Physics 212 – Statistical Mechanics

High and Low Temperature Expansions

In the previous lecture, we explored the phase diagram of the Ising model using a variational approximation scheme, mean field theory. That scheme made physical sense and gave qualitatively reasonable results. On the other hand, it used an uncontrolled approximation whose validity I left rather unclear. In the next few lectures, I will present more rigorous approaches to the evaluation of the Ising model partition function. This will give us some exact results and also a new set of concepts to bring to bear on problems of phase transitions.

In this lecture, I will present a method for deriving systematic Taylor series for the Ising model partition function, thermodynamic functions, and correlation functions. These have a geometric character that I hope you will find interesting. There is a close relation to the theory of random walks (which will appear on a future problem set). In this lecture, I will restrict myself to the Ising model on a 2-dimensional square lattice. This will allow me to represent the relevant Taylor series graphically. It will be clear, though, that the methods that I will introduce work in any number of dimensions. I will work at zero external field, $H = 0$, but the generalization to nonzero field is straightforward.

Let's begin with the high-temperature expansion of the Ising model partition function. As always, the partition function is

$$Z = \sum_{S_i=+1,-1} e^{\beta J \sum_{i\nu} S_i S_{i+\nu}} \tag{1}$$

Write this as a sum over a product of factors, each factor corresponding to one bond on the lattice,

$$Z = \sum_{S_i=+1,-1} \prod_{i,\nu} e^{\beta J S_i S_{i+\nu}} \tag{2}$$

At high temperature, $\beta \to 0$, so we can expand

$$e^{\beta J S_i S_j} = 1 + \beta J S_i S_j + \frac{1}{2!}(\beta J S_i S_j)^2 + \frac{1}{3!}(\beta J S_i S_j)^3 + \cdots \tag{3}$$

Actually, since $S_i^2 = 1$, we can simplify this expression

$$\begin{aligned} e^{\beta J S_i S_j} &= 1 + \beta J S_i S_j + \frac{1}{2!}(\beta J)^2 + \frac{1}{3!}(\beta J)^3 S_i S_j + \cdots \\ &= \cosh \beta J + S_i S_j \sinh \beta J \\ &= \cosh \beta J (1 + z S_i S_j) \end{aligned} \tag{4}$$

where

$$z = \tanh \beta J \tag{5}$$

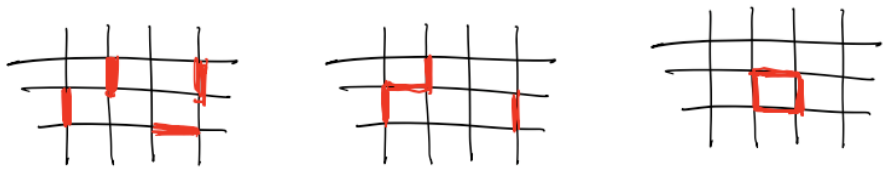
If we could not make this simplification, the method I am about to introduce would still work, but there would be more terms to sum up.

We now have put the partition function into the form

$$Z = (\cosh \beta J)^{dN} \sum_{S_i = +1, -1} \prod_{i,\nu} (1 + z S_i S_{i+\nu}) \tag{6}$$

I would now like to represent this expression as a Taylor series expansion in the parameter z which becomes small at high temperature. Imagine expanding the product and writing this out as a very large polynomial in z. The term with z^m is given by keeping the $zS_iS_{i+\nu}$ term in the expressions for m of the bonds and keeping the 1 term for all other bonds.

We can represent this term graphically in the following way: Draw the 2-dimensional lattice. Color the bonds for which we keep the $zS_iS_{i+\nu}$ term, and leave the other bonds uncolored. Then some typical configurations for the case $m = 4$ would be



(7)

The next step is to do the sum over the S_i for each configuration. We need the simple identities

$$\sum_{S_i} 1 = 2 \ , \quad \sum_{S_i} S_i = 0 \ , \ \sum_{S_i} S_i^2 = 2 \ , \ \ etc. \tag{8}$$

Then each configuration contributes 0 if there is any lattice site with 1 or 3 factors of S_i at that site. Equivalently, a lattice coloring would give 0 if any site has 1 or 3 colored bonds attached to that site. In the figure above, the first two configurations give 0, but the last one gives a nonzero value. If the value is nonzero, the sum over S_i at each site gives a factor 2, so the configuration has a total factor 2^{dN}.

We now arrive at the following rule for evaluating the term of order z^m in Z: Draw all possible colorings of the lattice with m colored bonds. Let C_m be the set of colorings such that an *even* number of colored bonds connect to each site of the lattice. Then

$$Z = (2 \cosh \beta J)^{dN} \sum_m \sum_{C_m} z^m \ . \tag{9}$$

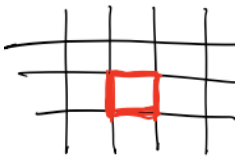
I would like to make one more simplification. The factor $(2 \cosh \beta J)^{dN}$ in front is an analytic function of β. It contributes to the free energy, but it cannot contribute

to a singularity in the free energy and so it is not relevant to the discussion of the singularities of thernodynamic functions at the critical point. Further, this factor will cancel out when we compute correlation functions of spins. So I will ignore this factor from here on. That is, I will write

$$Z = (2\cosh\beta J)^{dN} \cdot \overline{Z}(z) \tag{10}$$

and concentrate on developing a Taylor series representation of $\overline{Z}(z)$.

To do this, we must count nonzero colorings of the lattice. For the z^0 term, we leave all bonds uncolored. There is 1 such configuration. There are no allowed terms for $m = 1, 2, 3$. For the z^4 terms, there is one simple configuration of colored bonds, but this can appear anywhere on the lattice



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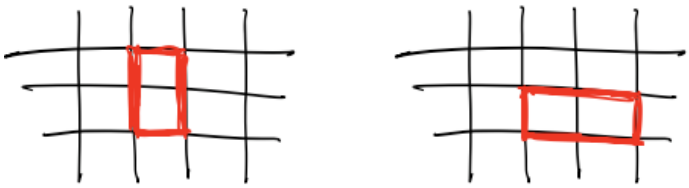
Thus, the number of colorings in C_4 is N. Similarly, for $m = 6$, there are $2N$ nonzero colorings



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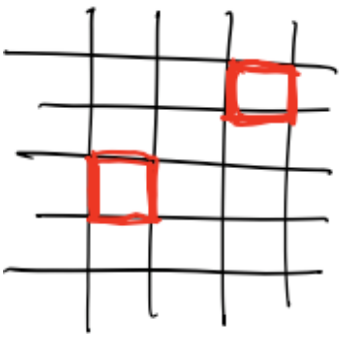
The contributions from C_8 require some extra thought. First, there are configurations consisting of 2 boxes, each at an arbitrary position on the lattice.



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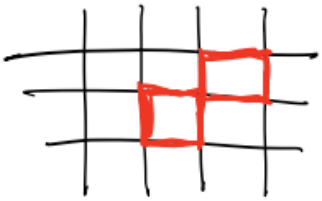
Swapping the positions of the two boxes does not result in a new coloring, so the total numer of these colorings is naively $N^2/2$. However, these boxes cannot be on top of one another or next-neighbors, since each bond can be colored only once. Thus, the correct number of these configurations is

$$\frac{1}{2}(N^2 - N - 4N) = \frac{N^2}{2} - \frac{5}{2}N \tag{14}$$

Notice the configuration



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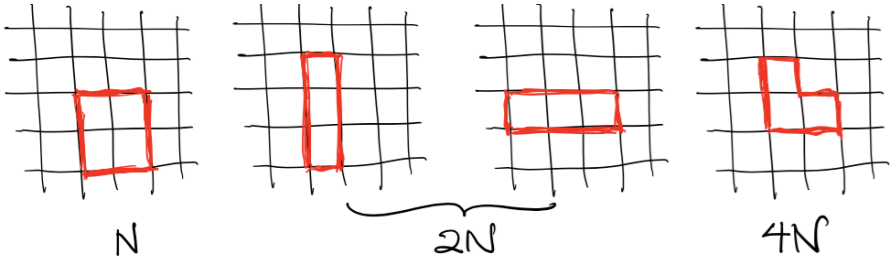
is perfectly acceptable. In addition, there are other colorings that kare not of the form of 2 simple boxes



(16)

In all, we find

$$\frac{1}{2}(N^2 - 5N) + N + 2N + 4N = \frac{N^2}{2} + \frac{9}{2}N \tag{17}$$

allowed colorings. Then, through order z^8, we find

$$\overline{Z} = 1 + Nz^4 + 2Nz^6 + (\frac{N^2}{2} + \frac{9}{2}N)z^8 + \cdots \ . \tag{18}$$

The term with N^2 seems incorrect. However, please remember that $\overline{Z}$ is the exponential of an extensive quantity. Thus, $\overline{Z}$ must resum to an expression of the form

$$\overline{Z} = \exp\Big[N f(z)\Big] \tag{19}$$

which would lead to an extensive expression for the free energy of the Ising model. Thus, finally,

$$\overline{Z} = \exp\Big[N\Big(z^4 + 2z^6 + \frac{9}{2}z^8 + \cdots\Big)\Big] \ . \tag{20}$$

Putting back the prefactor in (10), we find for the free energy of the model the expression

$$F = -\frac{Nd}{\beta}\log 2\cosh\beta J - \frac{N}{\beta}f(z) \tag{21}$$

where

$$f(z) = z^4 + 2z^6 + \frac{9}{2}z^8 + \cdots \ . \tag{22}$$

Working harder, and using a computer to assist with the counting, it is possible to work out the Taylor series for $f(z)$ to z^{20} or so. This gives a very precise quantitative accounting in the high-temperature region.

There is an interesting matter of principle to discuss here, but first I would like to generalize this analysis to compute the spin-spin correlation function, that is, the correlation function between individual spins at two lattice sites I and J,

$$\langle S_I S_J \rangle = \sum_{S_i} e^{\beta J \sum_{i,\nu} S_i S_{i+\nu}} S_I S_J \;/\; \sum_{S_i} e^{\beta J \sum_{i,\nu} S_i S_{i+\nu}} \tag{23}$$

We have already computed the denominator of this expression, and we can use the same set of tricks to derive a graphical representation of the numerator. Carrying out the same steps as led to (6), the numerator reduces to

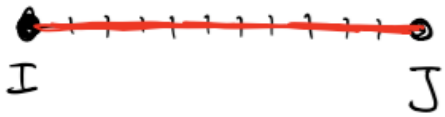
$$(\cosh \beta J)^{dN} \sum_{S_i = +1,-1} \prod_{i,\nu} (1 + z S_i S_{i+\nu}) \cdot S_I S_J \tag{24}$$

Notice the extra factors of S_I and S_J that appear in the sum. These imply that, when we do the sums over the S_i, we will get a nonzero result only if there are an *odd* number of colored bonds connecting to the sites I and J, with still an *even* number of colored bonds at all other sites. Then

$$\langle S_I S_J \rangle = \sum_n \sum_{C_n(I,J)} z^n \;/\; \sum_m \sum_{C_m} z^m \tag{25}$$

Here C_m is the set of colorings with m colored bonds and an even number of colored bonds at each site, and $C_n(I.J)$ is the set of colorings with an odd number of colored bonds at the sites I, J.

I would like to compute a few terms just for the simplest case, to give some ideas of this series expansion. Consider, then, the case $I = (0, 0)$ and $J = (n, 0)$. The first nonzero coloring is a straight line between I and J with n colored bonds



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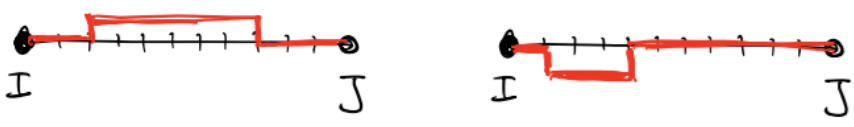
This is of order z^n. In the next order, z^{n+2}, some typical colorings are

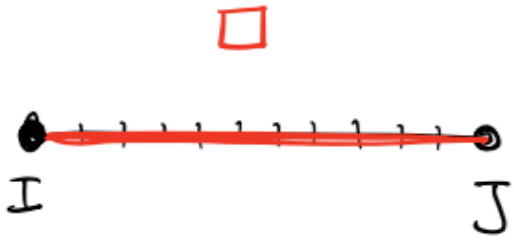


(27)

The total number of these is

$$2 \cdot \frac{n(n+1)}{2} \tag{28}$$

In order z^{n+4}, there are colorings with a separate box that can be anywhere on the lattice except for directed above or below the colored line between I and J



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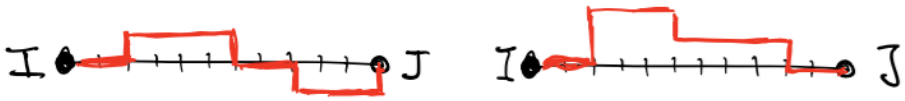
and additional colorings such as



(30)

The term proportional to Nz^{n+4} cancels out when the divide the numerator by the denominator

$$\langle S_I S_J \rangle = \left[z^n + n^2 z^{n+2} + (N - 2n + \cdots) z^{n+4} + \cdots \right] \; / \; \left[1 + 4N z^4 + \cdots \right] \tag{31}$$

Finally

$$\langle S_I S_J \rangle = z^n \cdot \left(1 + n^2 z^2 + \cdots \right) , \tag{32}$$

and this series is independent of N when the size of the system is much larger than n.

The leading term for the correlation function shows an exponential decay

$$\langle S_I S_J \rangle = z^n = \exp[-n \log \frac{1}{z}] \; . \tag{33}$$

and we can sum up the series in the form

$$\langle S_I S_J \rangle = \exp[-n g(z,n)] \; , \tag{34}$$

where, to the order we have computed

$$g(z,n) = \log \frac{1}{z} \cdot (1 - n z^2 + \cdots) \tag{35}$$

The spin-spin correlation function will play an important role in our discussion of the physics of phase transitions. I would like to say a little more about this here. In the leading order in z, we have seen that

$$\langle S_I S_J \rangle \to 0 \text{ as } |I - J| \to \infty \ . \tag{36}$$

This statement is actually an indicator that the system is in an unmagnetized state and that its global symmetry is preserved. In a magnetized state, $\langle S_I S_J \rangle$ would contain the effects of the local correlations between the spins at I and J, but it would also contain the overall correlation through the magnetization. In the limit $|I - J| \to \infty$, the local correlations would fall away, but the general spin orientation from the magnetization would remain. Thus, we would have, as $|I - J| \to \infty$,

$$\langle S_I S_J \rangle \to \langle S_I \rangle \langle S_J \rangle = m^2 \text{ where } m = M/N \tag{37}$$

More generally, if Q is the order parameter for a system with spontaneous symmetry breaking and has a local description,

$$Q = \int d^d x q(x) \tag{38}$$

we can study the correlation function

$$\langle q(x) q(y) \rangle \ . \tag{39}$$

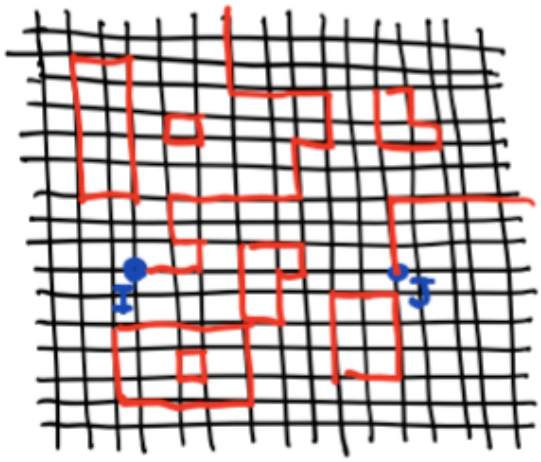
In the limit $|x - y| \to \infty$, this correlation function has the limit

$$\langle q(x) q(y) \rangle \to \langle q(x) \rangle \langle q(y) \rangle \tag{40}$$

If this limit is nonzero, Q has a thermodynamic expectation value and the symmetry of the model is spontaneously broken. If the limit is zero, the system is in a disordered phase and its symmetry is preserved.

The high-temperature series in z that I have described have a property that is not so obvious from my discussion so far but can be proved: For sufficiently small z, these series are convergent and thus define the free energy and the spin-spin correlation as analytic functions of the temperature. A way to see this for the spin-spin correlation function is that the diagrams contributing to $\langle S_I S_J \rangle$ are a subset of the diagrams contributing to the analogous quantity for a random walk on the lattice from I to J, in which a given bond can be covered multiple times, and thus $\langle S_I S_J \rangle$ is bounded above by the random walk expression. In any event, this result implies that, rigorously, there is a finite region of high temperatures $|z| < Z$ in which $\langle S_I S_J \rangle \to 0$ as $|I - J| \to 0$ and thus the system is in the symmetric phase. (Those of your who have studied Feynman diagrams will note that this is different from the situation of Feynman diagram perturbation theory, which has zero radius of convergence.)

The diagrams also suggest a way of thinking about the phase transition to a magnetized state. As z increases, the diagrams contributing to the spin-spin correlation function deviate more and more from the shortest-distance path. The environment also becomes full of closed-loop paths, making it easier for the path connected to the points I and J to wander away from the shortest line. We might imagine that at some value of z (of course, beyond the radius of convergence of the series), the path from I can wander off to infinity.



(41)

This is not at all rigorous, but it gives a nice intuitive picture. Visibly, the spin-spin correlation function has a piece that is uncorrelated between I and J

$$\langle S_I S_J \rangle = \langle S_I \rangle \langle S_J \rangle + \cdots \tag{42}$$

indicating spontaneous breaking of the symmetry.

Now that we have established that the Ising model has a high-temperature phase with zero magnetization, let's turn our attention to low temperatures. Here too there is a diagrammatic perturbation theory for $H = 0$ for which we can work out the details.

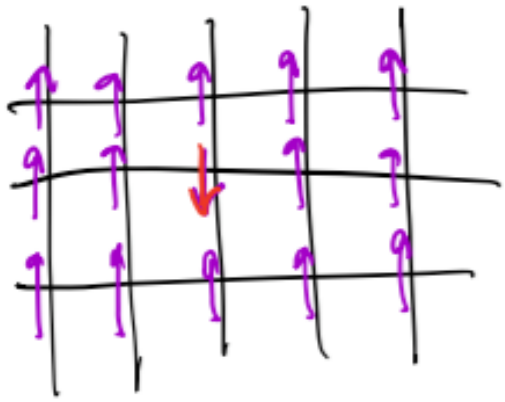
At zero temperature, $\beta \to \infty$ and all spins must be perfectly aligned. There are two ground states: $S_i = +1$ for all i, and $S_i = -1$ for all i. For definiteness, I will work with the state with all spins up. We can compute

$$Z = \sum_{S_i = \pm 1} e^{\beta J \sum_{i,\nu} S_i S_{i+\nu}} \tag{43}$$

systematically by starting with the state with all spins up and then accounting the contributions from states in which 1, 2, 3, *etc.* spins are flipped down. It is useful to factor out the result for all spins up and write

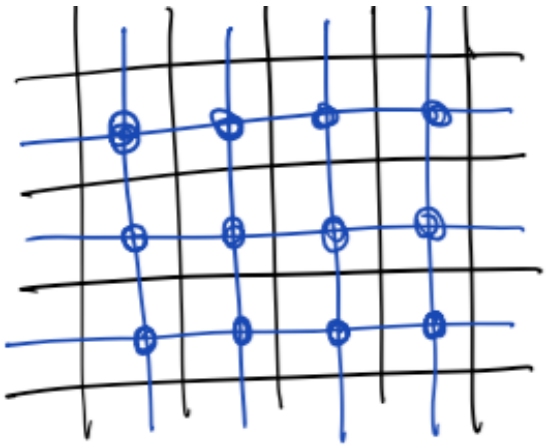
$$Z = e^{dJ\beta} \Big[1 + \cdots \Big] = e^{dJ\beta} \widetilde{Z} \ . \tag{44}$$

Consider the contribution to $\widetilde{Z}$ from states with 1 flipped spin



(45)

I will now introduce a rather formal way to describe this state that will nicely generalize to more complicated configurations. Given a lattice, we can define the *dual lattice* as the lattice of points at the centers of the simplices of the original lattice. For a 2-dimensional square lattice, the dual lattice is also a square lattice,

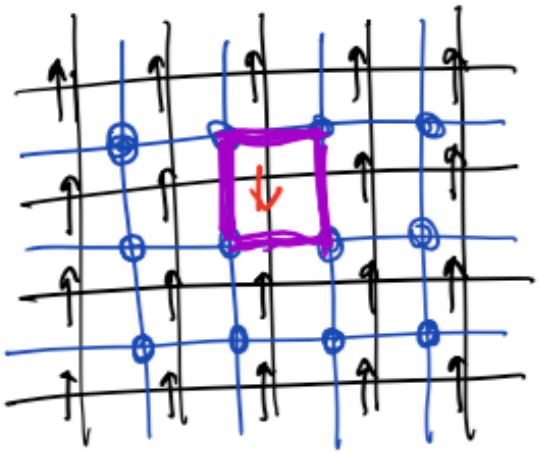


(46)

with the each bond of the dual lattice crossing a bond of the original lattice. Notice that this bond-to-bond correspondence is true only in 2 dimensions, so the analysis to follow will be correct only in 2 dimensions.

If we have a flipped spin on the original lattice, we can describe this situation as

having 4 mismatched bonds. These form a square on the dual lattice,



(47)

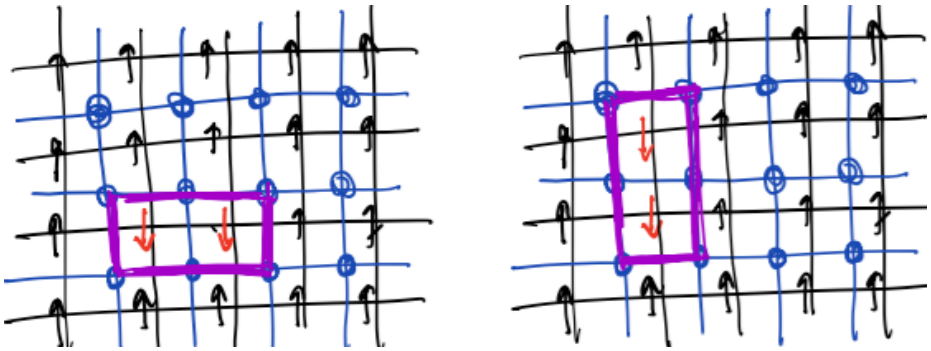
The contribution to $\widetilde{Z}$ from this configuration is

$$N(e^{-2\beta J})^4 \tag{48}$$

because each mismatched bond decreases $\mathcal{H}$ by $2J$ and the configuration can occur at any point on the lattice. It is convenient to write

$$w = e^{-2\beta J} \tag{49}$$

The next contributions are

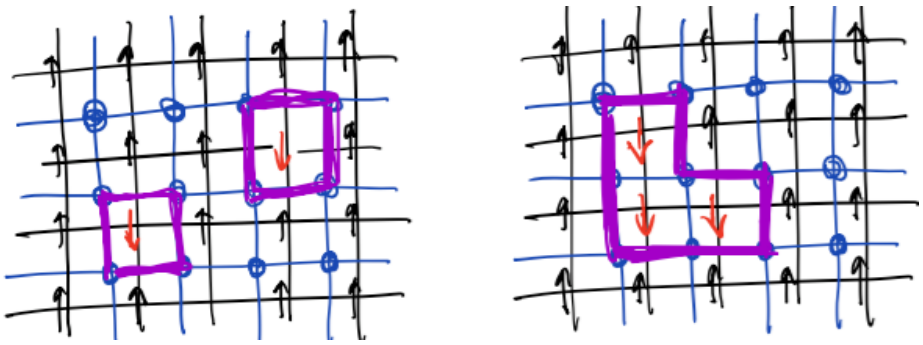


(50)

and these have the value

$$2Nw^6 \tag{51}$$

Typical configurations with 8 mismatched bonds are



(52)

Remarkably, the counting is exactly the same as for the calculation of the free energy at high temperatures! From our previous analysis, then

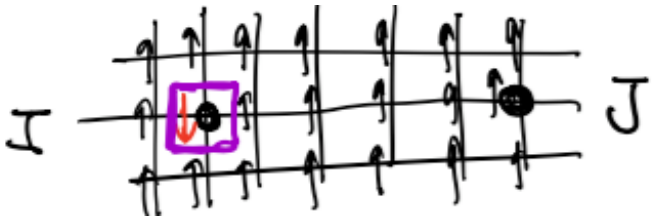
$$\begin{aligned}\widetilde{Z} &= 1 + Nw^4 + 2Nw^6 + (\frac{N^2}{2} + \frac{9}{2}N)w^8 + \cdots \ . \\ &= \exp\Big[N(w^4 + 2w^6 + \frac{9}{2}w^8 + \cdots)\Big] \ . \end{aligned} \tag{53}$$

Then

$$F = -2JN - \frac{N}{\beta} f(w) \ , \tag{54}$$

where $f(w)$ is the same function as defined in (22), but now a function of w rather than z. Since the Taylor series for $f(z)$ has a finite radius of convergence, this is actually an exact relation between the two expression for the free energy, valid for any temperature with $z = \tanh \beta J$, $w = \exp[-4\beta J]$.

We can compute the spin-spin correlation function using the same approach. The leading term in $\langle S_I S_j \rangle$ comes from

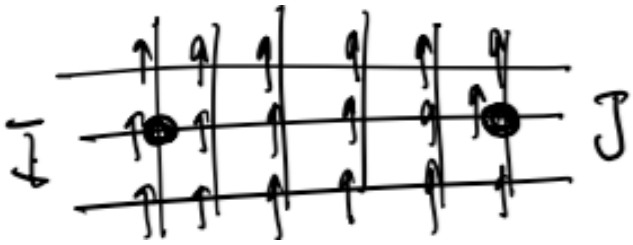


(55)

and gives

$$\langle S_I S_J \rangle = 1 \text{ for all } I, J \tag{56}$$

Adding the configurations of order w^4 in the numerator and denominator of (23)

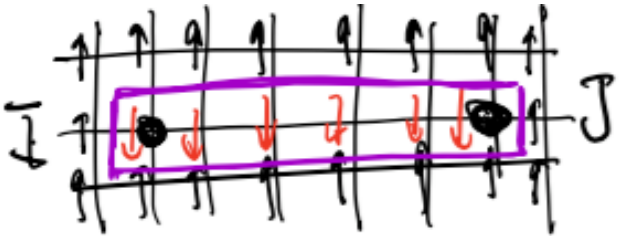


(57)

we find

$$\langle S_I S_J \rangle = 1 - 4w^4 + \cdots \ , \tag{58}$$

still indepenent of $|I-J|$ for $|I-J| > 1$. The first contribution to the connected correlation function is of very high order, w^{n+1}.



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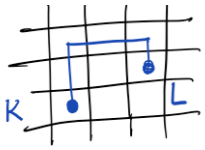
Since power series in w converge for small enough w, we conclude that

$$\langle S_I S_J \rangle \neq 0 \text{ as } |I-J| \to \infty \tag{60}$$

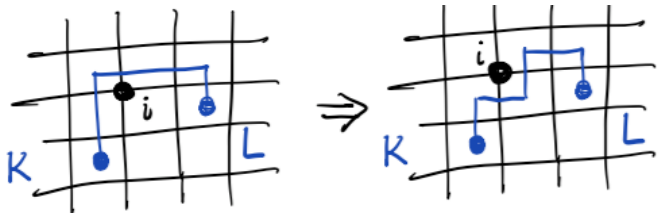
for sufficiently small but nonzero w. Thus, there is a low-temperature phase with nonzero magnetization. In 1936, Rudolf Peierls gave this argument and thus settled the question of whether the canonical ensemble could in principle give rise to a magnetized or broken symmetry state.

There is another correlation that is interesting to discuss in the region of small w; this has a behavior similar to that of the spin-spin correlation function at high temperatures. Let me define *disorder operators* Σ_K by the following prescription: Let K be a point on the dual lattice. Draw a path P on the dual lattice starting at K. Along this path, reverse the sign of the interaction on the cut bond of the original lattce from J to $-J$. The path could go off to infinity, or it could end at another site L of the dual lattice, which would then also carry a disorder operator Σ_L. We can represent the disorder correlation function $\langle \Sigma_K \Sigma_L \rangle$ by the diagram



(61)

It is important that this correlation function depends only on the positions K and L and not on the path P. We can change the path by a change of variables in the partition function sum. The change of variables $S_i \to -S_i$ loops the path over the site i.



(62)

The only place the line cannot move is at its endpoints K and L. Any path joining K to L gives an equivalent result. We then define

$$\langle \Sigma_K \Sigma_L \rangle = Z[P] \ / \ Z = \sum_{S_i} e^{-\beta \mathcal{H}[P]} \ / \ \sum_{S_i} e^{-\beta \mathcal{H}} \ , \tag{63}$$

where $\mathcal{H}[P]$ is the Ising model Hamiltonian with sign flips in the interactions along the path P.

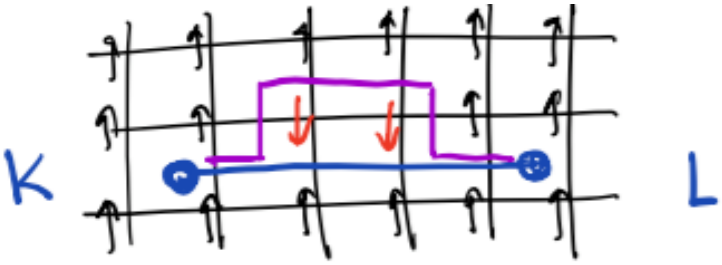
Lets now compute this in the w perturbation theory for $K = (0, 0)$ and $L = (n, 0)$ on the dual lattice. I have already explained how to compute the denominator in this expression, but now we need to compute the numerator. Choose P to be the straight line from K to L

(64)

In the leading configuration with all spins up, the n bonds crossing the line P are now mismatched, and so this configuration contributes w^n. At this level

$$\langle \Sigma_K \Sigma_L \rangle = w^n = \exp[-n \log \frac{1}{w}] \ . \tag{65}$$

At the next order, we would flip some spins above or below the line P. A typical configuration would be



(66)

These are directly analogous to (27) and give the contribution

$$2 \cdot \frac{n^2}{2}\, w^{n+2} \tag{67}$$

Going further, the contributions here are in 1-to-1 correspondence with the contributions that we found in the calculation of $\langle S_I S_J \rangle$. Thus,

$$\langle \Sigma_K \Sigma_L \rangle = \exp[-ng(w,n)] \ ,. \tag{68}$$

where $g(w,n)$ is exactly the function that appears in (34). In particular, in the phase of small w,

$$\langle \Sigma_K \Sigma_L \rangle \to 0 \text{ as } |I-J| \to \infty \ , \tag{69}$$

so the disorder operator has zero thermodynamic expectation value.

Thus, there is an exact duality between the high- and low-temperature phases of the 2-dimensional Ising model, reflected in the free energy and also in the correlation functions. This symmetry is called *Kramer-Wannier duality*, after Hendrik Kramers and Gregory Wannier, who announced it in a 1941 paper.

Kramers and Wannier pointed out that their duality could be used to find the exact critical temperature of the 2-dimensional Ising model. In mean field theory, we found that the free energy of the Ising model is an analytic function of T or β with only one singularity, at $T = T_c$. It is reasonable to assume that this statement is also true for the exact properties of the model. Then the high- and low-temperature expressions for the free energy must have their singularities at the same value of β. This is possible only if the functions $f(z(\beta))$ and $g(z(\beta))$ defined above have only one singularity, which must be located at the point $\beta = \beta_c$ at which

$$w(\beta) = z(\beta) \ . \tag{70}$$

This gives a simple equation for β_c

$$e^{-2\beta_c J} = \tanh \beta_c J = \frac{1 - e^{-2\beta_c J}}{1 + e^{-2\beta_c J}} \ . \tag{71}$$

Then

$$w_c = \frac{1 - w_c}{1 + w_c} \tag{72}$$

or

$$w_c^2 + 2w_c - 1 = 0 \ . \tag{73}$$

Choosing the positive solution of this equation

$$w_c = \sqrt{2} - 1 = (\sqrt{2} + 1)^{-1} \ . \tag{74}$$

Then

$$T_c = \frac{2J}{\log(\sqrt{2}+1)} = 2.26919\ J\ . \tag{75}$$

This value should be compared to the prediction $T_c = 4J$ from mean field theory. We now see that that value was only qualitatively correct. By magic, Kramers and Wannier found the exact location of the critical point for the 2-dimensional Ising model.

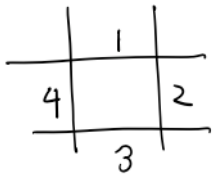
Here is some extra material for those who are curious about it:

Mathematically inclined students might want to see an exact transformation that relates the high- and low-temperature descriptions of the 2-dimensional Ising model. Here it is. The method of this derivation generalizes to a wide variety of other systems. It is an interesting exercise, left to the reader, to generalize this method to the 3-dimensional Ising model.

Begin from the form of the partition function (6)

$$Z = (\cosh \beta J)^{dN} \sum_{S_i=+1,-1} \prod_{i,\nu} (1 + z S_i S_{i+\nu}) \tag{76}$$

It is very tempting to turn the sum over the S_i into a sum over quantities $T_{i\nu} = S_i S_{i+\nu}$. The T_a are associated with bonds. They take the values ± 1. However, these quantities are not all independent variables. The product of the 4 T_a's around a square



(77)

satisfy the constraint

$$T_1 T_2 T_3 T_4 = 1\ . \tag{78}$$

We can acknowledge this constraint by introducing a delta function associated with each square

$$\delta_{1,\prod T} = \frac{1}{2} \sum_{U_K=\pm 1} \prod_a (\delta_{1,U_K} + \delta_{-1,U_K} T_a)\ . \tag{79}$$

This expression gives 1 when the product of the 4 T_a's equals 1 and 0 when the product equals zero.

Notice that the variable U_K is associated with a square and therefore sits at a point K of the dual lattice. The quantity in parentheses in (79) can be rewritten as

$$\delta_{1,U_K} + \delta_{-1,U_K} T_a = \delta_{1,T_a} + \delta_{-1,T_a} U_K \tag{80}$$

Let U_k, $U_{k+\nu}$ be the two U variables that sit on either side of the bond a. Summing over T_a,

$$\begin{aligned}
&\sum_{T_a}(\delta_{1,T_a}+\delta_{-1,T_a}U_K)(\delta_{1,T_a}+\delta_{-1,T_a}U_{K+\nu})(1+zT_a)\\
&\quad=(1+z)+(1-z)U_KU_{K+\nu}\\
&\quad=(1+z)\Big[1+\frac{(1-z)}{(1+z)}U_KU_{K+\nu}\Big]
\end{aligned}\tag{81}$$

For $z=\tanh\beta J$, we have

$$(1+z)=\frac{e^{\beta J}}{2\cosh\beta J}\qquad(1-z)=\frac{-e^{\beta J}}{2\cosh\beta J}\tag{82}$$

so

$$\frac{(1-z)}{(1+z)}=e^{-2\beta J}=w\tag{83}$$

Now we have rewritten the Ising model partition function as

$$Z=\Big(e^{\beta J}\Big)^{2N}\sum_{U_K=\pm1}\prod_{K,\nu}(1+wU_KU_{K+\nu})\ .\tag{84}$$

We have now converted the original Ising model partition function to an expression that is identical—up to the prefactor—with $z\to w$ and spin variables located on the dual lattice. This is the Kramers-Wannier duality.