Physics 212 - Problem Set #6
Solutions

1.) We need to compute the rate for spin flips and show that

$$\frac{\text{rate}(\downarrow \to \uparrow)}{\text{rate}(\uparrow \to \downarrow)} = \frac{e^{-\beta H(\uparrow)}}{e^{-\beta H(\downarrow)}}$$

(when all other spins of the lattice are held fixed). Assume $H(\uparrow) > H(\downarrow)$.

Then

$$\text{rate}(\uparrow \to \downarrow) = \text{probability } p \text{ of picking the site}$$

$$\text{rate}(\downarrow \to \uparrow) = p \cdot e^{-\beta \Delta E} \qquad \Delta E = H(\uparrow) - H(\downarrow)$$

so

$$\frac{\text{rate}(\downarrow \to \uparrow)}{\text{rate}(\uparrow \to \downarrow)} = \frac{p\, e^{-\beta\Delta E}}{p} = e^{-\beta[H(\uparrow) - H(\downarrow)]}$$

as required. The formula is symmetrical, so there is an identical argument for the case $H(\downarrow) > H(\uparrow)$.

Since the rate for flipping spins in one direction is as high as it can be, this procedure should reach equilibrium faster than the heat bath algorithm.

2.) My Java implementation of the Ising model with the Metropolis algorithm and periodic boundary conditions is given on the next page.

The following page shows snapshots at different temperatures.

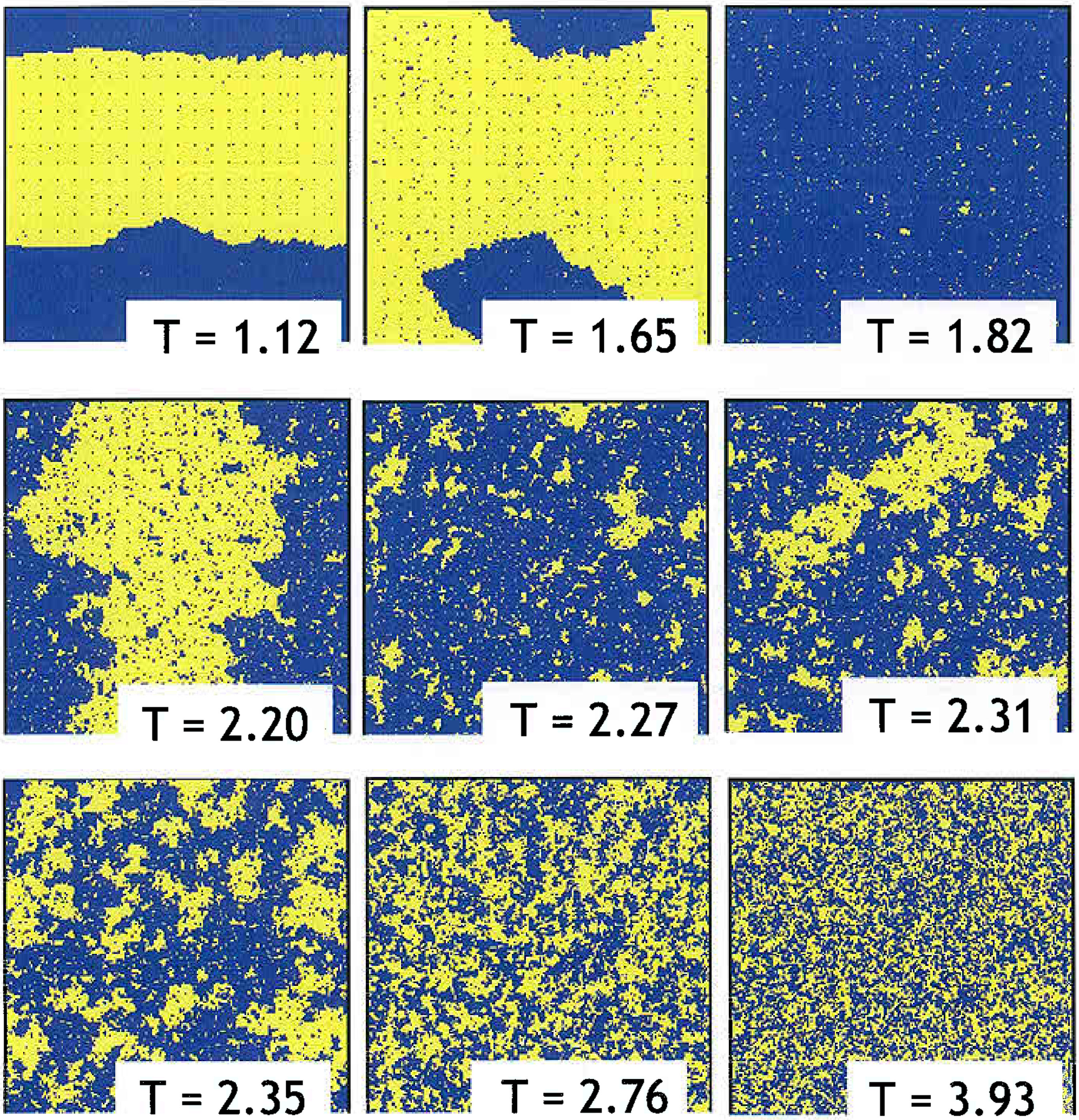
a) It is not so easy to judge the exact position of the phase transition by eye. From the snapshots, it seems to be at about $T = 2.3$ (between 2.31 and 2.35) for a 200×200 lattice. The Kramers-Wannier exact value for an infinite 2-d lattice is $T = 2.27$.

Below T_c, the pictures show phase coexistence. This is metastable, but it takes a very long time for one phase to take over.

b.) Imposing boundary conditions with all boundary spins up has very little effect for $T > T_c$. For $T < T_c$, this boundary condition stabilizes the phase with spin up and destabilizes the phase with spin down. Still, for $T > 2.0$, the spin down regions are stable for a long time.

```
import java.awt.*;
import java.awt.event.*;
import java.applet.Applet;

public class myIsing extends IsingGUI {

 /*     solve() carries out the Metropolis method for updating a
          2-dimensional lattice of spins.   The updating runs
           continuously until you push the Stop button of the
              applet.

         The spin values are given as the elements of an array of
            integers called

                  State[m][n]

         The entries of State should take the values 1 or -1.

         n and m range over the values  0, 1, 2, ...   Nx or Ny
           (If you call State[m][n] for m or n outside this
            range, bad things will happen.)

          Nx and Ny are set equal to 200; please do not change this.
             The program then simulates a 200 x 200 spin model.

         To implement fixed-spin boundary conditions, do Metropolis
              updates for   m, n = 1 .. Nx-1  only
         To implement periodic boundary conditions, do Metropolis
              updates for   m, n = 1 .. Nx-1  only
           and,
              when the 1 element is updated, copy it to the Nx element
              when the Nx-1 element is updated, copy it to the 0 element


          The temperature is available as a global variable called T.

          The method below is set up to simulate the thermodynamics of
              the Hamiltonian

                  H  =  -    sum_{nm}   S_{nm}/T

              corresponding to an external magnetic field  h = 1
               and no interaction.   You should change this Hamiltonian
                   appropriately to simulate the Ising model with J = 1 .

            The value of the energy/site will be reported in the applet
              if you implement the function   computeEnergy()  below

                                                                      */

    void solve(){
        /* intialization */
      int i,j;
      for (i = 1; i <= Nx; i++){
          for (j = 1; j <= Ny; j++){
              State[i][j] = 1;
          }
      }
        /*   sweep through the lattice and do Metropolis updating */
      int N = 0;
      while (true){
```

```
         N++;
             /* impose periodic boundary conditions */
        for (i = 2; i <= Nx-1; i++){
           State[i][0] = State[i][Ny-1];
           State[i][Ny] = State[i][1];
        }
        for (j = 2; j <= Ny-1; j++){
           State[0][j] = State[Nx-1][j];
            State[Nx][j] = State[1][j];
        }
                /* now sweep */
        for (i = 1; i < Nx; i++){
         for (j = 1; j < Ny; j++){
             int S = State[i][j];
             double Hnoflip = H(i,j,S);
             double Hflip = H(i,j,-S);
             if (Hflip < Hnoflip){
                 State[i][j] *= -1;
             }  else {
                 double r = ran();
                       /* gets a random number between 0 and 1 */
                 double ratio = Math.exp( - (Hflip - Hnoflip)/T);
                 if (r < ratio)  State[i][j] *= -1;
             }
         }
       }
         /* put a large number here to make the updating run slower */
       if (timetostop) break;
     if (N%8 == 0) refreshPicture();
     }
   }

   double H(int m, int n, int S){
       /*  value of H including only terms involving
                S = State[m][n]
            S is kept as an argument so we can flip it
            With more complicated Hamiltonian, the
                return value would depend on State[m+1][n]
                      and other neighboring spins       */
       return   - S * (State[m+1][n] + State[m-1][n] + State[m][n+1]
                                + State[m][n-1]);
   }

   double computeEnergy(){
       int i,j;
          /* should return  E/N   */
       double EE = 0.0;
       for (i = 1; i < Nx; i++){
         for (j = 1; j < Ny; j++){
              EE +=  H(i,j,State[i][j]);
         }
       }
       return EE/((Nx-1)*(Ny-1));
   }

}
```



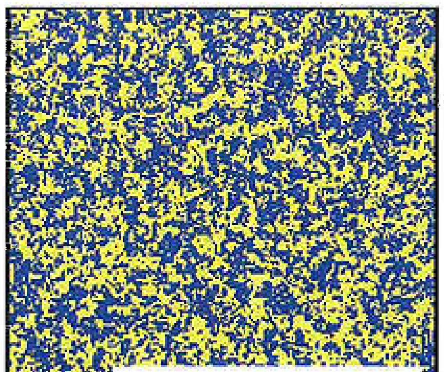
Ising Model Snapshots
200 x 200 lattice

c.) Looking at the snapshots, the correlation lengths are approximately

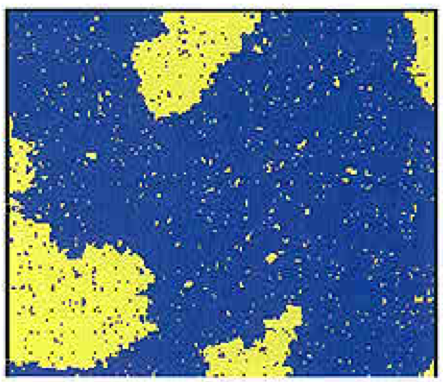
T	$\xi \cong$	
1.12	< 1 lattice spacing	
1.65	2-3	
1.82	3-4	↓ ξ increasing
2.20	6	
2.27	8-10	
2.31	10	
		— T_c
2.35	15	
2.76	4-5	↓ ξ decreasing
3.93	3	

d.) The antiperiodic boundary conditions have little effect above T_c. However, below T_c, the boundary conditions stabilize an equilibrium state with a domain wall.

See the snapshots on the next page.

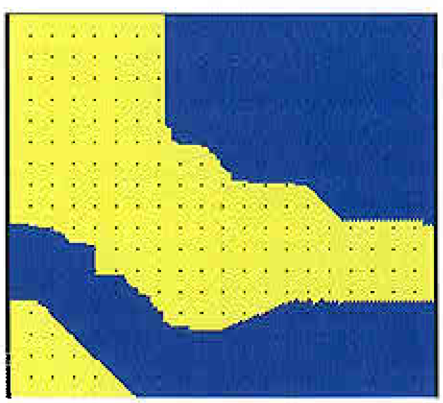


T = 3.24

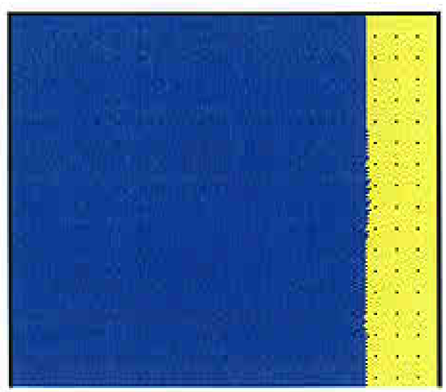


T = 1.93 - early

T = 1.93 - late



T = 0.58 - early



T = 0.58 - late

snapshots w. antiperiodic boundary conditions

3.) The partition function of the model is

$$Z = \prod_i \int ds_i \quad e^{\beta J \sum_{\langle ij \rangle} \vec{s}_i \vec{s}_j}$$

Parametrize $\vec{s}_i$ as $\qquad \vec{s}_i = (\cos\phi_i, \sin\phi_i)$

$$\vec{s}_i \cdot \vec{s}_j = \cos\phi_i \cos\phi_j + \sin\phi_i \sin\phi_j = \cos(\phi_i - \phi_j)$$

The spin s_0 sees the terms in Z

$$\int ds_0 \quad e^{\beta J \, \vec{s}_0 \cdot \sum_j \vec{s}_j} \qquad\qquad \int ds_0 = \int \frac{d\phi_0}{2\pi}$$

where the sum is over the $2d$ neighbors of the site 0.

For mean field theory, we replace

$$\vec{s}_j \to \langle \vec{s}_j \rangle \qquad (\text{independent of } j)$$

so

$$\langle \vec{s}_0 \rangle = \frac{\int ds_0 \quad e^{2d\beta J \, \vec{s}_0 \cdot \langle \vec{s} \rangle} \quad \vec{s}_0}{\int ds_0 \quad e^{2d\beta J \, \vec{s}_0 \cdot \langle \vec{s} \rangle}}$$

This is the mean field equation for $\langle \vec{s} \rangle$. The problem has rotational symmetry, so we can look for a solution where

$$\langle \vec{s} \rangle = (\langle s \rangle, 0)$$

Then $\qquad \vec{s}_0 \cdot \langle \vec{s} \rangle = \langle s \rangle \cdot \cos\phi_0$

The mean field equation becomes

$$\langle \vec{s}_0 \rangle = \frac{\int \frac{d\phi_0}{2\pi}\, e^{2d\beta J \langle s \rangle \cos\phi} \,(\cos\phi, \sin\phi)}{\int \frac{d\phi_0}{2\pi}\, e^{2d\beta J \langle s \rangle \cos\phi}}$$

The integral over $\sin\phi$ is zero by symmetry, so we find

$$\langle s \rangle = \frac{\int \frac{d\phi_0}{2\pi}\, e^{2d\beta J \langle s \rangle \cos\phi_0} \cdot \cos\phi_0}{\int \frac{d\phi_0}{2\pi}\, e^{2d\beta J \langle s \rangle \cos\phi_0}}$$

Using the identity in the problem set

$$\langle s \rangle = \frac{I_1(2d\beta J \langle s \rangle)}{I_0(2d\beta J \langle s \rangle)}$$

The $I_n(z)$ have the following behavior
(see, e.g. Abramowitz + Stegun section 9.6)

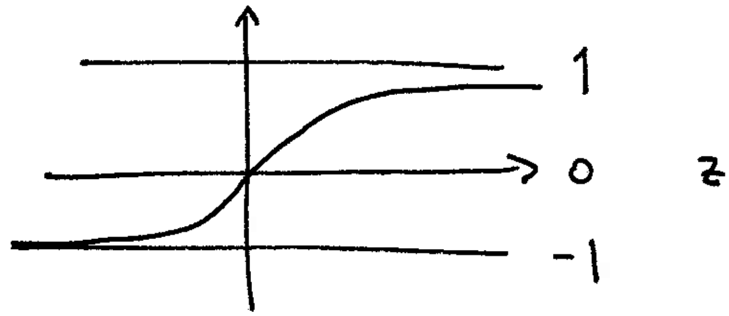
$$z \to 0 \qquad I_0(z) \sim 1 + O(z^2) \qquad I_1(z) \sim \tfrac{1}{2} z + O(z^3)$$

$$z \to \infty \qquad I_n(z) \sim \frac{e^z}{\sqrt{2\pi z}} \left(1 - \frac{4n^2 - 1}{8z} + \cdots \right)$$

so

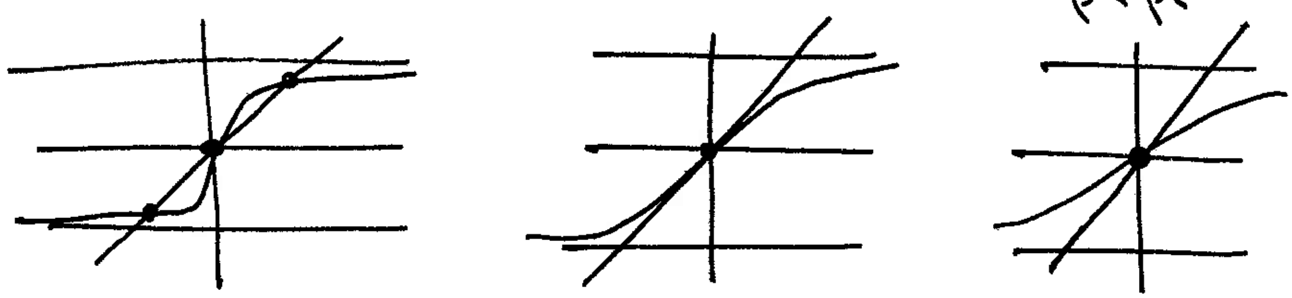
$$\frac{I_1(z)}{I_0(z)} \longrightarrow \begin{cases} \tfrac{1}{2} z + O(z^3) & \text{as } z \to 0 \\ 1 - O\left(\tfrac{1}{z}\right) & \text{as } z \to \infty \end{cases}$$

so $\dfrac{I_1(z)}{I_0(z)}$ has the qualitative form



and so the graphical solution of the mean-field equation works just as in the Ising case:

$T < T_c$, $\beta > \beta_c$ — $T = T_c$ — $T > T_c$, $\beta < \beta_c$



solution w. $\langle s \rangle \neq 0$ — $\langle s \rangle = 0$

$\downarrow$

the boundary case is that in which

$$\frac{I_1(2d\beta J\langle s\rangle)}{I_0(2d\beta J\langle s\rangle)}$$

has slope $= 1$ at $\langle s \rangle = 0$

$$\text{slope} = \tfrac{1}{2}\cdot 2d\beta J = d\beta J \quad \text{so} \quad \beta_c = \frac{1}{dJ}$$

$$T_c = dJ$$

To find the behavior of $\langle s \rangle$ for T just below T_c, we need one more term in the expansion of $I_n(z)$:

$$I_0(z) = 1 + \frac{1}{4} z^2 + \mathcal{O}(z^4)$$

$$I_1(z) = \frac{1}{2} z \left(1 + \frac{1}{8} z^2 + \mathcal{O}(z^4) \right)$$

so

$$\langle s \rangle = \frac{I_1(z)}{I_0(z)} \bigg|_{z = 2d\beta J \langle s \rangle} = \frac{1}{2} z \left(1 - \frac{1}{8} z^2 + \cdots \right) \bigg|_{z = 2d\beta J \langle s \rangle}$$

$$\langle s \rangle = d\beta J \langle s \rangle \left(1 - \frac{1}{2} (d\beta J \langle s \rangle)^2 + \cdots \right)$$

$$(d\beta J - \underbrace{d\beta_c J}_{=1}) \langle s \rangle \simeq \frac{1}{2} (d\beta J)^3 \langle s \rangle^3$$

$$2 \frac{(\beta - \beta_c)}{\beta^3 (dJ)^2} = \langle s \rangle^2$$

$$2 \left(\frac{T}{dJ} \right)^2 \left(1 - \frac{T}{T_c} \right) = \langle s \rangle^2$$

for $T \approx T_c$ $\quad \frac{T}{dJ} \approx 1$

$$\langle s \rangle = \sqrt{2} \left(1 - \frac{T}{T_c} \right)^{1/2}$$

$$M = \sqrt{2} N \left(1 - \frac{T}{T_c} \right)^{1/2}$$

4.) Now let $\vec{s}_i$ be an N-component unit vector.
Following the logic of the previous problem, the mean field equation is

$$\langle \vec{s} \rangle = \frac{\int d\vec{s}_0 \; e^{2dJ\beta \, \vec{s}_0 \cdot \langle \vec{s} \rangle} \; \vec{s}_0}{\int d\vec{s}_0 \; e^{2dJ\beta \, \vec{s}_0 \cdot \langle \vec{s} \rangle}}$$

Again, by symmetry, we can look for solutions where

$$\langle \vec{s} \rangle = \langle s \rangle \cdot \hat{1} = (\langle s \rangle, 0 \, 0 \cdots 0)$$

Then

$$\langle s \rangle \cdot \hat{1} = \frac{\int d\vec{s}_0 \; e^{2dJ\beta \langle s \rangle \, \vec{s}_0 \cdot \hat{1}} \; \vec{s}_0}{\int d\vec{s}_0 \; e^{2dJ\beta \langle s \rangle \, \vec{s}_0 \cdot \hat{1}}}$$

The numerator will be in the direction $\hat{1}$, so we will get an equation of the form

$$\langle s \rangle = f(2dJ\beta \langle s \rangle)$$

The condition for T_c is that the slope of $f(2dJ\beta\langle s \rangle)$ should be $\underline{1}$ at $\beta = \beta_c$, $T = T_c$. To determine the magnetization for $T < T_c$ we will need to expand

$f(z)$ to two terms.

So write

$$\hat{1}\ f(z) = \frac{\int d\vec{s}_0\ e^{z\,\vec{s}_0\cdot\hat{1}}\ \vec{s}_0}{\int d\vec{s}_0\ e^{z\vec{s}_0\cdot\hat{1}}}$$

We need the expansion of $f(z)$ in powers of z. Work on the denominator first.

$$D = \int d\vec{s}_0\ e^{z\vec{s}_0\cdot\hat{1}} = \int d\vec{s}_0\ \Big\{1 + z\,\vec{s}_0\cdot\hat{1} + \tfrac{1}{2}z^2(\vec{s}_0\cdot\hat{1})^2 + \tfrac{1}{3!}z^3(\vec{s}_0\cdot\hat{1})^3 + \tfrac{1}{4!}z^4(\vec{s}_0\cdot\hat{1})^4 + \dots\Big\}$$

Define the integral over unit vectors so that

$$\int d\vec{s}_0 = 1$$

By symmetry

$$\int d\vec{s}_0\ s_0^i = 0 \qquad \int d\vec{s}_0\ s_0^i s_0^j s_0^k = 0$$

since the integral should be unchanged if we let $s_0^i \to -s_0^i$.

$$\int d\vec{s}_0\ s_0^i s_0^j \text{ must be proportional to } \delta^{ij}$$

To evaluate the constant of proportionality, use $|\vec{s}_0|^2 = 1$

Write $\int d\vec{s}_0\ s_0^i s_0^j = A\ \delta^{ij}$

set $i=j$ and sum

$$1 = \int d\vec{s}_0 \sum_{i=1}^{N} s_0^i s_0^i = A \cdot N \quad \text{so} \quad A = \frac{1}{N}$$

then

$$D = 1 + \frac{1}{2N} z^2 + \mathcal{O}(z^4)$$

For the numerator, we will also need the formula for integrating over 4 so's. This is obtained in a similar way:

$$\int d\vec{s}_0 \; s_0^i s_0^j s_0^k s_0^l = B\left[\delta^{ij}\delta^{kl} + \delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}\right]$$

$$1 = \int d\vec{s}_0 \; \vec{s}_0\cdot\vec{s}_0 \; \vec{s}_0\cdot\vec{s}_0 = (\text{above w. } i=j \;\; k=l)$$

$$= B\left[N\cdot N + N + N\right]$$

so $$B = \frac{1}{N(N+2)}$$

Now, the numerator of the formula on p.13 is

$$\int d\vec{s}_0 \; \vec{s}_0 \; e^{z\vec{s}_0\cdot\hat{1}}$$

$$= \int d\vec{s}_0 \; \vec{s}_0 \left(1 + z\vec{s}_0\cdot\hat{1} + \tfrac{1}{2}(z\vec{s}_0\cdot\hat{1})^2 + \tfrac{1}{3!}(z\vec{s}_0\cdot\hat{1})^3 + \cdots\right)$$

$$= 0 + z\cdot\frac{1}{N}\cdot\hat{1} + 0 + \frac{z^3}{6}\,\underbrace{\frac{1}{N(N+2)}\cdot 3}_{\text{above w. } i=j=k=l=1}\;\hat{1} + \cdots$$

$$\langle s\rangle = \frac{\frac{2d\beta J}{N}\langle s\rangle + \frac{(2d\beta J\langle s\rangle)^3}{2N(N+2)} + \cdots}{1 + \frac{1}{2N}(2d\beta J\langle s\rangle)^2}$$

$$\langle s\rangle = \frac{2d\beta J}{N}\langle s\rangle \left(1 - \frac{1}{2}\left(\frac{1}{N} - \frac{1}{(N+2)}\right)(2d\beta J\langle s\rangle)^2 + \cdots\right)$$

$$\langle s\rangle = \frac{2d\beta J}{N}\langle s\rangle \left(1 - \frac{1}{N(N+2)}(2d\beta J\langle s\rangle)^2 + \cdots\right)$$

The slope at $\langle s\rangle = 0$ is given by $\frac{2d\beta J}{N}$

so $\frac{2d\beta_c J}{N} = 1$ or $T_c = \frac{2dJ}{N}$

For $T \lesssim T_c$

$$\left(\left(\frac{\beta}{\beta_c}\right) - 1\right)\langle s\rangle \cong \frac{N}{N+2}\langle s\rangle^3$$

so $\langle s\rangle \cong \left[\frac{N+2}{N}\left(1 - \frac{T}{T_c}\right)\right]^{1/2}$

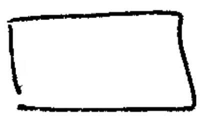
setting $N=2$, we recover the results of problem #3.

5.) The high-temperature expansion follows from the formula for the Ising model partition function:

$$Z = (\cosh \beta J)^{2N} \sum_{\{s_i\}} \prod_{\langle ij \rangle} (1 + s_i s_j \tanh \beta J)$$

$$= 2^N (\cosh \beta J)^{2N} \left(1 + (\text{diagrams})\right)$$

where (diagrams) are terms with $z = \tanh \beta J$

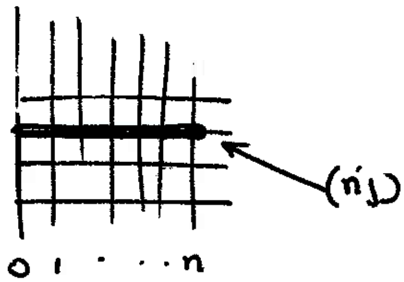
$[1 + (\text{diagrams})] =$  $+$ 

$$1 \quad + \quad N z^4 \quad + \cdots$$

Now compute

$$\langle s_{nj} \rangle = \frac{\sum_{\{s_i\}} \prod_{\langle ij \rangle} (1 + s_i s_j z) \cdot s_{nj}}{\sum_{\{s_i\}} \prod_{\langle ij \rangle} (1 + s_i s_j z)}$$

To get a nonzero result in the numerator, we need diagrams in which an <u>odd</u> number of z bonds end on the site (nj). Since we do not sum over boundary spins, an odd number of z bonds can also end on sites on the boundary. The leading term contributes to the numerator is then



$$= \quad z^n$$

To leading order

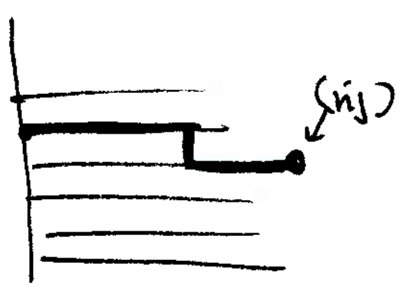
$$\langle s_{nj} \rangle = \frac{z^n}{1+\cdots} = \exp[-n/\xi]$$

where $$\xi = \frac{1}{\log \frac{1}{z}} = \frac{1}{\log(\coth \beta J)}$$

as $\beta \to 0$ $$\coth \beta J \sim \frac{1}{\beta J}$$

so $$\xi \sim \frac{1}{-\log(\beta J)} \to 0 \quad \text{as} \quad \beta \to 0$$

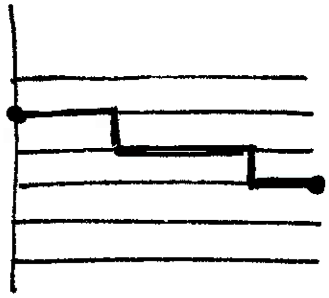
b.) The next term in the expansion of the numerator are



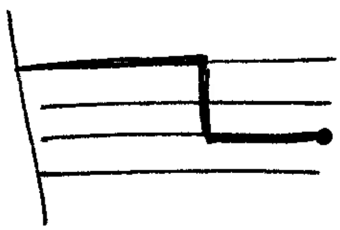
$$= 2n\, z^{n+1}$$

$\uparrow$ up or down

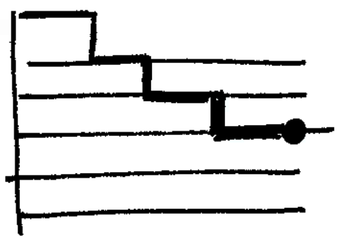
(Note that we do not have a factor $(1+s_is_jz)$ for bonds on the boundary.)



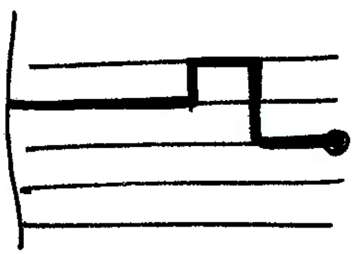
$$4\,\frac{n(n-1)}{2}\,z^{n+2}$$



$$2n\;z^{n+2}$$



$$8\,\frac{n(n-1)(n-2)}{3!}\,z^{n+3}$$

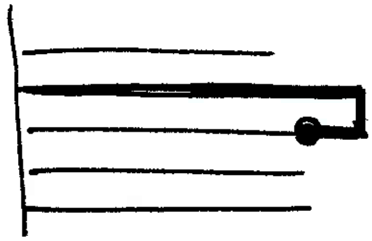


$$4\,\frac{n(n-1)}{2}\,z^{n+3}$$

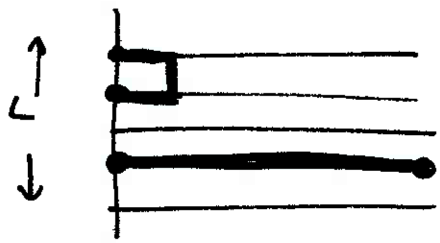
(large step to right)

$$4\,\frac{n(n-1)}{2}\,z^{n+3}$$

(large step to left)

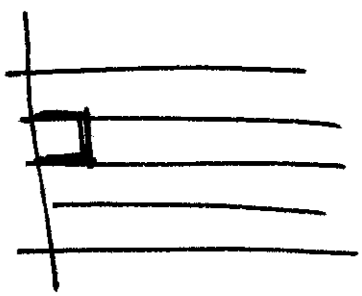


$2 \cdot z^{n+3}$



$(T_1 - 2)\, z^{n+3}$

The denominator gets a contribution at order z^3



$= \quad T_1 \cdot z^3$

so

$$\langle S_{nj} \rangle = z^n \Big(1 + 2nz + \frac{4n(n-1)}{2} z^2 + 2n\, z^2 + \frac{8n(n-1)(n-2)}{6} z^3 + 4n(n-1)\, z^3 + 2z^3 + (T_1 - 2)\, z^3 + \cdots \Big)$$

$$\div \left(1 + T_1 z^3 + \cdots \right)$$

$$\langle s_{nj} \rangle = z^n \Big(1 + 2nz + \frac{4n^2 z^2}{2}$$

$$+ \frac{8n^3}{3!} z^3 + z^3 \Big[-\frac{3 \cdot 8}{6} n^2 + \frac{2 \cdot 8}{6} n$$

$$+ 4n^2 - 4n + 2 - 2 \Big]$$

$$+ \cdots \Big)$$

$$= z^n \Big(1 + 2nz + \frac{1}{2}(2nz)^2 + \frac{1}{3!}(2nz)^3 + \cdots$$

$$+ z^3 \Big[-4n^2 + \frac{8}{3} n + 4n^2 - 4n \Big]$$

$$+ \cdots \Big)$$

$$= z^n \exp \Big[2nz - \frac{4}{3} n z^3 + \cdots \Big]$$

$$= \exp \Big[-n \Big(\log \frac{1}{z} - 2z + \frac{4}{3} z^3 + \cdots \Big) \Big]$$

so $$\xi^{-1} = \log \frac{1}{z} - 2z + \frac{4}{3} z^3 + \cdots$$

with $z = \tanh \beta J$