Oct. 3

Physics 212 – Statistical Mechanics

Mean Field Theory for the Ising Model

In the previous lecture, I gave an intuitive discussion of the physics of the phase diagram of the Ising model. In this lecture, I will calculate the free energy of the Ising model using an approximation scheme called "mean field theory". This method will give us a quantitative accounting of the properties of the various phases. The mean field method has important strengths, which will be apparent in this lecture, and also weaknesses, which will become more apparent as the course goes on.

Let me begin by writing again the Hamiltonian of the Ising model

$$\mathcal{H} = -J \sum_{i,\nu} S_i S_{i+\nu} - H \sum_i S_i \tag{1}$$

where each S_i can take the values $+1$ or -1.

A simple way to analyze this model is to treat each spin S_i in the *mean field approximation*. In the Hamiltonian, each spin appears together with other spins at neighboring sites. In the mean field approximation, we treat each spin independently, replacing the other spins that it interacts with by their expectation values. At the end of the analysis, we determine these expectation values self-consistently by setting them equal to the expectation value computed for the spin under discussion.

Here is the explicit analysis for the Ising model. Assume that, at temperature T and magnetic field H, the expectation value of each spin is

$$\langle S_i \rangle = s \tag{2}$$

Then we can analyze the spins individually. The partition function for the spin at site i is

$$Z_i = \sum_{S_i=+1,-1} \exp[\beta(J\ 2d\ sS_i + HS_i)] \tag{3}$$

where d is the dimension of the (cubic) lattice. Note that each lattice point has $2d$ nearest neighbors in d dimensions. The partition function evaluates to

$$Z = 2\cosh\Big(\beta(dJs + H)\Big) \tag{4}$$

or

$$F_i = -\frac{1}{\beta} \log\Big(\beta(2dJs + H)\Big) \tag{5}$$

From this we can derive

$$\langle S_i \rangle = -\frac{\partial F}{\partial H} = \tanh\Big(\beta(2dJs + H)\Big) \tag{6}$$

The self-consistency condition is then

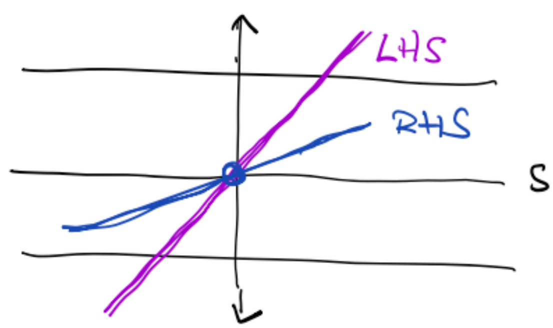
$$s = \tanh\Big(\beta(2dJs + H)\Big) \ , \tag{7}$$

and this is an equation that we can solve for s.

It is easiest to solve this equation graphically, by graphing the function on the left-hand side, LHS $= s$, on top of the function on the right-hand side. Let's do this first for the case $H = 0$.

$$s = \tanh\Big(\beta(2dJs)\Big) \ , \tag{8}$$

Then RHS $= \tanh(2dJ\beta s)$. For small values of β or high T, the comparison looks like



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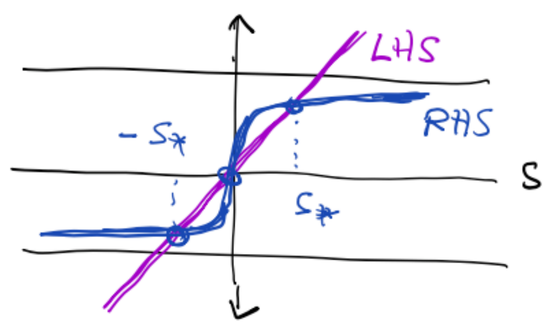
There is a unique solution at $s = 0$. However, For large values of β, low T, the comparison looks like



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There are 3 solutions. I will argue to you in a moment that the nontrivial solutions $s = \pm s_*$ are preferred.

We can study the transition between these two situations by expanding the equation (7) for small s. For $H = 0$, this gives

$$s = \tanh 2dJ\beta s = 2dJ\beta s - \frac{1}{3}(2dJ\beta s)^3 + \cdots \tag{11}$$

When the coefficient of s on the right-hand side equals 1, the two curves are tangent to one another. This is the dividing point between the two solutions. Call this temperature T_c or write $\beta_c = 1/T_c$. The value is given by

$$1 = 2dJ\beta_c \qquad \text{or} \qquad T_c = 2dJ \ . \tag{12}$$

For $\beta < \beta_c$, the two curves intersect only once, at $s = 0$. For $\beta > \beta_c$, write $\Delta\beta = (\beta - \beta_c)$ and take into account the the cubic term in (11) assuming that β is close to β_c. Then we find

$$s = s + \Delta\beta \cdot 2dJs - \frac{1}{3}s^3 + \cdots \tag{13}$$

which has the nontrivial solutions

$$s_* = \pm\Big[2dJ\Delta\beta\Big]^{1/2} \ . \tag{14}$$

Thus, mean-field theory predicts that, at $T < T_c$ and $H = 0$, there are two equivalent nontrivial thermodynamic states with

$$M = Ns_*(T) \ . \tag{15}$$

I still owe you can explanation of why, for $T < T_c$, the nontrivial solutions $s = \pm s_*$ are preferred over the trivial solution $s = 0$. To understand this, we can use the variational principle of statistical mechanics. Recall that, if $\mathcal{H}$ is the Hamiltonian we wish to analyze and $\mathcal{H}_a$ is a family of Hamiltonians that are easier to solve, the free energy F of $\mathcal{H}$ is bounded above by

$$F \leq F_a + \langle \mathcal{H} - \mathcal{H}_a \rangle_a \tag{16}$$

and we can choose the best representative for $\mathcal{H}$ by minimizing the right-hand side over a.

We would like to apply an approximation in which each spin fluctuates independently in the mean field of the others. So, try for the variational approximate Hamiltonians

$$\mathcal{H}_h = -\sum_i hS_i \tag{17}$$

where h is an effective magnetic field applied at each site. In the previous lecture, I derived that, for this Hamiltonian,

$$F_h = -\frac{N}{\beta}\log 2\cosh\beta h \qquad \langle S_i \rangle = \tanh\beta h \ . \tag{18}$$

The logic is essentially as the same as that used to derive $\langle S_i \rangle$ for mean field theory above. Then

$$\langle H \rangle_h = -NdJ(\tanh \beta h)^2 - Nh \tanh \beta h \tag{19}$$

and so (16) reads, for this choice of $\mathcal{H}_h$,

$$F \leq -\frac{N}{\beta} \log 2 \cosh \beta h - NdJ(\tanh \beta h)^2 - N(H-h) \tanh \beta h \tag{20}$$

Differentiate this with respect to h. This gives the minimization equation

$$0 = -N \tanh \beta h - (2dNJ \tanh \beta h + N(H-h))(\frac{d \tanh \beta h}{dh}) + N \tanh \beta h \tag{21}$$

The first and last terms cancel. The minimization criterion then becomes

$$h = 2dJ \tanh \beta h + H \tag{22}$$

Defining a new variable $\mathcal{S}$ by $\mathcal{S} = \tanh \beta h$, this equation becomes

$$\frac{1}{\beta} \tanh^{-1} \mathcal{S} = 2dJ\mathcal{S} + H \tag{23}$$

which is exactly the mean field self-consistency equation

$$\mathcal{S} = \tanh \beta(2dJ\mathcal{S} + H) \ . \tag{24}$$

This alternative derivation of the mean field equation gives us a little more power. Now we can evaluate the right-hand side of (16) for the various solutions to the equation and see which are preferred. To do this, it is useful to rewrite the minimization equation (21) as follows: Let $F_{RHS}(h)$ represent the right-hand side of (20). Then

$$\frac{d}{dh} F_{RHS}(h) = N(\Big(h - (2dJ\mathcal{S} + H)\Big) \cdot \frac{d\mathcal{S}}{dh} \tag{25}$$

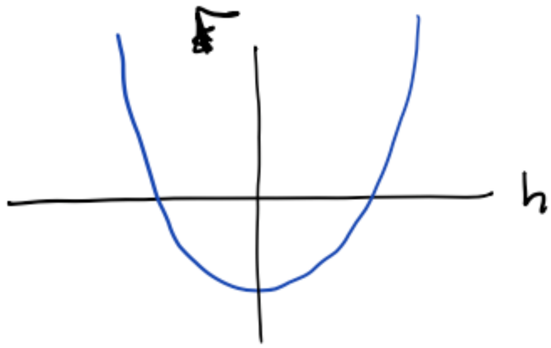
Notice that $d\mathcal{S}/dh$ is always positive, so this quantity is positive or negative according to the sign of the term in parentheses.

Consider first the case $H = 0$. The term that determines the sign of (25) is

$$h - 2dJ\mathcal{S}(h) \tag{26}$$

As noted above, this equation is exactly equivalent to the mean field equation (7). Thus, for $T > T_c$ it has one zero at $h = 0, \mathcal{S} = 0$, and for $T < T_c$ it has three zeros at $\mathcal{S} = 0, \pm s_*$. Notice also that both terms in this expression are an odd functions of h and so the expression is antisymmetric under $h \to -h$.

First, let's study $T > T_c$. Since $|\mathcal{S}| \leq 1$, the term (26) is negative for large negative h and positive for large positive h. For $T > T_c$, the equation has one zero, located at $\mathcal{S}(h) = 0$. Then the function $F_{RHS}(h)$ must have the form



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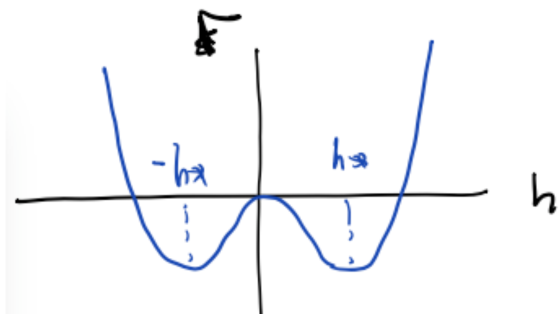
with a minimum at $h = 0, \mathcal{S} = 0$.

For $T < T_c$, the expression (26) is negative for $h < -h_*$, where h_* is defined by $\mathcal{S}(h_*) = s_*$. Above h_*, the expression turns positive. At $h = 0$ there is another zero, and the expression turns negative again. Finally, at $h = +h_*$, there is a third sign change and the expression is positive for all larger values of h. Then the function $F_{RHS}(h)$ must have the form



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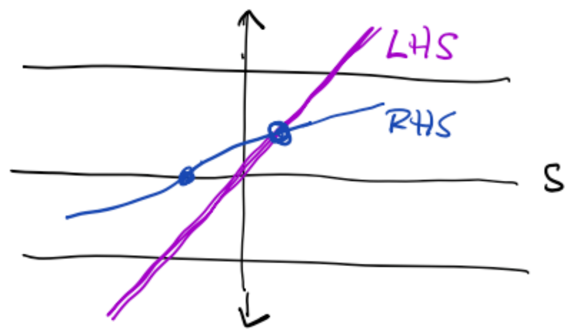
with symmetrical minima at $h = \pm h_*$ and a *maximum* at $h = 0$. Now we see clearly that $h = \pm h_*$, $\mathcal{S} = \pm s_*$ give the preferred solutions.

For $H > 0$, the self-consistency equation becomes

$$s = \tanh(2dJs\beta + H) \tag{29}$$

The graphical solution for s still has two cases. For small β or high T, it takes the form



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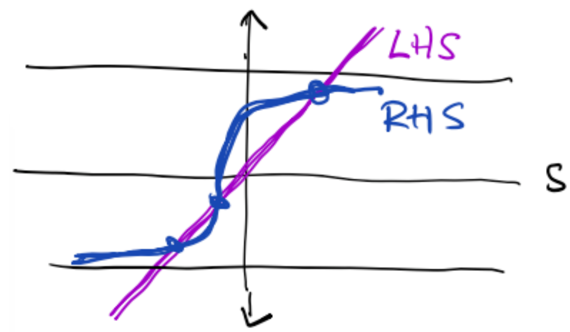
and there is one solution For large β or low T, it takes the form



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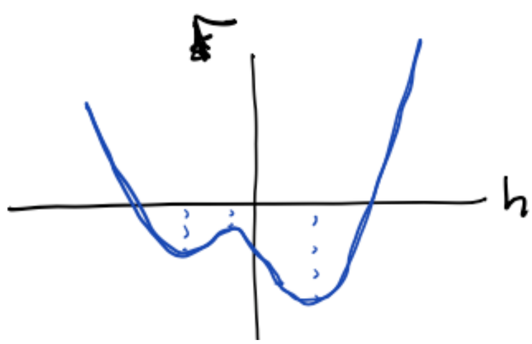
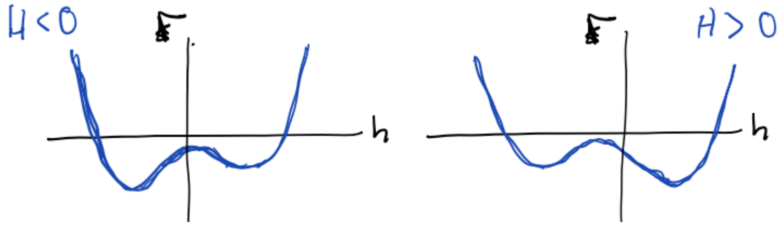
and there are three solutions. However, the positive solution is clearly preferred. If we construct $F_{RHS}(h)$ for this case, as we did above, it has the form



(32)

The extrema are at the solutions of (29), and the solution at positive h has the deepest minimum.

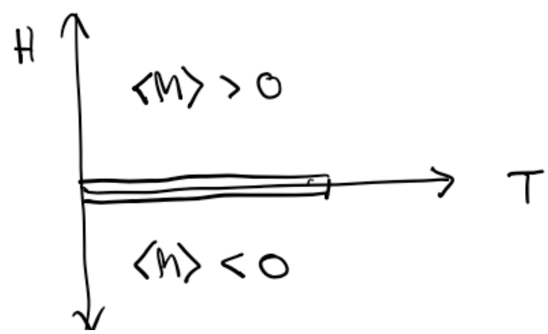
There is a similar story for $H < 0$. Notice that the expression for $F_{RHS}(h)$ is not symmetric in either case. However, for the magnetic fields H and $-H$, the two functions are mirror images of one another,



(33)

In particular, for $|H|$ very small and $T < T_c$. The preferred minimum flips from the left to the right when H crosses from negative to positive values.

I have now shown that mean field theory predicts exactly the phase diagram that we imagined in the previous lecture.



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The thermodyanic functions are continuous and, actually, analytic in T and H at all points in the phase diagram except for the points on the $H = 0$ axis for $T \leq T_c$. Actually, in mean field theory, the magnetization and energy are analytic separately in the phases above and below the line $H = 0$. Aside from the fact that the two phases meet discontinuously, the only place where the thermodyanic functions are non-analytic is just at the point $H = 0$, $T = T_c$. It is interesting to work out the dependences of the various quantities as we approach this point.

Consider first the magnetization. We have already seen in (14) that, for $H = 0$ and T just below T_c, $s_* \sim (\Delta\beta)^{1/2}$. In terms of temperature

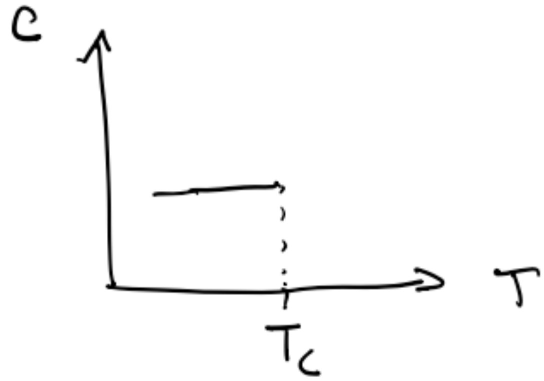
$$M = N s_* \sim (T_c - T)^{1/2} \ . \tag{35}$$

Also, at $H = 0$, mean field theory gives for $E = \langle \mathcal{H} \rangle$,

$$E = -NdJs^2 = \begin{cases} 0 & T > T_c \\ -NdJs_*^2 \sim -(T_c - T) & T < T_c \end{cases} \tag{36}$$

Differentiating with respect to T, the specific heat is a nonzero constant as $T \to T_c$

from below and then is 0 above T_c. So C has a discontiuity at T_c.



$$(37)$$

Next, take $\Delta\beta < 0$, $T > T_c$, and turn on a small field H. The self-consistency equation (7) becomes

$$\begin{aligned} s &= \tanh(\beta_c + \Delta\beta)(2dJs + H) \\ &= s - 2dJ|\Delta\beta|s + \beta_c H + \cdots \end{aligned} \tag{38}$$

or

$$s \sim \frac{H}{T - T_c} \tag{39}$$

This implies

$$M \; \frac{H}{T - T_c} \qquad \text{or} \qquad \chi = \left.\frac{\partial M}{\partial H}\right|_T \sim (T - T_c)^{-1} \tag{40}$$

The same singularity in χ appears for $T < T_c$.

Finally, consider $\beta = \beta_c$ with nonzero H. The self-consistency equation becomes

$$\begin{aligned} s &= \beta_c(2dJs + H) - \frac{1}{3}(\beta_c(2dJs + H)^3 + \cdots \\ &= s + \beta_c H - \frac{1}{3}s^3 + \cdots \end{aligned} \tag{41}$$

so that

$$s \sim H^{1/3} \qquad \text{or} \qquad M \sim H^{1/3} \ . \tag{42}$$

Let me summarize. The various thermodynamic functions are non-analytic at the point $T = T_c$, $H = 0$ with the singular behavior

$$\begin{aligned} \text{at } H = 0,\ T \to T_c \ : &\qquad M \sim (T_c - T)^{1/2} \ ,\ \chi \sim |T - T_c|^{-1} \\ \text{at } T = T_c \ : &\qquad M \sim H^{1/3} \ ,\ C \text{ discontinuous} \end{aligned} \tag{43}$$

You may be wondering why I am giving so much attention to this non-analytic behavior. Later in the course, you will see that it deserves even more attention.

It is not much more difficult to solve for the phase diagrams of all of the magnets defined in the previous lecture using mean field theory. Consider

$$\mathcal{H} = -J \sum_{i,\nu} \vec{S}_i \cdot \vec{S}_{i+\nu} - \vec{H} \cdot \sum_i \vec{S}_i \ . \tag{44}$$

Again we assume that we can concentrate on the statistical mechanics of the spin one site while replacing the spins at the neighboring sites by their average values

$$\langle S_i \rangle = \vec{s} \tag{45}$$

If $\vec{S}_i$ is an n-component unit vector, then also $\vec{H}$ is n-component. For $\vec{H} = 0$, the problem is rotationally symmetric and we are free to take $\vec{s}$ to be parallel to the $\hat{1}$ axis. If we turn on $\vec{H}$ parallel to $\hat{1}$, the external field will steer $\vec{s}$ into the $\hat{1}$ direction: $\vec{s} = (s^1, \vec{0})$.

Let S^1 be the 1 component of the unit vector $\vec{S}_i$, and, instead of s^1, write simply s. Then the self-consistency equation is

$$s = \int d\Omega_n \ e^{\beta(2dJs+H)S^1} \ S^1 \ / \ \int d\Omega_n \ e^{\beta(2dJs+H)S^1} \ . \tag{46}$$

where $d\Omega_n$ is an integral over the unit sphere in n dimensions.

Let's study this equation for $H = 0$. In the Ising case ($n = 1$), we found T_c by examining the slope of the right-hand side near $s = 0$ and finding the value of β for which this slope was equal to 1. The same criterion will apply here. We then should expand the numerator and denominator in a Taylor series in s.

To work this out, expand

$$e^{2dJ\beta s S^1} = 1 + (2dJ\beta s)S^1 + \frac{1}{2}(2dJ\beta s)^2 (S^1)^2 + \cdots \tag{47}$$

In the denominator, the leading term is

$$\int d\Omega_n \ [1 + \cdots] \tag{48}$$

Choose a normalization for the integral so that this equals 1. In numerator, the leading terms are

$$\int d\Omega_n \Big[\ 1 + (2dJ\beta s)S^1 + \cdots \Big] \ S^1 \ . \tag{49}$$

The first term vanishes by symmetry, and the second term gives

$$(2dJ\beta s) \left\langle S^1 \ S^1 \right\rangle \tag{50}$$

By rotational symmetry, the integral of the square of components of a unit vector must have the form

$$\left\langle S^a \ S^b \right\rangle = c \cdot \delta^{ab} \tag{51}$$

and, since $\vec{S}$ is a unit vector, it must also satisfy

$$\sum_a \langle S^a \ S^a \rangle = 1 \tag{52}$$

Then

$$\left\langle S^1 \ S^1 \right\rangle = 1/n \tag{53}$$

and (46) becomes

$$s = (2dJ\beta)\frac{1}{n} \ s + \cdots \tag{54}$$

The critical temperature is the temperature at which the coefficient on the right-hand side equals 1; hence, for the n-component model,

$$T_c = \frac{2dJ}{n} \tag{55}$$

By reflection symmetry, the next term in the expansion of the self-consistency equation will be

$$s = \frac{2dJ\beta}{n} s - (\mathrm{const}) \cdot s^3 + \cdots \tag{56}$$

So the qualitative form of the solution to the self-consistency equation will be the same as we found in the Ising case, and the prediction for the form of the phase diagram is the same. Even further, this equation will give the same non-analytic power laws as $T \to T_c$ that we found in the Ising case. For example,

$$M \sim (T_c - T)^{1/2} \ , \ M \sim H^{1/3} \text{ at } T_c \ . \tag{57}$$

I will refer to these expressions as exhibiting the “mean field critical exponents”.

Here is some extra material for those who are curious about it:

To study the whole phase diagram more quantitatively in the n-component case, it woud be good to have explicit expressions for the integrals in (46). These are given in terms of modified Bessel functions. There are several more points in this course where we will meet modified Bessel functions, so it it is useful to review their properties.

Consider first the denominator in (46), in the case $H = 0$. Choosing polar coordinates on the unit sphere, this denominator can be written as the integral

$$\mathcal{D} = \int d\Omega_n \ e^{B\cos\theta} \tag{58}$$

where $B = 2dJ\beta s$ and

$$\int d\Omega_n = \int_0^\pi d\theta \ (\sin\theta)^{n-2} \mathcal{A}(n-1) \tag{59}$$

and $\mathcal{A}(n-1)$ is the area of the unit sphere in $(n-1)$ dimensions. Changing variables,

$$\begin{aligned} \int d\Omega_n &= \int_{-1}^1 d\cos\theta \ (1-\cos^2\theta)^{(n-3)/2} \mathcal{A}(n-1) \\ &= \int_{-1}^1 dt \ (1-t^2)^{(n-2)/2-1/2} \mathcal{A}(n-1) \end{aligned} \tag{60}$$

The factor $\mathcal{A}(n-1)$ will cancel between numerator and denominator in (46), so I will drop it from here on. Then

$$\mathcal{D} = \int_{-1}^1 dt (1-t^2)^{(n-2)/2-1/2} e^{Bt} \ . \tag{61}$$

You can compare this to the integral representation for the modifed Bessel function $I_\nu(z)$,

$$I_\nu(z) = \int_{-1}^1 dt (1-t^2)^{\nu-1/2} e^{zt} \ . \tag{62}$$

so that

$$\mathcal{D} \sim I_\nu(2dJ\beta s) \qquad \text{with} \qquad \nu = \frac{(n-2)}{2} \tag{63}$$

The expectation value of $\cos\theta$ is given by

$$\langle \cos\theta \rangle = \frac{1}{\mathcal{D}} \frac{\partial}{\partial B} \mathcal{D} \ . \tag{64}$$

Now, it is a property of the modified Bessel function that

$$\frac{\partial}{\partial z} \Big\{ z^{-\nu} I_\nu(z) \Big\} = z^{-\nu} I_{\nu+1}(z) \ . \tag{65}$$

This implies

$$s = \langle \cos\theta \rangle = I_{n/2}(2dJ\beta s) / I_{(n-2)/2}(2dJ\beta s) \tag{66}$$

The Taylor expansion of $I_\nu(z)$ is

$$I_\nu(z) = \frac{z/2}{\Gamma(\nu+1)} \Big[1 + \frac{(z/2)^2}{\nu+1} + \mathcal{O}(z^4) \Big] \tag{67}$$

So, for small s, this expression for $\langle \cos\theta \rangle$ becomes

$$\langle \cos\theta \rangle = \frac{(2dJ\beta s/2)}{n/2} + \cdots = \frac{2dJ\beta s}{n} + \cdots \tag{68}$$

which gives a nice check on the formula for $\langle \cos\theta \rangle$ that we found in (54).

For $z \to \infty$,

$$I_\nu(z) \sim \frac{e^z}{\sqrt{2\pi z}}\left(1 - \frac{4\nu^2 - 1}{8z} + \cdots\right) \tag{69}$$

so for $\beta \to \infty$, $T \to 0$, or, restoring H, $H \to \infty$,

$$s \to 1 \ , \tag{70}$$

which is as it should be in the limit of zero temperature or extremely strong field.