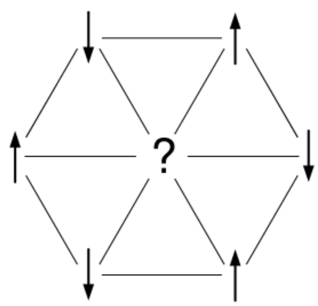


Figure 5.12: The six nearest neighbors of the central spin on a hexagonal lattice are successively antiparallel, corresponding to the lowest energy of interaction for an Ising antiferromagnet. The central spin cannot be antiparallel to all its neighbors and is said to be *frustrated*.

Figure 1: Caption

Question 1

So far we have considered the ferromagnetic Ising model for which the energy of interaction between two nearest neighbor spins is $J > 0$. Hence, all spins are parallel in the ground state of the ferromagnetic Ising model. In contrast, if $J < 0$, nearest neighbor spins must be antiparallel to minimize their energy of interaction.

Question 1.a

Sketch the ground state of the one-dimensional antiferromagnetic Ising model. Then do the same for the antiferromagnetic Ising model on a square lattice. What is the value of M for the ground state of an Ising antiferromagnet?

The ground state is simply the least energy configuration. This is when we have alternating spins as nearest neighbors.

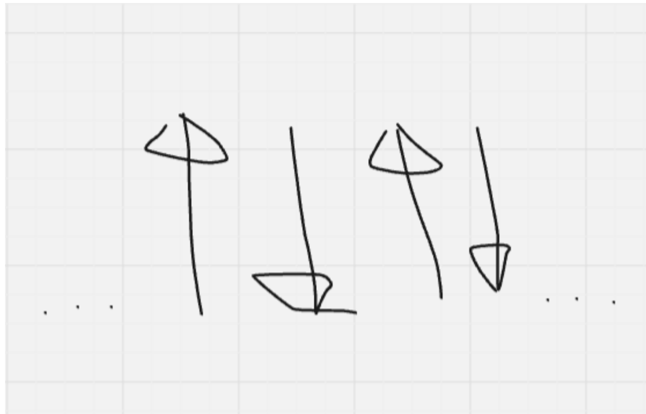


Figure 2: sketch of the ground state of the 1-D antiferromagnetic Ising model

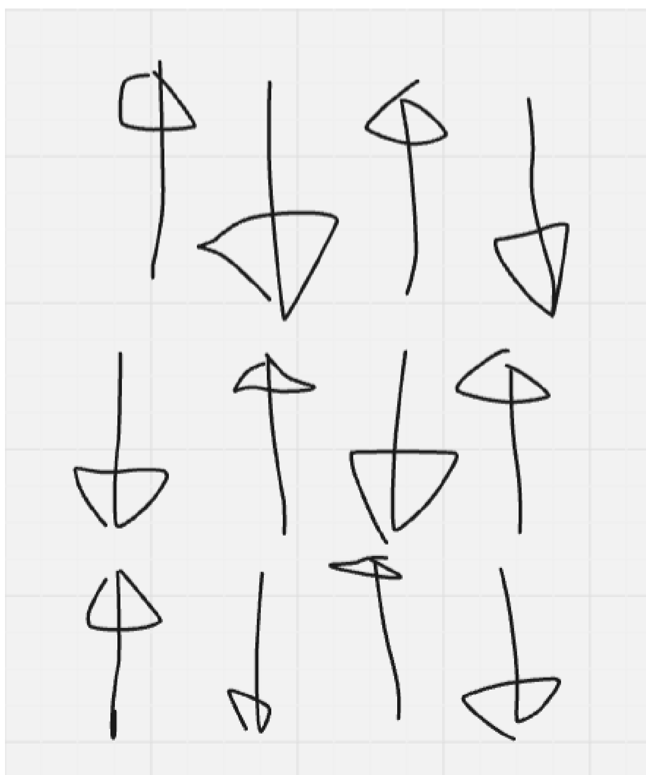


Figure 3: sketch of the ground state of the antiferromagnetic Ising model

The value of M is then $M = 0$ since the magnetization is zero.

Question 1.b

Use Program `IsingAnitferromagnetSquareLattice` to simulate the antiferromagnetic Ising model on a square lattice at various temperatures and describe its qualitative behavior. Does the system have a phase transition at $T > 0$? Does the value of M show evidence of a phase transition?

For very low values of the temperature ($0.1K$). We get a checkerboard of spin states. Slowly increasing the temperature we get small perturbations but a general checkerboard look. At around $T = 2K$ the checkerboard goes away with higher temperatures complete chaos and spin states flipping. This means that there is a phase transition at $T > 0$ where the value of M does not show any evidence of it. This is because M is largely unchanged by changing the temperature around the critical temperature.

Question 1.c

In addition to the usual thermodynamic quantities the program calculates the staggered magnetization and the staggered susceptibility. The staggered magnetization is calculated by considering the square lattice as a checkerboard with black and red sites so that each black site has four red sites as nearest neighbors and vice versa. The staggered magnetization is calculated from $\sum c_i s_i$ where $c_i = +1$ for a black site and $c_i = -1$ for a red site. Describe the behavior of these quantities and compare them to the behavior of M and χ for the ferromagnetic Ising model.

The staggered susceptibility is relatively low for high and low T but spikes at the critical temperature. The staggered magnetization is high for low T and then lowers to zero at and after the critical temperature.The behaviour of M in the ferromagnetic model is then anaolgous to the staggered magnetization behavior and the behavior of χ in ferromagnetic is anaolgous to the staggered susceptibility.

Question 1.d

Consider the Ising antiferromagnetic model on a hexagonal lattice (see Figure 5.11), for which each spin has six nearest neighbors. The ground state in this case is not unique because of frustration (see Figure 5.12). Convince yourself that there are multiple ground states. Is the entropy zero or nonzero at T = 0? Use Program `IsingAntiferromagnetHexagonalLattice` to simulate the antiferromagnetic Ising model on a hexagonal lattice at various temperatures and describe its qualitative behavior. This system does not have a phase transition for $T > 0$. Are your results consistent with this behavior?

Because of the "frustrated" states that occur when you try to minimize the energy, the entropy is a nonzero value since at $T = 0$ there are more multiple ground states of frustrated spins. Testing for different T we don't get radically different behavior in the spin flips. It is a sea of flips no matter the temperature. This is consistent with no phase transitions.

Question 2

Minima of free energy

Question 2.a

To understand the meaning of the various solutions of (5.108), expand the free energy in (5.126) about $m = 0$ with $H = 0$ and show that the form of $f(m)$ near the critical point (small m) is given by

$$f(m) = a + b(1 - \beta qJ)m^2 + cm^4 \tag{2.1}$$

Determine a, b, and c

We have:

$$f(T, H) = \frac{1}{2}Jqm^2 - kT\ln(2\cosh((qJm + H)/(kT))) \tag{2.2}$$

Let's have $H = 0$ and do a taylor series expansion about $m = 0$ to fourth order since we need a m^4 factor.

$$f(m) \approx f(0) + \frac{f'(0)m}{1} + \frac{f''(0)m^2}{2} + \frac{f'''(0)m^3}{6} + \frac{f''''(0)m^4}{24} \tag{2.3}$$

We can see that

$$f(0) = 0 - kT\ln(2\cosh[(qJ(0) + H)/kT]) \to 0 - kT\ln(2) \tag{2.4}$$

$$f'(0) = 0 - \frac{2kT}{2kT}\left(\frac{1}{\cosh[(qJ(0) + H)/kT]}\right)qJ\sinh((qJ(0) + H)/kT) = 0 - 0 = 0 \tag{2.5}$$

$$f''(0) = Jq - \frac{1}{kT}(qJ)^2\left(sech^2[(qJ(0) + H)/kT]\right) = Jq - \frac{1}{kT}(qJ)^2 = Jq\left(1 - \frac{1}{kT}qJ\right) \tag{2.6}$$

$$f'''(0) = -\beta(qJ)^2(-2sech^2[(qJ(0) + H)/kT])(\tanh[(qJ(0) + H)/kT])(\frac{qJ}{kT}) = 0 \tag{2.7}$$

$$f''''(0) = 2\beta^2(qJ)^3\Bigg((-2sech^2[(qJ(0) + H)/kT])(\tanh[(qJ(0) + H)/kT])(tanh[(qJ(0) + H)/kT])\frac{qJ}{kT} + sech^4[(qJ(0) + H)/kT]\frac{q}{k} \tag{2.8}$$

This long expression then goes to:

$$2\beta^3(qJ)^4(0 + 1) \tag{2.9}$$

We finally get:

$$a = f(0) = -kT\ln(2) \tag{2.10}$$

$$b = \frac{qJ}{2} \tag{2.11}$$

$$c = \frac{1}{12}(qJ)^4\beta^3 \tag{2.12}$$

Question 2.b

If H is nonzero but small, show that there is an additional term $-mH$ in 2.1

In the linear term we have:

$$f'(m) = 2Jqm - qJ\tanh([(qJm + H)/kT]) \tag{2.13}$$

When setting m to zero but have small H we can use the small angle approximation to get:

$$\tanh([(H)/kT]) \approx \frac{H}{kT} \tag{2.14}$$

So now we have a term

$$-qJ\beta mH \tag{2.15}$$

Question 2.c

Show that the minimum free energy for $T > T_c$ and $H = 0$ is at $m = 0$, and that $m = \pm m_0$ corresponds to a lower free energy for $T < T_c$.

For $T > T_c$, we have that the coefficients of $f(m)$ are all positive. This then makes the function shaped like m^2 and m^4 which have a minima at the origin. For $T < T_c$, we have that the function's squared term is:

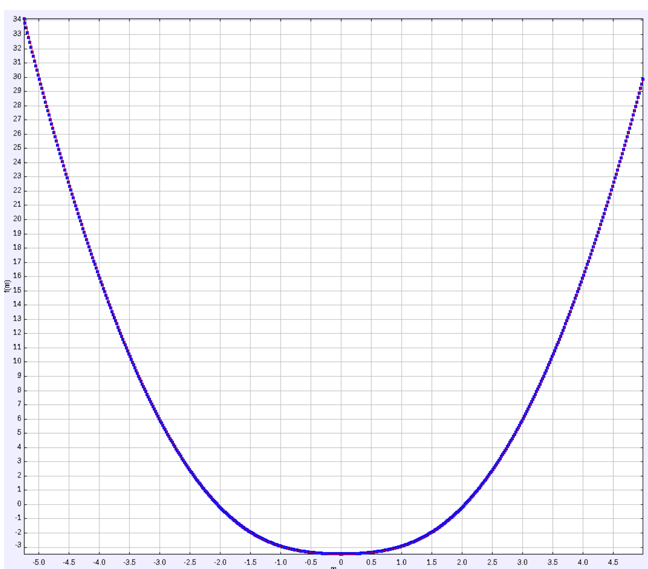
$$qJm^2/2 - \beta qJm^2 \tag{2.16}$$

So now we have a point where they are equal (but oppsite) for two different m, which gives the two minima.

Question 2.d

Use program `IsingMeanField` to plot $f(m)$ as a function of m for $T > T_c$ and $H = 0$. For what value of m does $f(m)$ have a minimum?

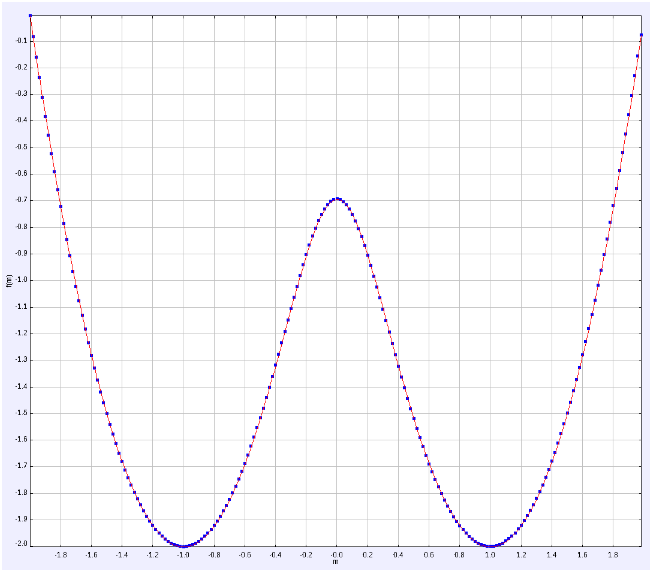
$f(m)$ has a minimum at $m = 0$



Question 2.e

Plot $f(m)$ FOR $T = 1$ and $H = 0$. Where are the minima of $f(m)$? Do they have the same depth? If so, what is the meaning of this result?

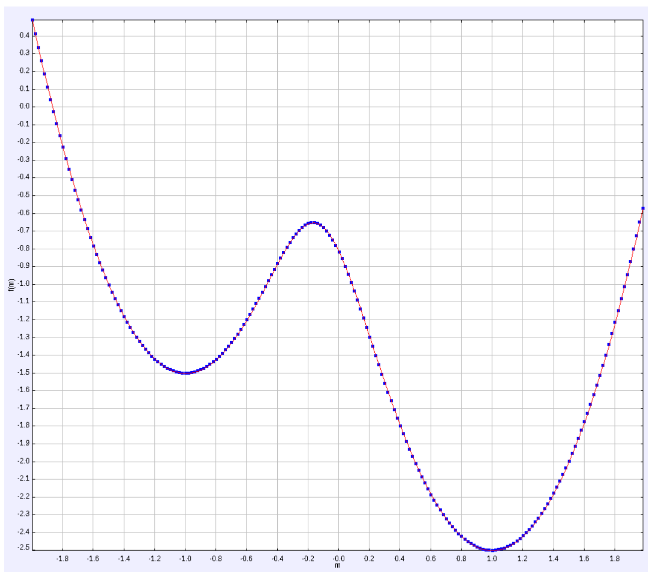
$f(m)$ has two minima at $m = \pm 1$. They have the same result which means that the free energy is minimized for two equal but opposite m.



Question 2.f

Choose $H = 0.5$ and $T = 1$. Do the two minima have the same depth? The global minimum corresponds to the equilibrium or stable phase. If we quickly "flip" the field and let $H \to -0.5$, the minimum at $m \approx 1$ will become a local minimum. The system will remain in this local minimum for some time before it switches to the global minimum.

The two minima do not have the same depth.



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