#1

P-1

Problem #1

Physics 114: Week 9

by David Lazore '16

G& T Problem 5.2

a)

The partition function of a lattice of Magnetic dipoles with interaction energy E_0

$$Z = \sum_s e^{-\beta(E_{s,0} - MB_s)}$$

Taking the first and second derivatives,

$$\frac{\partial Z}{\partial B} = \sum_s \beta M e^{-\beta(E_{s,0} - MB_s)}$$

$$\frac{\partial^2 Z}{\partial B^2} = \sum_s \beta^2 M^2 e^{-\beta(E_{s,0} - MB_s)}$$

We can use these to write $\overline{M}$ and $\overline{M^2}$ in terms of these derivatives:

$$\overline{M} = \frac{1}{Z}\sum_s M e^{-\beta(E_{s,0} - MB_s)} = \frac{1}{\beta Z}\frac{\partial Z}{\partial B} = \frac{1}{\beta}\frac{\partial \ln Z}{\partial B}$$

$$\overline{M^2} = \frac{1}{Z}\sum_s M^2 e^{-\beta(E_{s,0} - MB_s)} = \frac{1}{\beta^2 Z}\frac{\partial^2 Z}{\partial B^2}$$

Now taking the identity

$$\chi = \left(\frac{\partial \overline{M}}{\partial B}\right)_T$$

We can write

$$\chi = \frac{\partial}{\partial B}\left[\frac{1}{\beta}\frac{\partial \ln Z}{\partial B}\right]_T = \frac{1}{\beta}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial B^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial B}\right)^2\right] = \frac{1}{\beta}\left[\beta^2\overline{M^2} - \beta^2\overline{M}^2\right]$$

$$= \frac{1}{kT}\left[\overline{M^2} - \overline{M}^2\right]$$

b)

G& T also tell us that $\chi = N\mu^2\beta sech^2(\beta\mu B)$

Combining this with our result from part a), we get that

$$\overline{M^2} - \overline{M}^2 = N\mu^2 sech^2(\beta\mu B)$$

c)

Setting $\mu = 1$,

$$\begin{aligned}
\overline{M^2} - \overline{M}^2 &= N sech^2(\beta B) \\
&= N\left(\frac{2}{e^{\beta B} + e^{-\beta B}}\right)^2 \\
&= 4N\frac{1}{(e^{\beta B} + e^{-\beta B})^2} \\
&= 4N\frac{e^{\beta B}e^{-\beta B}}{(e^{\beta B} + e^{-\beta B})^2} \\
&= 4N\left(\frac{e^{\beta B}}{e^{\beta B} + e^{-\beta B}}\right)\left(\frac{e^{-\beta B}}{e^{\beta B} + e^{-\beta B}}\right) \\
&= 4Npq \quad \text{where} \\
&p = \frac{e^{\beta B}}{Z}, \quad q = 1 - p = \frac{e^{-\beta B}}{Z}
\end{aligned} \tag{1}$$

Which is the same variance as a binomial distribution!

and $Z = e^{\beta B} + e^{-\beta B}$

Problem
#2

G+T 5.6

Thermo of 1D Ising model:

(a) To find: Ground state of Ising Chain...

If $H=0$, There are two ...↑↑↑↑... or ...↓↓↓↓...

However, if $H=0^+$, just ...↑↑↑↑↑...

(b) We could use G+T Eq (5.47) but we'll do That below. For now, observe That

$$S = k\ln\Omega = \begin{cases} k\ln 1 = 0 & T\to 0,\ H=0^+ \\ k\ln 2^N = Nk\ln 2 & T\to\infty \end{cases}$$

(c) Now, start with

$$F = -NkT\ln(2\cosh\beta J) \quad (5.48)$$

to find/confirm S, $\bar{E}$ & C equations....

$$S = -\left(\frac{\partial F}{\partial T}\right)_{B,N} \text{ so}$$

$$S = +Nk\ln(2\cosh\beta J) - NkT\frac{\sinh\beta J}{\cosh\beta J}\underbrace{\frac{J}{kT^2}}_{=\frac{\partial\beta}{\partial T}}$$

so
$$S = Nk\ln(2\cosh\beta J) - Nk\left(\frac{J}{kT}\right)\tanh\beta J$$

Does this equal

$$S \stackrel{?}{=} Nk\left[\ln\left(e^{2\beta J}+1\right) - \frac{2\beta J}{1+e^{-2\beta J}}\right] \quad (5.49)$$

Yes... algebraically equivalent.

Now $E = F + TS$

$$= -NkT\ln(2\cosh\beta J)$$
$$+ NkT\left[\ln(2\cosh\beta J) - \left(\frac{J}{kT}\right)\tanh\beta J\right]$$

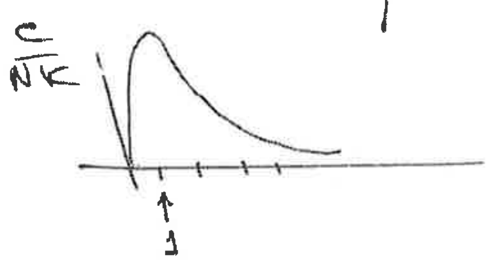
$$E = -NJ\tanh\beta J \quad ✓ \qquad (5.50)$$

$$C = \frac{\partial E}{\partial T} = -\frac{1}{kT^2}\frac{\partial E}{\partial \beta}$$

$$= \frac{-NJ}{kT^2} J\,\mathrm{sech}^2\beta J$$

$$C = Nk(\beta J)^2\,\mathrm{sech}^2\beta J \quad ✓ \quad (5.51)$$

(d) Why



$\frac{kT}{J} \equiv x$

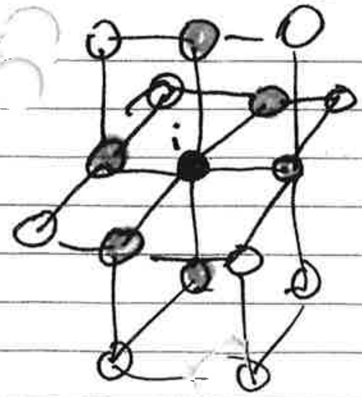
$$C = Nk\left(\frac{J}{kT}\right)^2 \mathrm{sech}^2\frac{J}{kT}$$

$$= \frac{Nk}{x^2}\,\mathrm{sech}^2\frac{1}{x} \qquad x = \frac{kT}{J}$$

Around 0, $C \to 0$ (Third law)
States are finite ... only 2^N of them &
as $T\to\infty$ $E \to 0$ spins random $\Rightarrow C \to 0$. | These limits (or >1 peak!)

Around $kT = J$, we begin to excite out of gs so $C > 0$. Thus must $\exists$ a peak btwn

Amy Intro to #3, G+T 5.18



Mean field Theory

Each spin has q neighbors (Schroeder uses "n" ... some other books use "z")

Spin i feels effective field

$$H_{eff} = J \sum_{j=1}^{q} s_j + H$$

Let's take mean effective field

$$\bar{H}_{eff} = J q \bar{s}_j + H$$

assume all s_j are same

$$= J q m + H$$

prettier notation... $\bar{s}_j = m$

Thence $$Z_1 = \sum_{s_i = \pm 1} e^{+\beta s_i \bar{H}_{eff}};$$

$$Z_1 = 2\cosh[\beta(Jqm + H)]$$

$$f = -kT \ln Z_1;$$

$$f = -kT \ln\left(2\cosh[\beta(Jqm+H)]\right) \quad (1)$$

Thus $$-\frac{\partial f}{\partial H} = \tanh[\beta(Jqm+H)] = m \quad (2)$$

Eq (2) must be solved self consistently ... it is subject of Prob 3 this week (G+T 5.18)

That problem even goes further ... Lets us "improve" on mean field as described in (G+T 5.17)

Improvement: $s_i = m + \Delta_i$; $s_j = m + \Delta_j$ (↑ smallish)

$$\Rightarrow E = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i$$

$$= +J \sum_{\langle ij \rangle} m^2 - J m \sum_{\langle ij \rangle} (s_i + s_j) - H \sum_i s_i$$

To 1st order in Δ_i

$$E = +\frac{JqNm^2}{2} - (Jqm + H) \sum_{i=1}^{N} s_i$$

$$\Rightarrow Z(T,V,N) = e^{-\beta \frac{JqNm^2}{2}} \left[2\cosh[\beta(Jqm+H)] \right]^N$$

Eq (3) is improved

$$\Rightarrow \boxed{f = \frac{1}{2} Jqm^2 - kT \ln \left\{ 2\cosh\left[\beta(Jqm+H)\right] \right\}} \quad (3)$$

($\frac{1}{2} Jqm^2$:) add'l term not present in Eq. (1)

Further fruits of Mean Field Theory:

⇨ Expand Eq (2) about $m = 0$
To see there {are 3 real roots form $T < T_c$ / is 1 real root when $T > T_c$}

p. 272 of G&T do this ... $m = 0, \pm\sqrt{3}\frac{T}{T_c}\left(\frac{T_c - T}{T_c}\right)^{1/2}$

∴ Critical exponent $\beta = 1/2$

⇒ Take derivative w.r.t. H of Eq. (2) to get

$$\chi = \lim_{H \to 0} \frac{\partial m}{\partial H}$$

and expand χ around $m = 0$.

p. 272 of G+T does this...
they find

$$\chi = \begin{cases} \dfrac{1}{k(T-T_c)} & T > T_c \\ \dfrac{1}{2k(T_c-T)} & T < T_c \end{cases}$$

Thus $\chi \sim |T_c - T|^{-1}$

So we have

<u>Critical exponent</u> $\gamma = 1$

3 Prob G & T 5.18 MFOy

Want to understand sol'ns of (5.108)

$$m = -\frac{df}{dH} = \tanh\left(\frac{Jqm + H}{kT}\right)$$

To do so, begin with (5.126) & expand around $m=0$, holding $H=0$

(a) $f(T,H) = \frac{1}{2}Jqm^2 - kT\ln\left[2\cosh\left(\frac{qJm}{kT}\right)\right]$

where m is s.t. f is minimized.

Thus $f(T) = \frac{1}{2}Jqm^2 - kT\ln 2 - kT\ln\left[\cosh\left(\frac{qJm}{kT}\right)\right]$

Now, want $m \approx 0$ *

$$f(T) \approx \frac{1}{2}Jqm^2 - kT\ln 2 - kT\ln\left[1 + \frac{1}{2!}\left(\frac{qJm}{kT}\right)^2 + \frac{1}{4!}\left(\frac{qJm}{kT}\right)^4\right]$$

(expansion of cosh)

Now, need to make self-consistent expansion of

$$\ln[1+\epsilon] = \epsilon - \frac{\epsilon^2}{2} + \frac{\epsilon^3}{3}$$

Thus,

$$f(T) \approx \frac{1}{2}Jqm^2 - kT\ln 2 - kT\left[\frac{1}{2}\left(\frac{qJm}{kT}\right)^2 - \frac{1}{8}\left(\frac{qJm}{kT}\right)^4 + \frac{1}{24}\left(\frac{qJm}{kT}\right)^4 + \cdots\right]$$

so up to ord (m^4)

$$f(T) \approx -kT\ln 2 + \frac{1}{2}Jqm^2\left(1 - \frac{Jq}{kT}\right) + \frac{m^4}{12}kT\left(\frac{Jq}{kT}\right)^4 + \cdots$$

* Note: Though we are just examining region around $m=0$, can look to larger m. Must bear in mind that physically, $|m| \leq 1$. See pages beyond for some plots.

This is of the form

$$f(m) = a + b\left(1 - \frac{T_c}{T}\right)m^2 + c\,m^4$$

where $a = -kT\ln 2$

$$b = \frac{1}{2}Jq = \frac{1}{2}kT_c$$

where $T_c = \frac{Jq}{k}$ $\quad c = \frac{1}{12}k\frac{T_c^4}{T^3}$

(b) For $H \neq 0$, argue that $f(T,H)$ has a two-variable Taylor expansion...

$$f(T,H) = f(T,0) + \left(\frac{\partial f}{\partial H}\right)_T H + \cdots$$

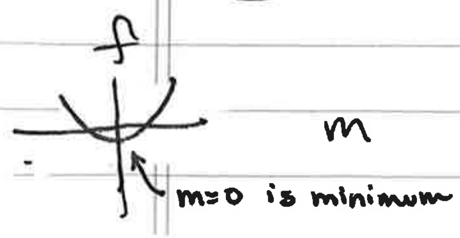
Since $\left(\frac{\partial f}{\partial H}\right)_T = -m$, it follows that $f(T,H) = f(T,0) - mH$

Alternative: Using $T_c = qJ/k$ you can expand $f(T,H)$ from first expression on p. 3-1 and you will get that $f(T,H) = f(T,0) - mH$ to 1st order in m & H.

(c) Spose $T > T_c$. Then

$$f = a + b\left(1 - \frac{T_c}{T}\right)m^2 + cm^4$$

(This coeff > 0)



For $T < T_c$:

$$f = a + b\left(1 - \frac{T_c}{T}\right)m^2 + cm^4$$

This coeff < 0

So nonzero m has smaller free energy than $f(m=0)$

Please see Mathematica plots ...

For these see next page ... 4

(d) $T > T_c$ $H = 0$

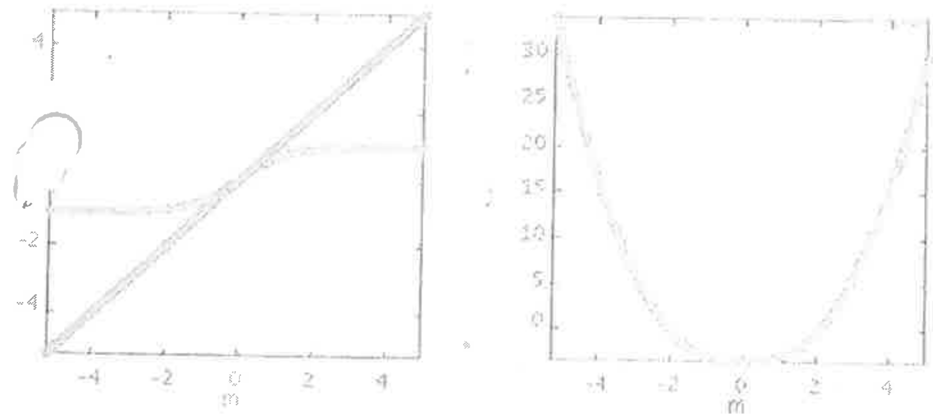
(e) $T = 1$ $H = 0$

(e′) $T = 3$ $H = 0$

(f) $T = 1$ $H = 0.5$

Note: If flipped H field quickly to $H = -0.5$ for example, local min at $m \approx 1$ becomes the global min, but it will take some time for system to "catch on" and switch to state reflecting the new global minimum

3-4



File Edit Display Help

Input Parameters

Name	Value
J	5.0
q	4.0
H	0.0

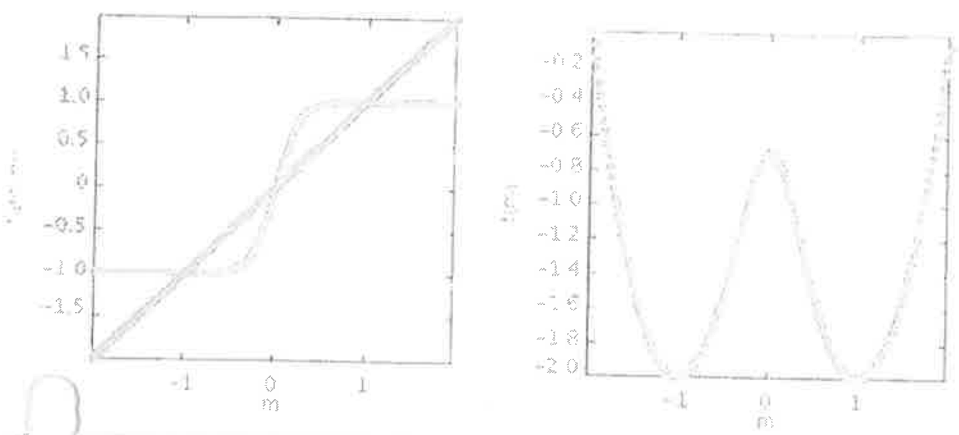
(d)

Calculate Reset

Messages

Root = 0.000

File Edit Display Tools Views Help File Edit Display Tools Views Help File Edit Display Help



Input Parameters

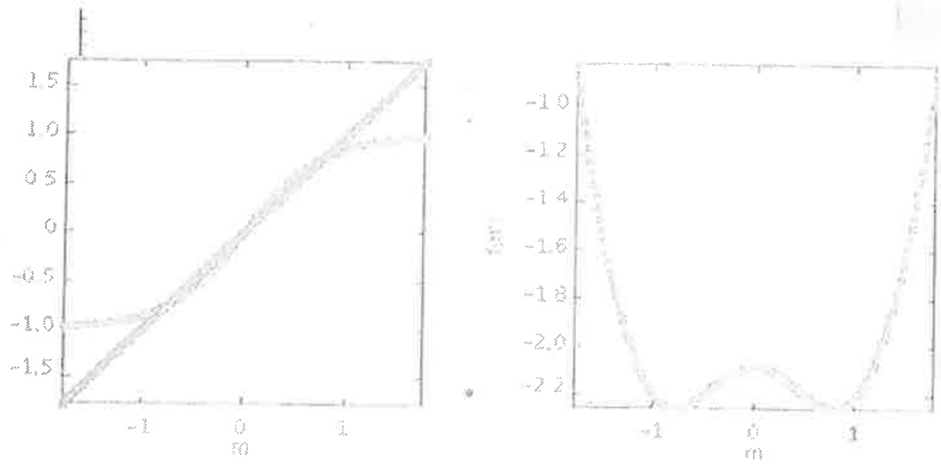
Name	Value
J	1.0
q	4.0
H	0.0

(e)

Calculate Reset

Messages

Root 0 = 0.999
Root 1 = 0.000
Root 2 = 0.999



Input Parameters

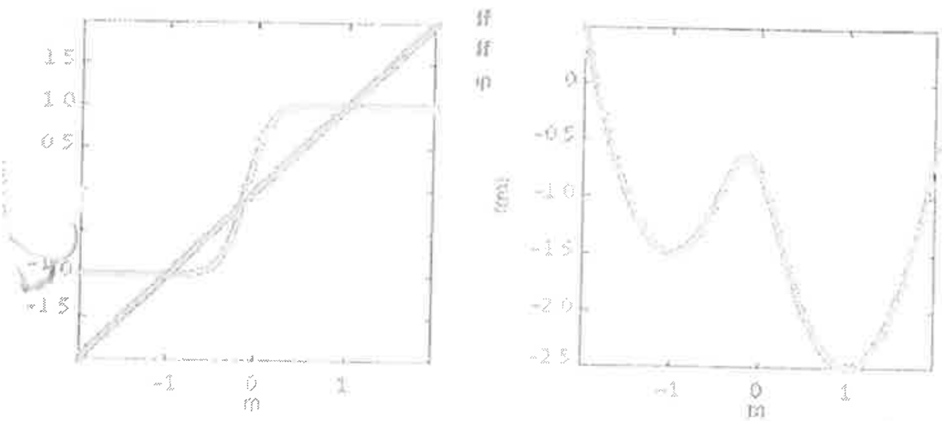
Name	Value
J	
q	4.0
H	0.0

(e′)

Calculate Reset

Messages

Root 0 = 0.776
Root 1 = -0.000
Root 2 = 0.776



Input Parameters

Name	Value
J	1.0
q	4.0
H	

Calculate Reset (J

Messages

Root 0 = 0.998
Root 1 = 0.167
Root 2 = 1

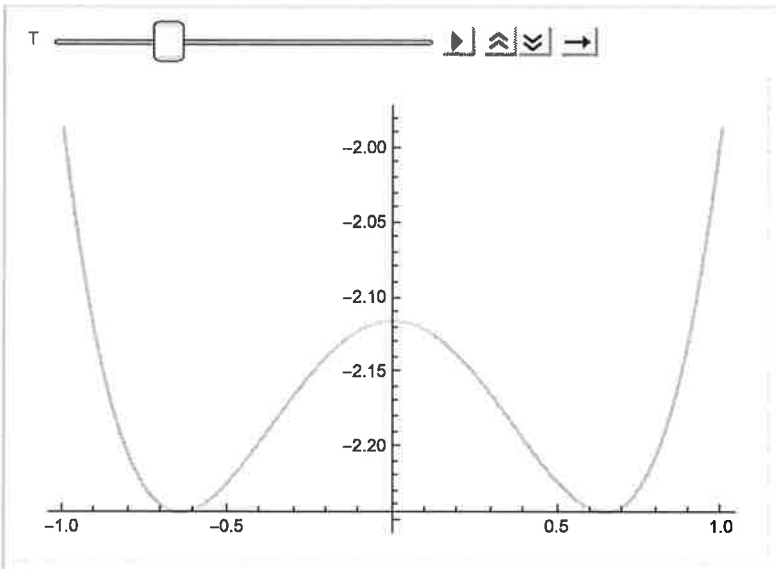
3-5

```
Tc = 4; TcOverT[T_] := Tc / T
cc[T_] := 1 / 12 Tc^4 / T^3;
a[T_] := -T Log[2];
b = Tc / 2;
```

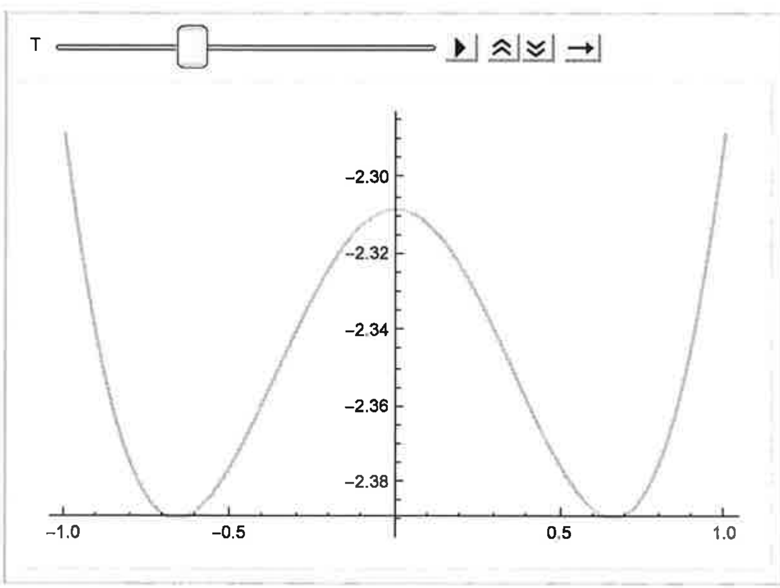
In[45]:=

```
Animate[Plot[a[T] + b * (1 - TcOverT[T]) * m^2 + cc[T] * m^4, {m, -1, 1}],
 {T, 2, 6}, AnimationRunning → False]
```

Out[45]=




```
Animate[Plot[.5 * Tc m^2 - T * Log[2 * Cosh[TcOverT [T] * m]], {m, -1, 1}],
 {T, 2, 6}, AnimationRunning → False]
```



Problem #4

Individual

4: **Transfer matrix solution of 1d Ising chain**
Please fill in some steps in the derivation so that everyone understands this technique. In particular:

i) Show that the definition $\mathbb{T} = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix}$ implies G&T Eq. (5.76), that $Z_N = Tr(\mathbb{T}^N)$.

Ok pals. Recall the relation,

$$Z_N = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}} \quad (1)$$

We define T as $T_{s,s'} = e^{\beta [J s s' + \frac{1}{2} B (s+s')]}$.

The 1D Ising model's energy can be written

$$E = -J \sum_{i=1}^{N} s_i s_{i+1} - \frac{1}{2} B \sum_{i=1}^{N} (s_i + s_{i+1})$$

The above, combined with equation (1) yields

$$Z_N = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} T_{s_1,s_2} T_{s_2,s_3} \cdots T_{s_N,s_1} \quad (2)$$

Note by the matrix multiplication definition,

$$(T^N)_{s_1,s_{N+1}} = \sum_{s_2} \cdots \sum_{s_N} T_{s_1} \cdots T_{s_N,s_{N+1}}$$

We set periodic boundary conditions,

let $s_1 = s_{N+1}$. Summing over s_1,

$$\sum_{s_1} (T^N)_{s_1, s_1} = \sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} T_{s_1, s_2} \cdots T_{s_N, s_1}$$

but this is just Z_N (see ②).

We now have $\sum_{s_1} (T^N)_{s_1, s_1} = Z_N$.

But the trace is the sum of the diagonals!

$(T^N)_{s_1, s_1}$ is the diagonal with index s_1.

$$Z_N = \mathrm{tr}(T^N).$$

ii) Find the eigenvalues of T which are given in Eq. (5.80).

$$\begin{vmatrix} e^{\beta(J+B)} - \lambda & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-B)} - \lambda \end{vmatrix} = 0 \quad , \text{ standard method.}$$

```
In[2]:= (E^(β (J+B)) - λ) (E^(β (J-B)) - λ) - (E^(-β J))^2 // FullSimplify
Out[2]= λ^2 - 2 E^(J β) λ Cosh[B β] + 2 Sinh[2 J β]
```
$= 0$

This is a simple quadratic in λ. By quadratic formula,

$$\lambda_{\pm} = e^{\beta J} \cos \beta B \pm \sqrt{e^{-2\beta J} + e^{2\beta J} \sinh^2 \beta B}$$

iii) Show that Eq. (5.81) follows, so that only the larger eigenvalue λ_+ is important in the thermodynamic limit.

$Z_N = \mathrm{Tr}(T^N)$ from earlier. But it's a theorem that **Trace = $\sum$ eigenvalues**

and also $(\text{eigenvalues}(A))^N = (\text{eigenvalues}(A^N))$

↑ this assertion is bad I know

Then $Z_N = \lambda_+^N + \lambda_-^N$.

We can write

$$\frac{1}{N}\ln Z_N = \frac{1}{N}\ln(\lambda_+^N + \lambda_-^N)$$

$$= \frac{1}{N}\ln\left[\lambda_+^N\left(1 + \frac{\lambda_-^N}{\lambda_+^N}\right)\right] \quad \text{(factoring)}$$

$$= \frac{1}{N}\ln \lambda_+^N + \frac{1}{N}\ln\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right]$$

$$= \ln \lambda_+ + \frac{1}{N}\ln\left[1 + \left(\frac{\lambda_-}{\lambda_+}\right)^N\right]$$

As $N \to \infty$, we have $\ln \lambda_+$, since the right term $\to 0$.

iv) Do the algebraic manipulations necessary to find $m(T)$ as in Eq. (5.83). Plot f this function: $m(T)$ vs. T for cases $H = 0$ and $H = 1$. For each case, use $J = 0, 0.5, 2.0$ and 4.0 to show us how this function looks.

Starting = with $\int m\{\tau\}\, dV$

$$f(T,H) = -kT \ln\left[e^{\beta J}\cosh\beta H + \left(e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}\right)^{1/2}\right]$$

$$m = \frac{\partial}{\partial T}$$

we simply take the derivative,

$$\frac{\partial f}{\partial H} =$$

```
In[33]:= f = -k T Log[E^(β J) Cosh[β H] + (E^(2 β J) Sinh[β H]^2 + E^(-2 β J))^(1/2)]

Out[33]= -k T Log[e^(J β) Cosh[H β] + Sqrt[e^(-2 J β) + e^(2 J β) Sinh[H β]^2]]

In[36]:= D[f, H] // FullSimplify

Out[36]= -(e^(J β) k T β Sinh[H β]) / Sqrt[e^(-2 J β) + e^(2 J β) Sinh[H β]^2]
```

Cancelling $e^{\beta J}$ from the top / bottom, we have the desired expression of (5.83).

For $H=0$, $m=0$. Otherwise:

m /. {H → 0}

0

m /. {H → 1, β → 1/T}

$$\frac{\mathrm{Sinh}\left[\frac{1}{T}\right]}{\sqrt{e^{-\frac{4J}{T}} + \mathrm{Sinh}\left[\frac{1}{T}\right]^2}}$$

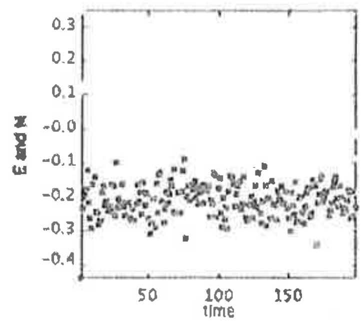
mh1 = $\frac{\mathrm{Sinh}\left[\frac{1}{T}\right]}{\sqrt{e^{-\frac{4J}{T}} + \mathrm{Sinh}\left[\frac{1}{T}\right]^2}}$;

```
Plot[ {mh1 /. {J → 0}, mh1 /. {J → 0.5}, mh1 /. {J → 2}, mh1 /. {J → 4}},
  {T, 0, 15}]
```

Physics 114
Assigned Problem
Chrissy McGinn

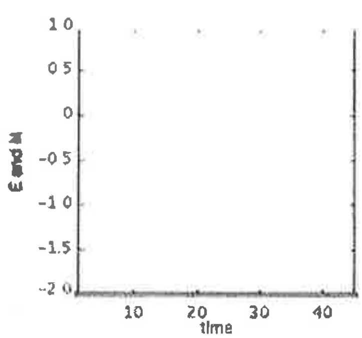
G & T 5.13

a) For $T = 10$, $H = 0$, and $N = L^2 = 32^2 = 1024$, the following plots were generated:

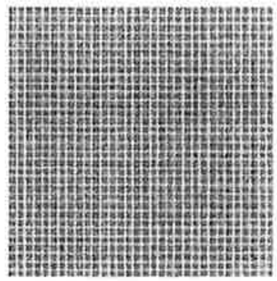


The orientation of spins is random such that the mean magnetization is approximately zero since the mean magnetization is around 0.009 in the simulation. The typical size of a domain of parallel spins is about 10-15 spins.

b) For $T = 0.5$, the simulation looks as follows:



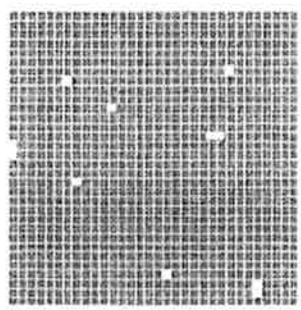
5-2

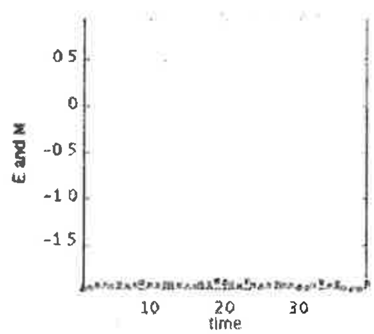


For this simulation, the average magnetization $M = 1$ which is not equal to zero, unlike the simulation for $T = 10$. For sufficiently high T then the average magnetization is zero but for low T it is not.

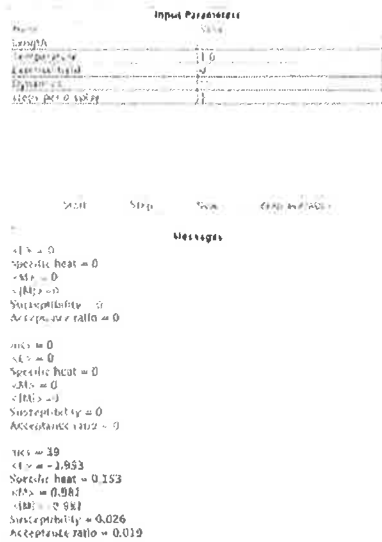
c)

$T = 1.6$

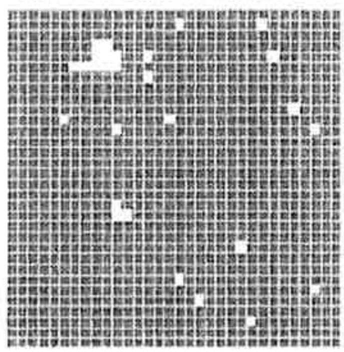


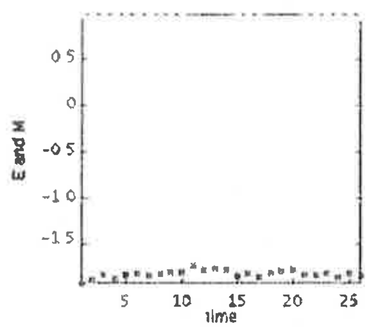


5-3

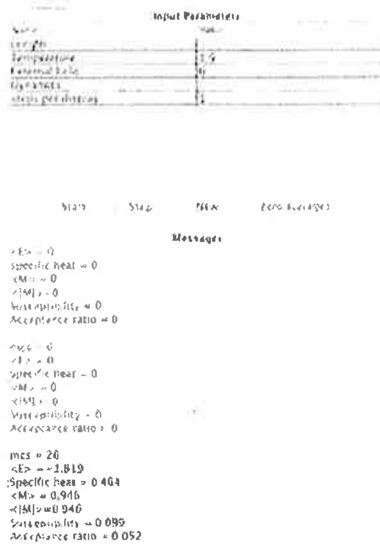

Input Parameters
Messages
mcs = 39
Specific heat = 0.153
Susceptibility = 0.026
Acceptance ratio = 0.019

$T = 1.9$



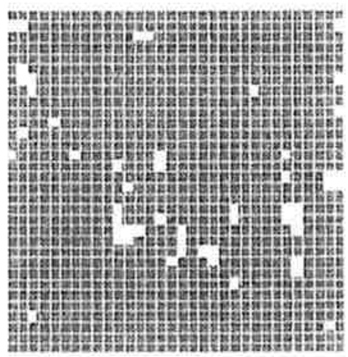

0.5
0
-0.5
-1.0
-1.5
E and M
5
10
15
20
25
time

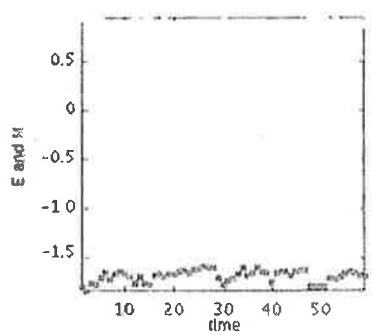
5-4



Input Parameters
Messages
specific heat = 0
Acceptance ratio = 0
mcs = 20
<E> = -1.819
Specific heat = 0.464
<M> = 0.946
<|M|> = 0.946
Susceptibility = 0.095
Acceptance ratio = 0.052

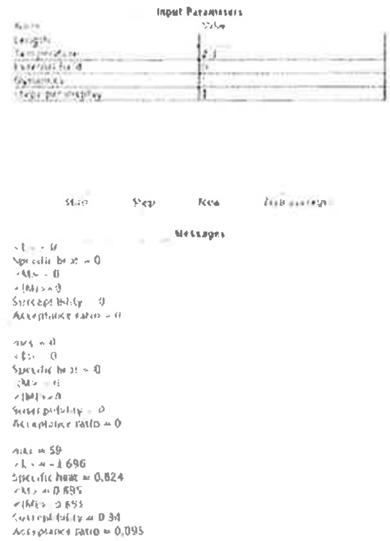
$T = 2.1$



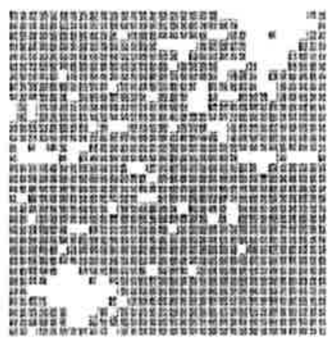


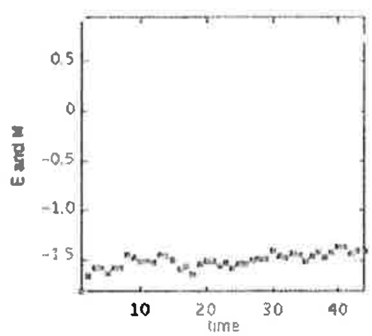
0.5
0
-0.5
-1.0
-1.5
E and M
10
20
30
40
50
time

5-5


Input Parameters
Messages
Specific heat = 0.824
Acceptance ratio = 0.095

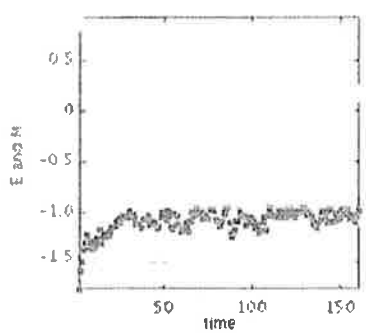
$T = 2.3$




0.5
0
-0.5
-1.0
-1.5
E and M
10
20
30
40
time


Input Parameters
Start
Step
New
Zero averages
Messages
Specific heat = 0
Specific heat = 0
mcs = 44
Specific heat = 1.358
Susceptibility = 1.74

$T = 2.6$


0.5
0
-0.5
-1.0
-1.5
E and M
50
100
150
time

S-7

Input Parameters

[illegible]	[illegible]
Length	[illegible]
Temperature	2.6
External field	0
Steps	[illegible]
steps per display	[illegible]

Start Step New Zero averages

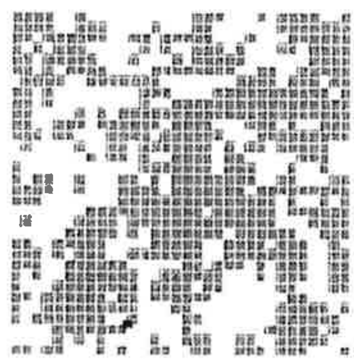
Messages

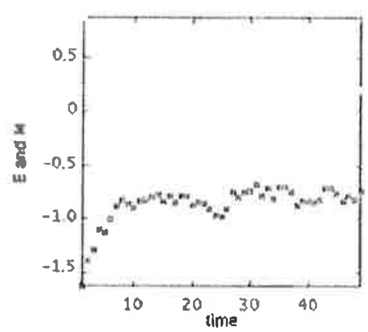
<E> = 0
specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 0
<E> = 0
specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 161
<E> = −1.098
specific heat = 1.985
<M> = 0.308
<|M|> = 0.311
Susceptibility = 15.551
Acceptance ratio = 0.33

$T = 3.1$





Input Parameters

Name	Value
Length	
Temperature	3.6
External field	0
Dynamics	
Steps per display	1

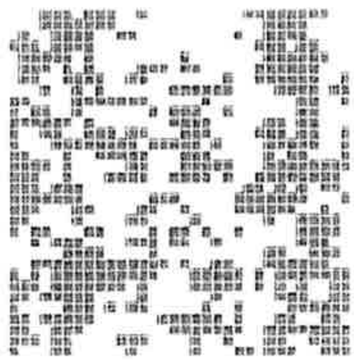
Messages

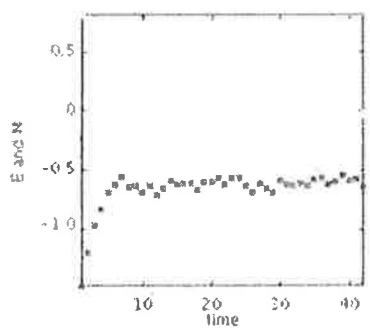
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 0
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

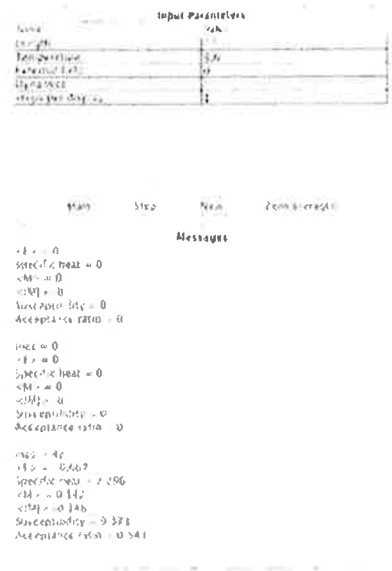
mcs = 49
<E> = -0.869
Specific heat = 3.256
<M> = 0.256
<|M|> = 0.256
Susceptibility = 12.37
Acceptance ratio = 0.442

$T = 3.6$





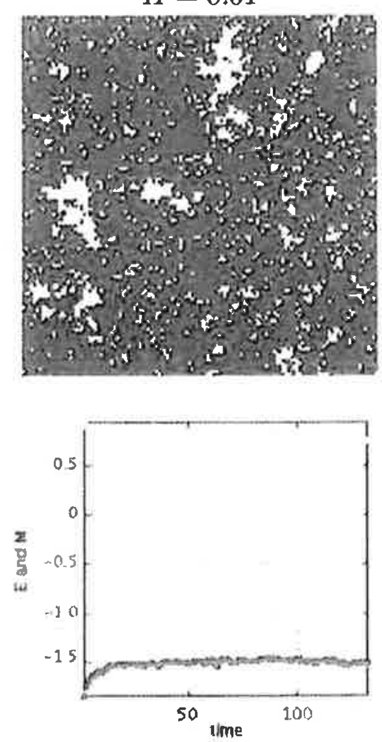
5-9



The mean magnetization decreases with increasing temperature. The average energy also decreases with increasing temperature. The heat capacity increases to its maximum at around $T = 3.1$ until it decreases. The susceptibility also peaks at $T = 2.6$.

d)

$H = 0.01$



5-10

Input Parameters

Name	Value
Length	[illegible]
Temperature	2.269
External field	0.02
Dynamics	[illegible]
Steps per display	1

Start   Step   New   Zero averages

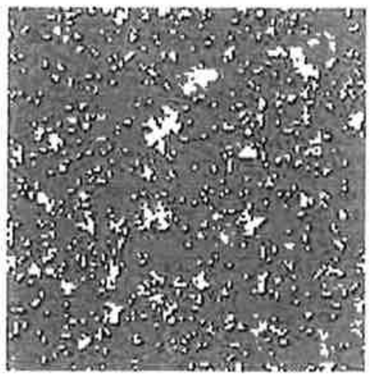
Messages

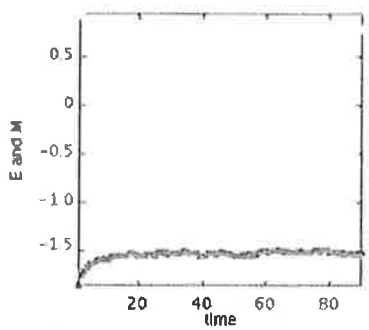
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 0
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 133
<E> = -1.512
Specific heat = 8.741
<M> = 0.760
<|M|> = 0.760
Susceptibility = 31.545
Acceptance ratio = 0.166

$H = 0.02$

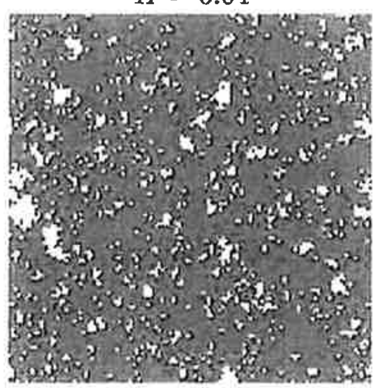


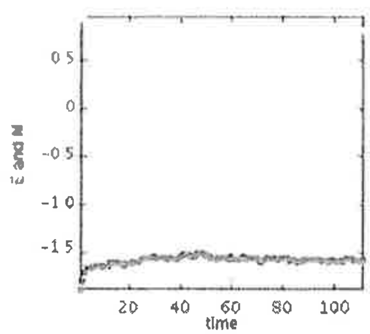


5-11

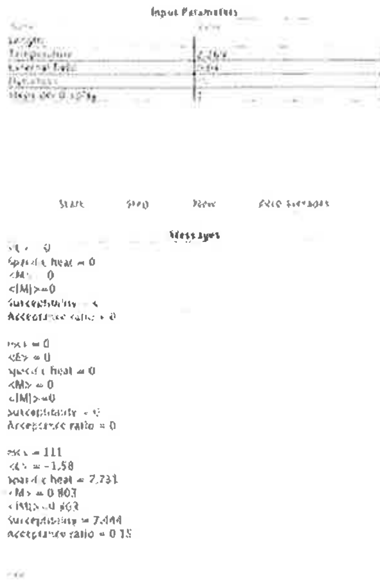

Input Parameters
Messages
Specific heat = 0
<M> = 0

$H = 0.04$

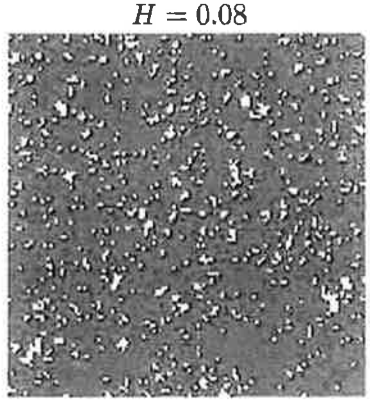


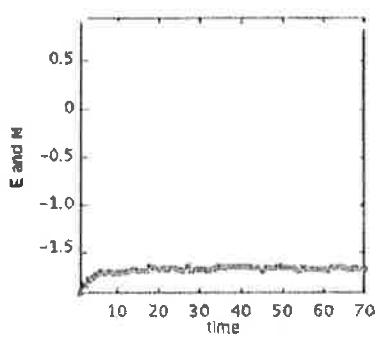

0.5
0
-0.5
-1.0
-1.5
20
40
60
80
100
time

5-12


Input Parameters
Start
Step
New
Messages
Specific heat = 0
<|M|>=0
Acceptance ratio = 0
mcs = 0
<E> = 0
specific heat = 0
<M> = 0
<|M|>=0
Acceptance ratio = 0
mcs = 111
<E> = -1.58
specific heat = 7.731
Susceptibility = 7.444
acceptance ratio = 0.15

$H = 0.08$




0.5
0
-0.5
-1.0
-1.5
E and M
10
20
30
40
50
60
70
time

Input Parameters

Name	Value
Length	[illegible]
Temperature	2.269
External field	[illegible]
Dynamics	[illegible]
Steps per display	[illegible]

Start Step New Zero averages

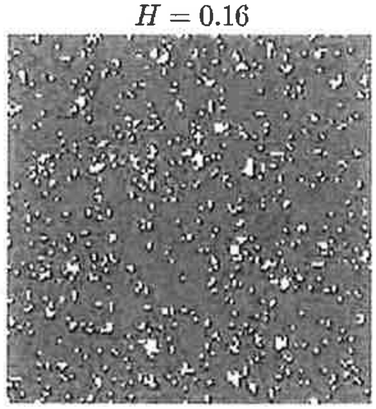
Messages

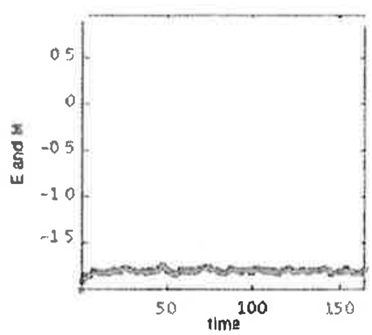
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 0
<E> = 0
Specific heat = 0
<M> = 0
<|M|> = 0
Susceptibility = 0
Acceptance ratio = 0

mcs = 70
<E> = -1.662
Specific heat = [illegible]
<M> = 0.856
<|M|> = 0.858
Susceptibility = 2.62
Acceptance ratio = 0.125

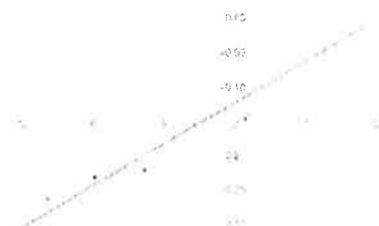
$H = 0.16$



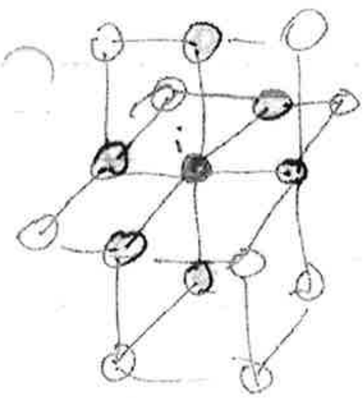


5-14

The log log plot of m and H is below:



The fit for this plot is $m = H^{0.0612}$. Then $\delta = 1/0.0612 = 16.34$.



Mean field Theory

Each spin has q neighbors (Schroeder uses "n" ... some other books use "z")

Spin i feels effective field

$$H_{eff} = J \sum_{j=1}^{q} s_j + H$$

let's take mean effective field

$$\bar{H}_{eff} = Jq\bar{s}_j + H$$ assume all s_j are same

$$= Jqm + H$$

problem notn... $\bar{s}_j = m$

Thence $Z_1 = \sum_{s_i = \pm 1} e^{+\beta s_i \bar{H}_{eff}}$;

$$Z_1 = 2\cosh[\beta(Jqm + H)]$$

$$f = -kT \ln Z_1 ;$$

$$f = -kT \ln(2\cosh[\beta(Jqm + H)])$$

Thus $\dfrac{-\partial f}{\partial H} = \tanh[\beta(Jqm + H)] = m$

This must be solved self consistently ... it is subject of Prob 3/ This week (G+T 5.18)

That problem even goes further .... Lets us "improve" on mean field as described in (G+T 5.17 Problem)

Improvement: $s_i = m + \Delta_i$; $s_j = m + \Delta_j$

smallish

$$\Rightarrow E = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i$$

$$= +J\sum_{\langle ij\rangle} m^2 - Jm\sum_{\langle ij\rangle}(s_i + s_j) - H\sum_i s_i$$

To 1st order in Δ_i

$$E = +\frac{JqNm^2}{2} - (Jqm + H)\sum_{i=1}^{N} s_i$$

$$\Rightarrow Z(T,V,N) = e^{-\beta \frac{JqNm^2}{2}} \left[2\cosh[\beta(Jqm+H)]\right]^N$$

$$\Rightarrow f = \frac{1}{2}Jqm^2 - kT\ln\left\{2\cosh\left[\beta(Jqm+H)\right]\right\}$$

improved →

add'l term not on p. 1

Problem #6

ii)

Presentation Problem

Jacob Greenberg

1 G&T 5.7

We have three magnetic dipoles, and want to calculate the correlation functions, $G(r=1)$ and $G(r=2)$. There is no external field, so the energy of the system depends only on the orientations of the two pairs. Starting at $k=1$, the spin spin correleation is,

$$G(r) = \overline{s_1 s_{1+r}} - \bar{s}_1 \bar{s}_{1+r} = \overline{s_1 s_{1+r}} - 0, \tag{1}$$

since there are just as many states a given dipole is pointing up as those it points down. Equation 5.60 in G&T gives us the general form for this for 1 dimension. To calculate $\overline{s_1 s_{1+r}}$, we need the partition function. We know from the Ising model that $Z = 8\cosh^2 \beta J$. Then we need to calculate $s_1 s_{1+r} e^{-\beta E}$ for each state. There are only 8 states, so it isn't too hard to work out by hand, and 4 of those states are just reflections of others, and have the same energy in absence of an external field. As an example, for the state ↑↑↑, we have two pairs of dipoles pointing in the same direction, giving an energy of $E = -(s_1 s_2 J + s_2 s_3 J) = -2J$. The state ↑↑↓ has energy $E = -(J - J) = 0$. Then these contribute to the correlation of the first and second spins with $e^{2\beta J}$ and 1 respectively. We find that,

$$G(r=1) = \overline{s_1 s_2} = \frac{1}{8\cosh^2 \beta J}\left(2e^{+2\beta J} - 2e^{-2\beta J}\right) \tag{2}$$

$$= \frac{+4\sinh 2\beta J}{8\cosh^2 \beta J} \tag{3}$$

$$= \frac{2\sinh \beta J \cosh \beta J}{2\cosh^2 \beta J} \tag{4}$$

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

$$G(r=2) = \overline{s_1 s_3} = \frac{1}{8\cosh^2 \beta J}\left(2e^{+2\beta J} + 2e^{-2\beta J} - 4\right) \tag{6}$$

$$= \frac{4\cosh 2\beta J - 4}{8\cosh^2 \beta J} \tag{7}$$

$$= \frac{2\sinh^\beta J + 1 - 1}{2\cosh^2 \beta J} \tag{8}$$

$$= \tanh^2 \beta J \tag{9}$$

These agree with the solution in G&T, $G(r) = \tanh^r \beta J$.

Amy

17

6. (4) G&T problem 5.36

N=4 spins in H field with periodic BCs

* This makes no sense to me ... are we meant to double bonds this way?

I'll say no

(a) Count states to find Z

State	Energy	State	Energy
↑↑ / ↑↑ (all up)	−4H − 4J	↑↓ / ↓↑ (more two down two up?)	−4J
↑↑ / ↑↓	−2H	↑↑ / ↓↓	−4J
↑↑ / ↓↑	−2H	↓↓ / ↓↑	2H
↑↓ / ↑↑	−2H	↓↓ / ↑↓ (three down one up)	2H
↓↑ / ↑↑	−2H	↓↑ / ↓↓	2H
↑↑ / ↓↓ (two down two up)	0	↑↓ / ↓↓	2H
↑↓ / ↑↓	0	↓↓ / ↓↓ (all down)	4H − 4J
↑↑ / ↓↓	0		
↓↑ / ↓↑	0		

Thus, $Z = e^{\beta(4J+4H)} + e^{\beta(4J-4H)} + 4e^{\beta 2H} + 4e^{-\beta 2H} + 2e^{-\beta 4J} + 4$

(b) $\Omega(E) = ?$ Let $H = 0$ (prev.)

E	$\Omega(E)$
$-4J$	2
0	12
$4J$	2

Broad peak around $E = 0$. Should become relatively more sharp if had more spins & thus more options.

(c) There are four states with energy $\pm 4J$. Twelve states have zero energy. Idea: T_c will be s.t.

$Z_{disordered} = Z_{ordered}$

Thus $2e^{\beta 4J} + 2e^{-\beta 4J} = 12$

```
NSolve[Sinh[x] == 3, x]
NSolve::ifun : Inverse functions are b
    solutions may not be found; u
{{x → 1.81845}}
1.818 / 4
.45
1 / %
2.20022
```

$\cosh 4\beta J = 3$

$4\beta J = 1.76275$

$\Rightarrow \frac{J}{kT_c} = 0.44$

$\Rightarrow T_c = 2.27 \frac{J}{k}$

Not bad :)

Problem #7

Critical temps ...

Critical Exponents

For this, we don't explicitly need p. 2 ....

The Para → Ferro transition happens at a special T_c where spontaneous magnetiz^n occurs. Thus $m(H \equiv 0) \neq 0$ for $T < T_c$.

This problem will tell us what Mean field theory predicts T_c to be, and how it compares with some exact 2D results.

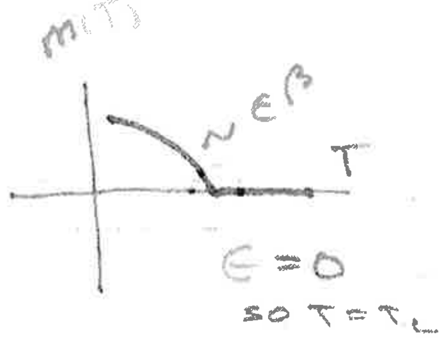
Also, as we let $T \to T_c$, there are power laws that important quantities obey.

eg.

$$m(T) = \begin{cases} 0 & T \geq T_c \\ \text{const.} \left(\frac{T_c - T}{T_c}\right)^\beta & T < T_c \end{cases}$$

$\frac{T_c - T}{T_c} \equiv \epsilon$ a small number.

So

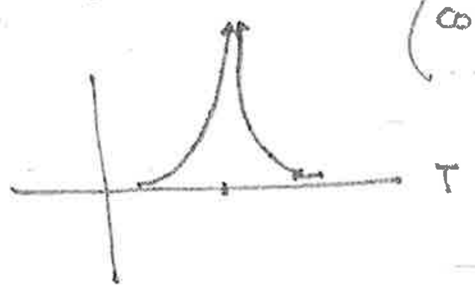


β is a critical exponent

These exponents are same $\forall$ lattices in a certain spatial dimension. Also, above a certain critical dimensionality, they are equal to their mean field values.

This talk will tell us how to find the mean field value of β.

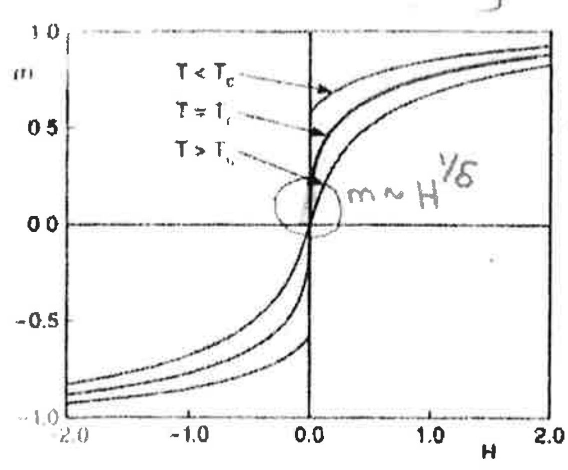
Also we'll see γ: $\chi(\epsilon) = \begin{cases} \text{const. } \epsilon^{-\gamma} & \epsilon < 0 \ (T > T_c) \\ \text{const.}' \epsilon^{-\gamma} & \epsilon > 0 \ (T < T_c) \end{cases}$



Finally, we'll see δ. This one involves being at T_c, and varying H

$m(T=T_c, H) \sim H^{1/\delta}$

i.e. $H \underset{T=T_c}{\sim} m^{\delta}$



Problem #7 addendum

Critical Temp and Exponents

(a) MFEq says $m = -\frac{\partial f}{\partial H} = \tanh\left[(Jqm+H)/kT\right]$

We find T_c as soon as there are nonzero solutions for m. This is, for $H=0$,

when $m = \tanh\left[\frac{Jq}{kT} m\right] \Rightarrow \frac{Jq}{kT} = 1 \Rightarrow T_c = \frac{Jq}{k}$

(b) injection

		vs. exact
Thus for square ($q=z=4$)	$T_c = 4J/k$	$2.269\ J/k$
triangular (6)	$T_c = 6J/k$	3.641 "
hex (3)	$T_c = 3J/k$	1.519 "

right trend at least!

back to (a)

What about β, γ & δ?

β: expand $\tanh x \approx x - \frac{1}{3}x^3$

$$\Rightarrow \quad m = \frac{Jqm}{kT} - \frac{1}{3}\frac{Jq}{kT}m^3$$

$$m = \frac{T_c}{T}m - \frac{1}{3}\frac{T_c}{T}m^3$$

Assuming $m \neq 0$: $m(1 - T_c/T) = -\frac{1}{3}\frac{T_c}{T}m^3$

$$m\left(\frac{T-T_c}{T}\right) = -\frac{1}{3}\frac{T_c}{T}m^3$$

$$m\left(\frac{T_c-T}{T}\right) = \frac{1}{3}\frac{T_c}{T}m^3$$

$T_c \approx T$

$$3\left(\frac{T_c-T}{T}\right) = m^2$$

$$m \sim \left(\frac{T_c-T}{T}\right)^{1/2} = \epsilon^{1/2}$$

$\Rightarrow \beta = 1/2$ cf. real value $1/8$

Now γ

$$\chi = \lim_{H\to 0} \frac{\partial m}{\partial H} \underset{m\ \text{small}}{=} \frac{1-m^2}{kT - Jq(1-m^2)}$$ G+T (5.114)

case $T \geq T_c \Rightarrow m = 0$

$$\Rightarrow \chi = \frac{1}{k(T-T_c)}$$

$$= \frac{T_c}{k}\left(\frac{T-T_c}{T_c}\right)^{-1}$$

$$\sim \epsilon^{-1} \qquad \underline{\gamma = 1}$$ cf. 2d real value 7/4

~~Now γ~~

case $T \leq T_c$, use $m \sim \left(\frac{T_c - T}{T_c}\right)^{1/2}$

more precisely $\Rightarrow m^2 \approx 3\left(\frac{T_c - T}{T_c}\right)$

so $$\chi = \frac{1-m^2}{k\left[T - T_c(1-m^2)\right]}$$

$$\approx \frac{1}{k\left[T - T_c\left(1 - \frac{3(T_c - T)}{T_c}\right)\right]}$$

$$\approx \frac{1}{k\left[T - 3T + 2T_c\right]}$$

$$\approx \frac{1}{k\,2\left[T_c - T\right]^1}$$ so again $\gamma = 1$

Lastly, δ:

Again, expand tanh:

$$m = \tanh\left[\frac{T_c m}{T} + \frac{H}{kT}\right]$$

$T \equiv T_c$ $\quad m \stackrel{\sim}{=} m + \frac{H}{kT_c} - \frac{1}{3}\left(m + \frac{H}{kT_c}\right)^3$

$$\Rightarrow \frac{H}{kT_c} \sim \frac{1}{3}\left(m + \frac{H}{kT_c}\right)^3$$

$m \sim H^{1/3}$ $\quad 1/\delta = 1/3$ cf. $\delta = 15$ exact

$\Rightarrow \delta = 3$

Back to b)

MFA does not care about lattice type, only # of nn's q for T_c.

It doesn't care about spatial dimension either.

For exponents: It is indep of q, lattice type AND spatial dimension.

Problem #8 Onsager Sol'n ...

$$Z_N(H=0) = \left[2\cosh(\beta J)\, e^{I}\right]^N$$

where $I = \frac{1}{2\pi}\int_0^{\pi} \ln\left[\frac{1}{2}\left(1+(1-\kappa^2\sin^2\phi)^{1/2}\right)\right]$

and $\kappa(\beta J) = \dfrac{2\sinh(2\beta J)}{\cosh^2(2\beta J)}$

a) If $I=0$

$$Z_N(H=0) = \left[2\cosh(\beta J)\right]^N$$

Which is partition function for the 1d Ising chain

$I=0 \Rightarrow T=\infty$

b) $\dfrac{F}{N} = -\dfrac{kT}{N}\log Z$

$$= -kT\log\left[2\cosh(\beta J)\, e^{I}\right]$$

$$\frac{F}{N} = -kT\log 2\cosh\beta J - kT\, I$$

c) G + T say

$$\frac{E}{N} = -2J\tanh 2\beta J - J\,\frac{\sinh^2 2\beta J - 1}{\sinh 2\beta J\cosh 2\beta J}\left[\frac{2}{\pi}K_1(\kappa)-1\right]$$

where $K_1(\kappa) = \displaystyle\int_0^{\pi/2}\frac{d\phi}{\sqrt{1-\kappa^2\sin^2\phi}}$ complete Elliptic Int of 1st kind

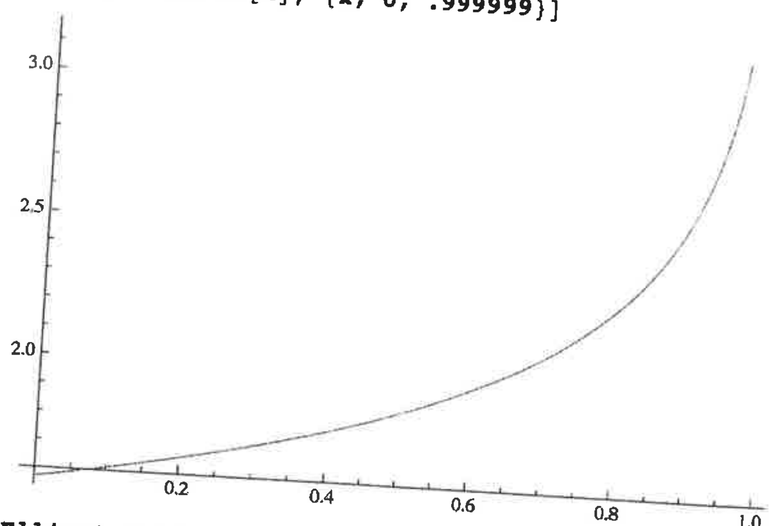
To show, this Sol does diverge at $k = 1$.

(Good thing that prefactor is zero!

ie $1 = \sinh^2 2\beta_c J$

$\Rightarrow \sinh \frac{2J}{kT_c} = 1$)


```
2 / Log[1 + 1.414]
2.26941
Plot[EllipticK[x], {x, 0, .999999}]
```




```
EllipticK[1]
ComplexInfinity
```

d) $K = \frac{2\sinh(2\beta J)}{\cosh^2(2\beta J)} = 1$

Us ID $\cosh^2 x - \sinh^2 x = 1$ w/ $u = 2\beta J$

$$K = \frac{2\sinh u}{1+\sinh^2 u} = 1$$

$$\Rightarrow 2\sinh u = 1 + \sinh^2 u$$

Clearly, sol'n is $\sinh u = 1$ QED :)

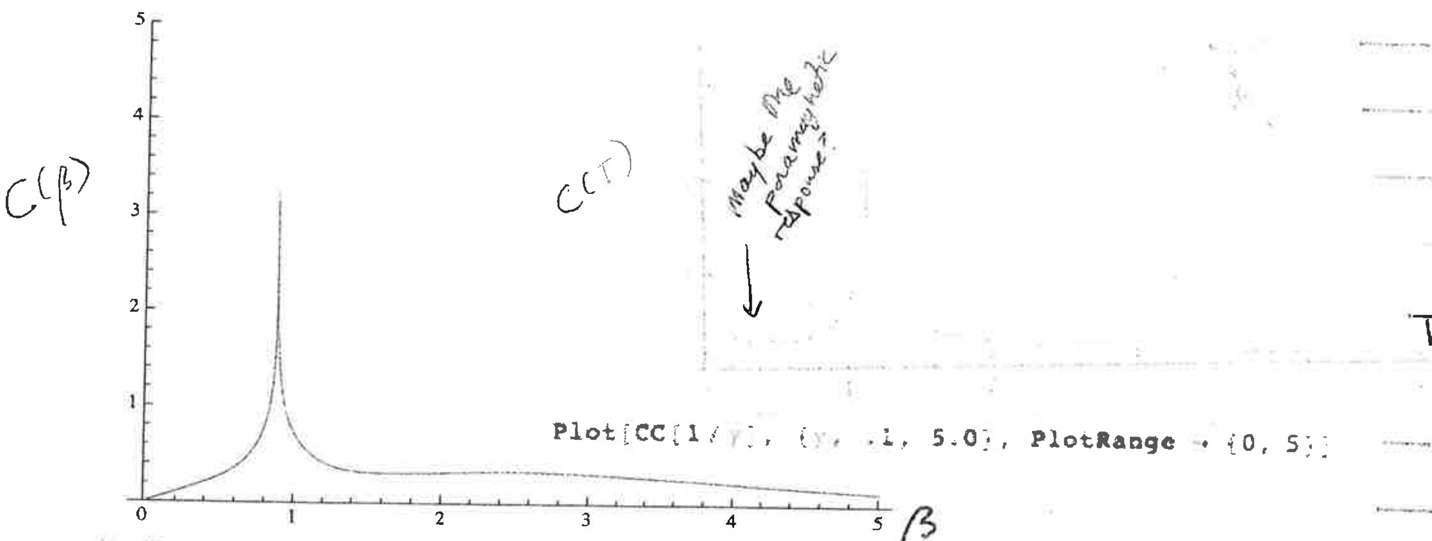
e) Mathematica below

x = 2 β J here; also use EllipticE[π/2, k] to get complete Elliptic integral of the second kind

```
kappa[x_] := 2 * Sinh[x] / (Cosh[x])^2

CC[x_] := (x / 2 * Coth[x])^2 (EllipticK[kappa[x]] - EllipticE[π / 2, kappa[x]] -
     (1 - Tanh[x]^2) * (π / 2 + (2 * Tanh[x]^2 - 1) * EllipticK[kappa[x]]))

Plot[CC[x], {x, 0.0, 5.0}, PlotRange → {0, 5}]
```



f) Blah blah blah... suddenly LOTS (like almost all in the system) of modes are getting accessible. Also, $\chi \sim \langle m^2\rangle - \langle m\rangle^2$ so fluctuations are growing enormous...