PROBLEM SET 4

Physics 219A, Spring 2014

Due Wednesday, May 14

[1.] Work out the mean field theory for the Blume-Capel model

$$H = -J \sum_{ij} S_i S_j + \Delta \sum_i S_i^2$$

where $S_i = 0, \pm 1$. Show that for a range of values of Δ the model has a first order phase transition, that is, the magnetization M is a discontinuous function of the temperature T. Sketch the phase diagram. Hints:
i. Write $S_i = M + (S_i - M)$ and substitute into H neglecting terms of order $(S - M)^2$.
ii. Calculate Z and F as a function of M.
iii. Sketch graphs of F versus M for various Δ and T. A crucial feature compared to the models we discussed in class will be the possibility that the M^4 term in F could be negative.

[2.] Solve the XY model in mean field theory. What is T_c for a 2-d square lattice, and how does it compare to the mean field solution for the Ising model? Can you argue why T_c is expected to be lower/higher?

Physics 219 Spring 2014

Homework 4

$\boxed{1}$ $E = -J \sum_{\langle ij \rangle} S_i S_j + \Delta \sum S_i^2 \qquad S_i = \pm 1, 0$

Before doing MFT, Let's think about limiting cases.

If Δ is large and negative, the ΔS_i^2 favors $S_i = \pm 1$.

In this limit, the Blume Capel model becomes the Ising model!

Meanwhile, in the limit of very low temperature

$E = -J\, z/2\, N + \Delta N \qquad$ if all $S_i = +1$

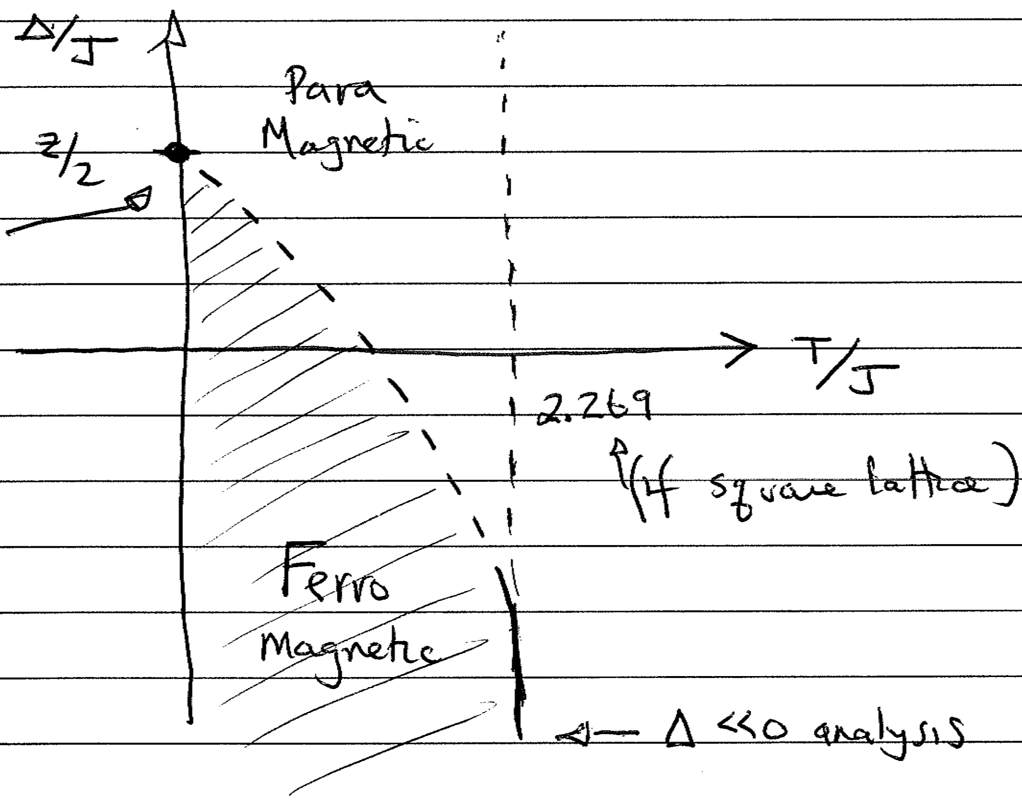
z ← coordination # (# of neighbors)

$E = 0 \qquad$ if all $S_i = \phi$

We see that as long as $Jz/2 > \Delta$ we favor ferromagnetism (all $S_i = +1$) at low T.

1-2

We can sketch the phase diagram from these two limits



T→0 analysis

1-3

Now let's do MFT

$$S_i \to m + (S_i - m) \qquad m = \langle S_i \rangle$$

$$E_{MFT} = -J \sum_{\langle ij \rangle} \left[(S_i - m) + m\right]\left[(S_j - m) + m\right] + \Delta \sum_i S_i^2$$

Do not do MFT on this term because

a) Unnecessary, already noninteracting

b) a bad approximation, fluctuations on different sites tend to average to zero, but not on same site.

$$= -J \sum_{\langle ij \rangle} \left\{ \cancel{(S_i - m)(S_j - m)} + m(S_j - m) + m(S_i - m) + m^2 \right\}$$

$$+ \Delta \sum_i S_i^2$$

Neglect

$$E_{MFT} = +J \sum_{\langle ij \rangle} m^2 - 2J \sum_{\langle ij \rangle} m S_i + \Delta \sum_i S_i^2$$

$$= J N \tfrac{z}{2} m^2 - J z m \sum S_i + \Delta \sum S_i^2$$

1-4

$$Z = e^{-\beta J N z m^2/2} \left[1 + e^{-\beta J z m - \beta\Delta} + e^{\beta J z m - \beta\Delta} \right]^N$$

$$f = \frac{-kT \ln Z}{N} = \frac{M^2 J z}{2} - kT \ln\left(1 + 2e^{-\beta\Delta} \cosh \beta J z m\right)$$

Could write self consistent eqn for m or alternately analyze by expanding f in powers of m.

Let's do the latter, I will abbreviate $e \equiv e^{-\beta\Delta}$

$$\cosh \beta J z m = 1 + \tfrac{1}{2} \beta^2 J^2 z^2 m^2 + \tfrac{1}{24} \beta^4 J^4 z^4 m^4 + \ldots$$

$$f = M^2 J z/2 - \tfrac{1}{\beta} \ln \left\{ 1 + 2e \left(\downarrow \right) \right\}$$

and expand $\ln(1+y) = y - \tfrac{1}{2} y^2 + \ldots$

$$f = M^2 J z/2 - \tfrac{1}{\beta} \ln(1+2e) \left\{ 1 + \frac{e \beta^2 J^2 z^2 m^2}{1+2e} + \frac{e/12\, \beta^4 J^4 z^4 m^4}{1+2e} + \ldots \right\}$$

$$= m^2 J z/2 - \tfrac{1}{\beta} \left\{ \ln(1+2e) + \frac{e \beta^2 J^2 z^2 m^2}{1+2e} + \frac{e/12\, \beta^4 J^4 z^4 m^4}{1+2e} - \frac{1}{2} \left(\frac{e \beta^2 J^2 z^2 m^2}{1+2e} \right)^2 + o(m^6) \right\}$$

$a(T)$

$$f = -k_B T \ln(1+2e) + \frac{m^2 Jz}{2}\left(1 - \frac{2e\beta Jz}{1+2e}\right)$$

$$+ \frac{z^4 m^4 J^4 \beta^3}{12}\left(6\frac{e^2}{(1+2e)^2} - e\frac{1}{(1+2e)}\right)$$

$b(T)$

$$+ o(m^6) \qquad \frac{e}{(1+2e)^2}(4e-1)$$

The key physics is this: If the m^4 coefficient is positive (the situation discussed in class) we have a second order phase transition when the m^2 coefficient $a(T)$ vanishes, that is, at

$$1 = 2e\beta Jz/1+2e$$

$$k_B T_c = \frac{2e}{1+2e} Jz$$

Notice that in the limit $\Delta \ll 0$ $e = e^{-\beta\Delta} \to$ large and we get $k_B T_c = Jz$, the Ising result, see discussion on pages 1-2 (except here we used exact Onsager T_c).

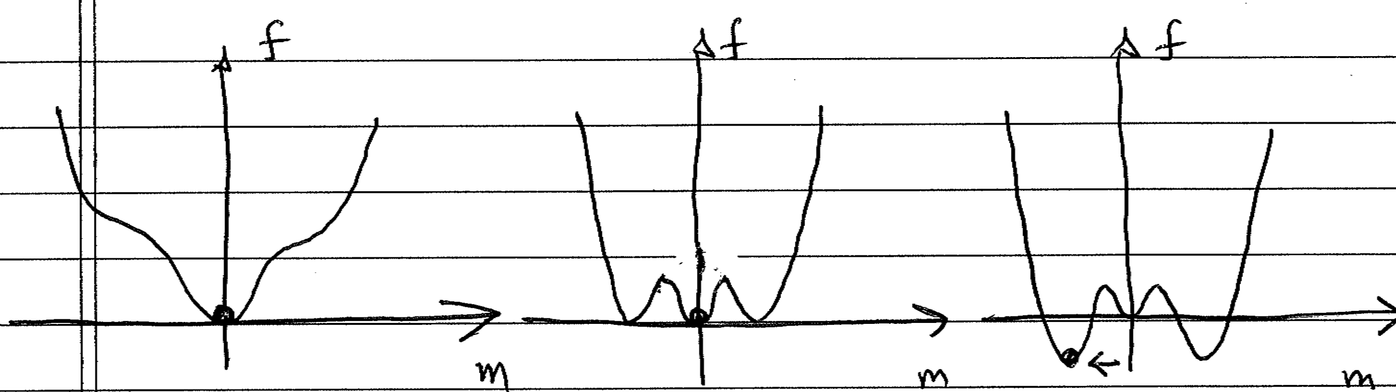
1-6.

Now this problem allows for another scenario.

We have $b(T) = e/(1+2e)^2 (4e-1)$

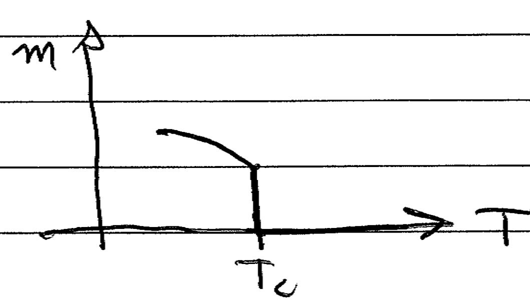
which could go negative!

The basic physics to recognize is that this allows for the possibility of a <u>First</u> <u>order</u> transition because the family of $f(m)$ curves could possibly look like this:

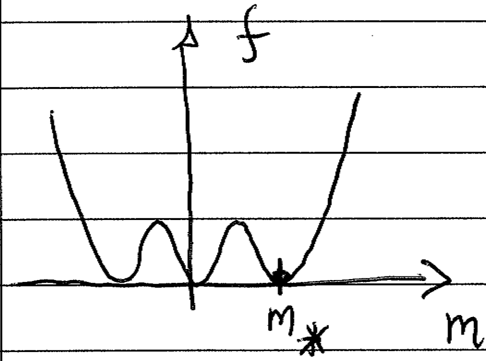


$\longrightarrow$ T decreases and $a > 0$ $b < 0$ $c > 0$

sudden jump in $f(m)$ minimum



It turns out to be pretty difficult to analyze this carefully, without a computer. One approach is to get T_c by demanding $\partial f / \partial m = 0$ to locate m_* and then require $f(m_*) = 0$



$$f = \underbrace{f_0}_{-k_B T \ln(1+2e)} + a m^2 + b m^4 + c m^6 + \dots$$

but even this is dangerous because it is not clear m_* is small.

The best way to do problem is numerically

① Write self consistent eqn for m and solve iteratively. See pages 1-8,

② plot $f(m)$ for various Δ/J and T/J, and look for pattern as on page 1-6.

I will do ① here.

Self consistent Eqn for m is obtained by

$$\partial f/\partial m = 0$$

or, equivalently computing $m = \langle S \rangle$ from MFT expression $E = JNz/2\, m^2 - Jzm\, S + \Delta S^2$

$$m = \langle S \rangle = Z^{-1}\left\{ 1 e^{-\beta E(S=1)} + 0 e^{-\beta E(S=0)} + (-1) e^{-\beta E(S=-1)} \right\}$$

$$= \frac{e^{\beta Jzm - \beta\Delta} - e^{-\beta Jzm - \beta\Delta}}{1 + e^{+\beta Jzm - \beta\Delta} + e^{-\beta Jzm - \beta\Delta}}$$

To solve, start with m_0 and iterate, ie

m_0 on rhs $\to$ m_1 on lhs
m_1 on rhs $\to$ m_2 on lhs
m_2 on rhs $\to$ m_3 on lhs
...

It is actually a bit better to use a "mixing parameter" ie when you get m_n from m_{n-1} stick $x\, m_n + (1-x) m_{n-1}$ into rhs rather than full m_n

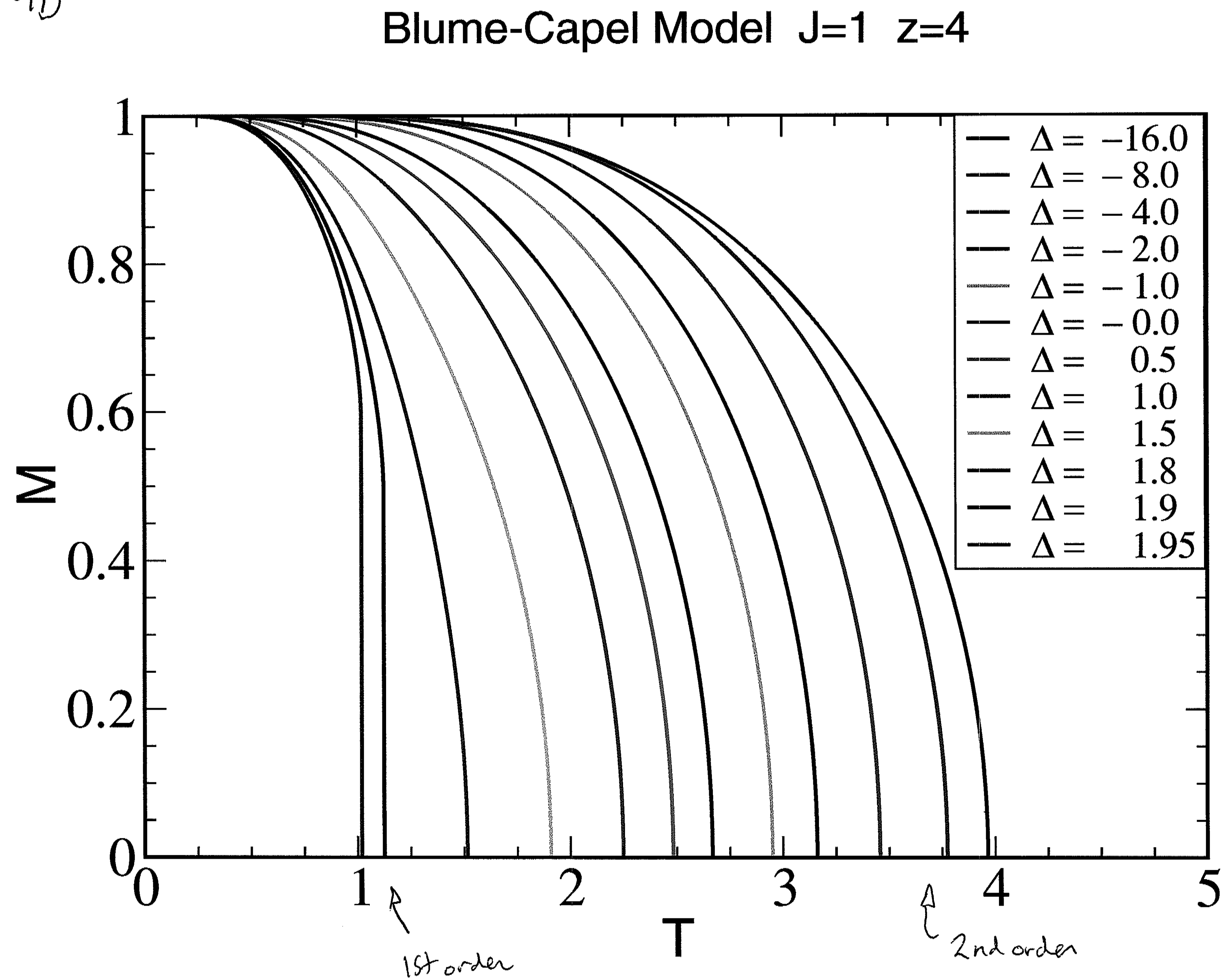
Alternately use Newtons Method

$\boxed{\text{See code}}$

i-9

```
c       SOLVE THE SELF CONSISTENT MFT EQ. FOR M IN THE BLUME-CAPEL MODEL.
c       main READS IN delta (J=1, z=4 ARE ASSUMED) AND
c            CONTAINS A LOOP OVER TEMPERATURES
c            FOR EACH T (beta) SUBROUTINE NEWTON ITERATES THE
c            SELF CONSISTENT EQUATION USING NEWTON'S METHOD.
c       DATA FOR M(T) WRITTEN TO fort.68.
c       MORE COMPLETE DATA SHOWING ITERATION WRITTEN TO fort.66

c       DECLARE VARIABLES

        implicit none
        real*8 delta,beta,m,m0,T
        integer i

c       READ IN delta AND STARTING MAGNETIZATION

        write (6,*) 'enter delta,m0'
        read  (5,*) delta,m0
        m=m0

c       LOOP OVER TEMPERATURES
c       SUBROUTINE newton ITERATES THE MF SELF-CONSISTENCY EQN.

        do 100 i=50,5000,1
            T=0.001d0*dfloat(i)
            beta=1.d0/T
            call newton(delta,beta,m)
            write (66,990) i,delta,T,beta,m
            write (68,991) T,m
100     continue
990     format(i6,4f10.4)
991     format(2f10.4)

        end


c        SOLVE  g(m) = m - 2 e^(-beta delta) sinh(z beta M)
c                 / [1 + 2 e^(-beta delta) cosh(z beta M) ] = 0

        subroutine newton(delta,beta,m)
        implicit none
        real*8 e,g,gp,beta,delta,m,enuff,z

        z=4.d0
        enuff=0.00001d0
        write (66,890) m
10      e = dexp(-beta*delta)
        g = m -  2.d0*e*dsinh(z*beta*m)/(1.d0+2.d0*e*dcosh(z*beta*m))
        gp= 1.d0 -  2.d0*z*beta*e*(2.d0*e+dcosh(z*beta*m))/
     1           (1.d0+2.d0*e*dcosh(z*beta*m))**2
        m=m-g/gp
        write (66,890) m
890        format(f12.6)
        if (dabs(g/gp).ge.enuff) go to 10
        write (66,*) ' '

        return
        end
```

1~1D


Blume-Capel Model J=1 z=4
M
T
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5
Δ = −16.0
Δ = − 8.0
Δ = − 4.0
Δ = − 2.0
Δ = − 1.0
Δ = − 0.0
Δ = 0.5
Δ = 1.0
Δ = 1.5
Δ = 1.8
Δ = 1.9
Δ = 1.95
1st order
2nd order

2-1

$\boxed{2}$ $$E = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$

There are different ways to do MFT. Let's first expand $\cos(\theta_i - \theta_j)$ before replacing things by $\langle\ \rangle$

$$= -J \sum_{\langle ij \rangle} \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j$$

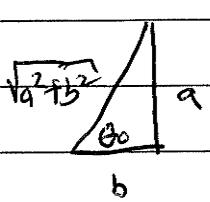
$$\xrightarrow[\text{MFT}]{} -J \sum_{\langle ij \rangle} \cos\theta_i \underbrace{m_x}_{\langle \cos\theta_j \rangle} + \sin\theta_i \underbrace{m_y}_{\langle \sin\theta_j \rangle}$$

$$E_{MFT} = -Jz \sum_i m_x \cos\theta_i + m_y \sin\theta_i$$

It is tempting to argue that one might as well choose axes so that $\langle \cos\theta_j \rangle = m$ and $\langle \sin\theta_j \rangle = 0$

ASIDE: This turns out to be true! We can prove it is okay by noting

$$\int_0^{2\pi} d\theta\, e^{a\cos\theta + b\sin\theta} = \int_0^{2\pi} d\theta\, e^{\sqrt{a^2+b^2}\left(\frac{a}{\sqrt{a^2+b^2}}\cos\theta + \frac{b}{\sqrt{a^2+b^2}}\sin\theta\right)}$$



$$= \int_0^{2\pi} d\theta\, e^{\sqrt{a^2+b^2}\,(\cos\theta_0 \cos\theta + \sin\theta_0 \sin\theta)} = \int_0^{2\pi} d\theta\, e^{\sqrt{a^2+b^2}\cos(\theta - \theta_0)}$$

$$= \int_0^{2\pi} e^{\sqrt{a^2+b^2}\cos\theta}\, d\theta.$$

$\hookrightarrow$ $\theta - \theta_0 \to \theta$

This proves an approach involving m_x and m_y is identical to one with m_x only (if M_x is $\sqrt{m_x^2 + m_y^2}$)

Self consistent Eqn for m

$$m = \langle \cos\theta \rangle = Z^{-1} \int_0^{2\pi} e^{\beta J z m \cos\theta} \cos\theta \, d\theta$$

Expanding exponential in powers of m:

$$Z = \int_0^{2\pi} e^{\beta J z m \cos\theta} \, d\theta$$

$$= \int_0^{2\pi} \left(1 + \beta J z m \cos\theta + \tfrac{1}{2} \beta^2 J^2 z^2 m^2 \cos^2\theta + \ldots \right) d\theta$$

$$= 2\pi \left\{ 1 + \tfrac{1}{4} \beta^2 J^2 z^2 m^2 + \ldots \right\}$$

Numerator is $\quad 2\pi \left\{ \beta J z m \tfrac{1}{2} + \ldots \right\}$

To lowest order in m we get

$$m = \beta J z m \tfrac{1}{2} + \ldots$$

So we need $\quad \beta J z \tfrac{1}{2} \geq 1 \quad$ for an $m \neq 0$ soln

Thus $\quad k_B T_c = \tfrac{1}{2} J z \quad \leftarrow \tfrac{1}{2}$ the Ising answer

We expect $T_c(XY) < T_c(\text{Ising})$
because continuous XY
spin has much more entropy.

2-3

It's not necessary, but we can write integrals out with no expansion

$$Z = \int_0^{2\pi} d\theta \, e^{\beta J z m \cos\theta}$$

$$= \int_0^{2\pi} d\theta \sum_n I_n(\beta J z m) e^{in\theta} = 2\pi I_0(\beta J z m)$$

Similarly

$$\int_0^{2\pi} d\theta \, e^{\beta J m z \cos\theta} \cos\theta$$

$$= \int_0^{2\pi} d\theta \sum_n I_n(\beta J z m) e^{in\theta} \tfrac{1}{2}(e^{i\theta} + e^{-i\theta})$$

$$= \pi\left[I_1(\beta J z m) + I_{-1}(\beta J z m)\right] = 2\pi I_1(\beta J z m)$$

so self consistent eqn is

$$m = I_1(\beta J z m) / I_0(\beta J z m)$$

I attach a small code to evaluate this so we can plot $m(T)$.