PROBLEM SET 3

Physics 219A, Spring 2014

Due Wednesday, April 30

[1.] Construct the high temperature expansion for the partition function Z of the 2-d Ising model on a *triangular* lattice. Go out to at least sixth order in $t = \tanh(\beta J)$. Evaluate the free energy F and show that all terms of higher power than linear in N cancel out, so that F is properly extensive.

[2.] Construct the high temperature expansion for the nearest neighbor spin-spin correlation function of the 2-d Ising model on a triangular lattice.

[3.] Construct the low temperature expansion for the partition function Z of the 2-d Ising model on a *triangular* lattice. Do the high and low temperature expansions look related, as is the case for a square lattice? Actually, the low T expansion of the Ising model on a triangular lattice is related to the high T expansion on a *different* lattice. What is that lattice?

[4.] Look up the Onsager solution of the 2-d Ising model on a square lattice, and plot the energy E as a function of temperature T. On the same graph, plot the high and low temperature expansion results for $E(T)$.

[5.] Solve the 1-d "XY" model by the transfer matrix technique. The Hamiltonian is

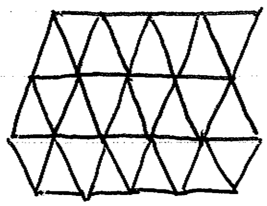
$$H = -J \sum_l \cos(\theta_l - \theta_{l+1}).$$

On each site l we have an angular variable θ_l which can take on any value $0 \leq \theta_l \leq 2\pi$. Unlike the Ising case, where the transfer matrix M is finite dimensional, in the XY model M is infinite dimensional. (But you have encountered such things already in quantum mechanics.) The eigenvalues are the solution of an appropriate integral equation.
Hint:

$$\exp(\, \beta J \cos(\theta - \theta'\,)\,) = \sum_n I_n(\beta J) \exp(\, in(\theta - \theta'\,)\,)$$

where $I_n(x)$ are Bessel functions. (Apparently they are everywhere!)

High T Expansion for Z for 2d Ising on a triangular lattice.



$$Z = \sum_{S_1}\sum_{S_2}\cdots\sum_{S_N} e^{-\beta H} = \sum_{S_1}\cdots\sum_{S_N} e^{+\beta J \sum_{\langle ij\rangle} S_i S_j}$$

$$= \sum_{S_1}\cdots\sum_{S_n}\prod_{\langle ij\rangle} e^{\beta J S_i S_j}$$

$$= \sum_{S_1}\cdots\sum_{S_n}\prod_{\langle ij\rangle}\left(c + s S_i S_j\right)$$

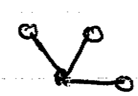
$s = \sinh\beta J$ $\qquad$ $c = \cosh\beta J$

as discussed in class; expand in closed loops

$$Z = 2^N c^{3N}\left[1 + 2Nt^3 + \dots\right]$$

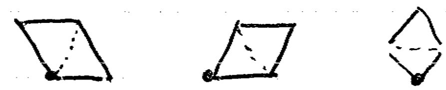
select all c from $(c + S_i S_j s)$

Note that all bonds are counted of 3 bonds taken from each of N vertex:



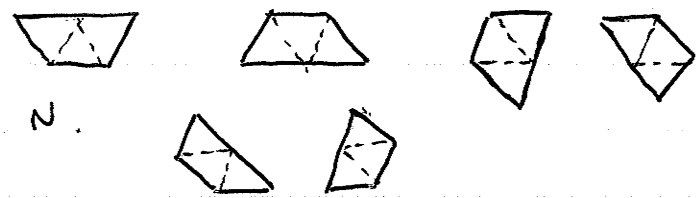
There are 2N triangles on N site lattice. If for any site you choose two plaquette shown, then all lattice is tiled

all t^4 terms are counted by choosing 3 quadralaterals for each site



$$Z = 2^N e^{3N}\left[1 + 2Nt^3 + 2Nt^4 + \dots\right]$$

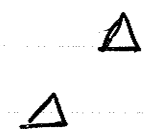
The t^5 terms look like:



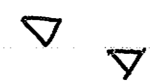
Each of these has a factor N.

So these give $6Nt^5$

Now let's do t^6. Clearly we have the "disconnected" pieces of 2 triangles which both point up: $\frac{N}{2}(N-1)\,t^6$

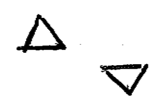


Similarly if both point down: $N/2\,(N-1)\,t^6$



Finally one up and one down triangle $N(N-3)\,t^6$

no factor of 1/2.



~~all together so far~~

$$\cancel{Z = 2^N e^{3N}\left[1 + 2Nt^3 + 2Nt^4 + 6Nt^5 + 2(N-1)t^6 + \dots\right]}$$

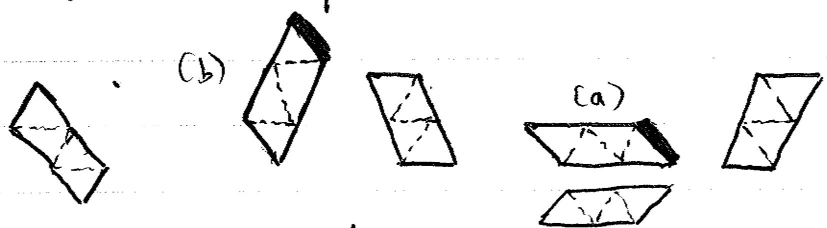
N.B. The disconnected pieces are a bit different from the square lattice case. We will check the coefficient with requirement $F \propto N$ with no N^2 terms.

Remaining t^6 diagrams: Hexagons  $\cdot\ Nt^6$

Hexagons with 2 pieces missing  $6Nt^6$

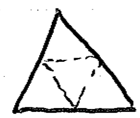
↑ 6 choices of 2 missing pieces

There are also quadrilaterals like:



$6Nt^6$

Given a bond can go to left (a) or down and to left (b) (going up + right or to right duplicates shapes)
Similar logic for other 2 bond orientations → 6 shapes

There are also triangles  Nt^6

all together:

$$\boxed{Z = 2^N c^{3N}\left[1 + 2Nt^3 + 3Nt^4 + 6Nt^5 + (2N^2+14N)t^6 + \dots\right]}$$

check by computing $f = F/N$

$$F = -kT \ln Z$$

use $\ln[1+x] = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 \dots$

$$F = -kTN\left\{ \ln 2 + 3\ln c + 2t^3 + 3t^4 + 6t^5 + (2N+14)t^6 - \frac{1}{2N}(2Nt^3 + 2Nt^4 + \dots)^2 \right\}$$

1-4.

$$f = \frac{F}{N} = -kT \{ \ln 2 + 3 \ln c + 2t^3 + 3t^4 + 6t^5 + (2N+14)t^6 - 2Nt^6 \}$$

This is good!

$$\boxed{f = -kT \{ \ln 2 + 3 \ln c + 2t^3 + 3t^4 + 6t^5 + 14t^6 + \dots \}}$$

Let's compute to t^5. The denominator is from problem #1

$$\langle S_1 S_j \rangle_{nn} = \left[1 + 2Nt^3 + 2Nt^4 + 6Nt^5 + \dots \right]^{-1} \left[\text{Numerator} \right]$$

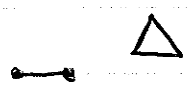
Through $o(t^3)$ is easy.

t

$2t^2$

$4t^3$

at t^4 we have disconnected pieces:

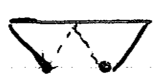


$(N-1)t^4$

and

$(N-1)t^4$

and connected ones:

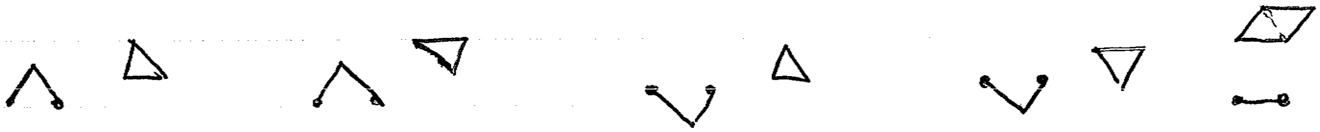


$2t^4$

$4t^4$

$4t^4$

$o(t^5)$ has disconnected diagrams



$(N-1)t^5$ $\quad$ $(N-2)t^5$ $\quad$ $(N-2)t^5$ $\quad$ $(N-1)t^5$ $\quad$ $2(N-2)t^5$

and a bunch of connected ones

$4t^5$ $\quad$ $4t^5$ $\quad$ $4t^5$ $\quad$ $4t^5$ $\quad$ $2t^5$

all together:

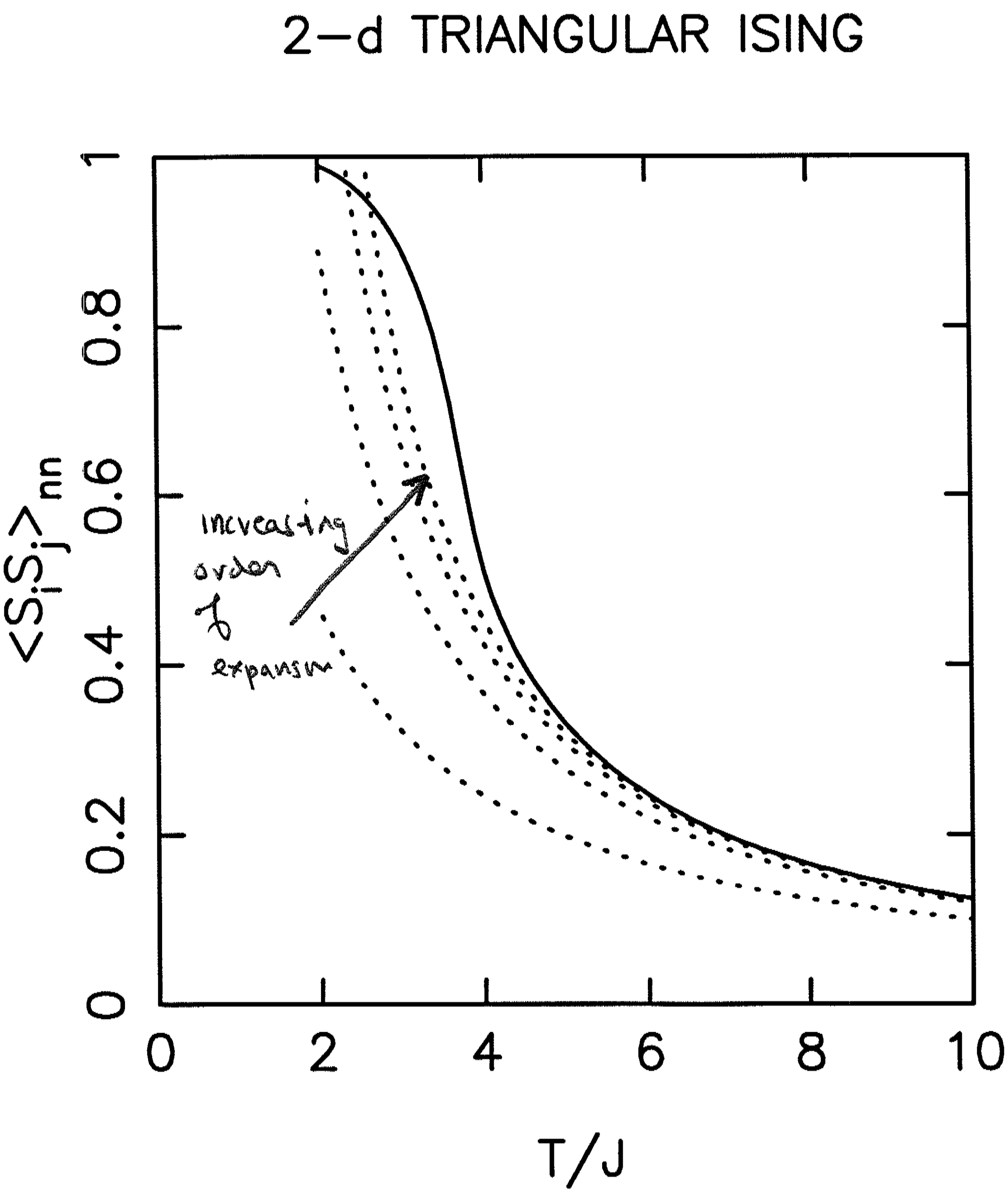
$$\langle S_i S_j \rangle_{nn} = \left[t + 2t^2 + 4t^3 + (2N+8)t^4 + (4N+8)t^5 + \ldots\right]$$

$$\left[1 - 2Nt^3 - 2Nt^4 - 6Nt^5 - \ldots\right]^{R}$$ (denominator)

$$= t + 2t^2 + 4t^3 + (2N+8)t^4 + (4N+8)t^5$$

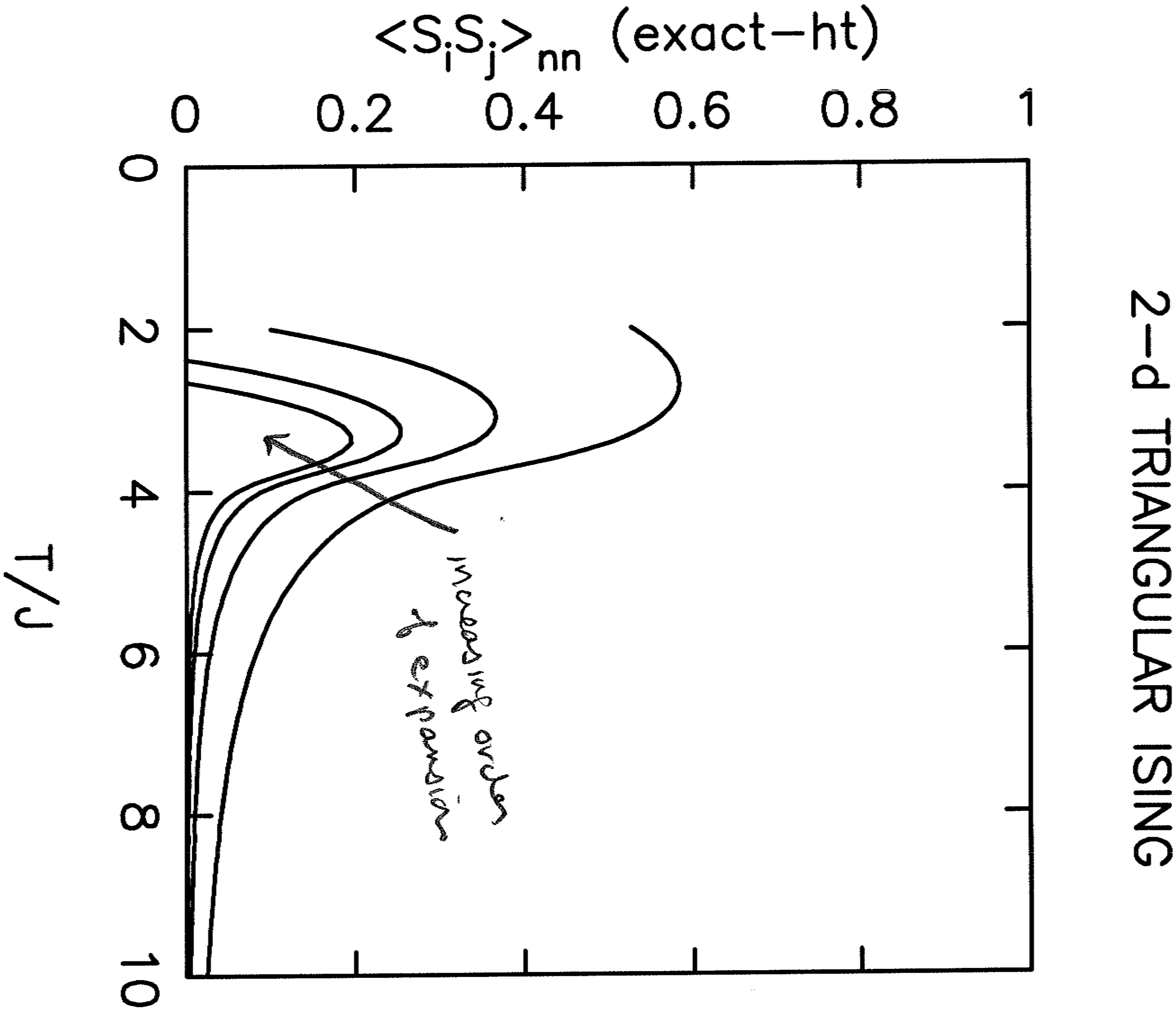
$$- 2Nt^4 - 4Nt^5 - 2Nt^5 \ldots$$

$$= t + 2t^2 + 4t^3 + 8t^4 + 8t^5 + \ldots$$



dashed lines
are various high T
expansions.
Solid curve is
Monte carlo simulation

2-4



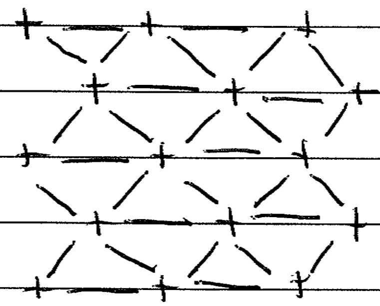
2−d TRIANGULAR ISING
<S_iS_j>_nn (exact−ht)
0
0.2
0.4
0.6
0.8
1
T/J
0
2
4
6
8
10
increasing order of expansion

3-1

Low T expansion, triangular lattice

Ground state is

Energy E_0 →



First excited state flips 1 spin $+ \to -$

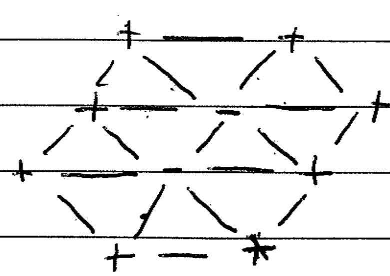
Each broken bond costs energy $2J$. There are 6 bonds

So energy is higher by $+12J$

$$Z = \underset{\substack{\uparrow \\ E_0 \text{ is ground} \\ \text{state (all +) energy}}}{2e^{-\beta E_0}} \left\{ 1 + N e^{-12\beta J} + \ldots \right\}$$

The next excited state flips 2 adjacent spins and

breaks 10 bonds :



For each spin

there are 6 neighbors

→ 3 unique adjacent neighbors (since a pair double counts

$3\text{-}1 \rightarrow 4\text{-}1$

Onsager's soln is:

$$\frac{1}{N}\langle E\rangle = -J\coth 2\beta J\left[1+\frac{2}{\pi}\left(2\tanh^2 2\beta J-1\right)K(k)\right]$$

$$K(k)=\int_0^{\pi/2} d\phi\left[1-k^2\sin^2\phi\right]^{-1/2} \leftarrow \text{(complete elliptic integral of first kind)}$$

$$k = 2\sinh 2\beta J/(\cosh 2\beta J)^2$$

What a mess! Nevertheless we can plot this along with our low and high T expansions:

$$\frac{1}{N}\langle E\rangle = -2J\left[\tanh\beta J + 2\tanh^3\beta J + 4\tanh^5\beta J + \dots\right]$$

(high T)

$$\frac{1}{N}\langle E\rangle = \underbrace{-2J}_{\frac{1}{N}E_0} + 8J\left[e^{-8\beta J}+3e^{-12\beta J}+9e^{-16\beta J}+\dots\right]$$

(low T)

I will chose $J=1$ to set scale of energies in the following plots. Also $k_B=1$.

$\ast$ NOTE: The <u>important point</u> is that the high and low T expansions even to the low orders to which we have calculated them, cover a very wide range of T in their validity. Only near T_c do they fail, and even so, one might easily make a fairly good guess in that region

3-2 → 4-2

Check onsager at high T:

βJ small : $k \approx 4\beta J$ is also small

$K(k) = \int_0^{\pi/2} d\phi \left[1 - k^2 \sin^2\phi\right]^{-1/2}$

$\approx \int_0^{\pi/2} d\phi \left[1 + \tfrac{1}{2} k^2 \sin^2\phi \cdots\right]$

$= \frac{\pi}{2} + \frac{\pi}{8} k^2 = \frac{\pi}{2}\left[1 + \frac{1}{4} 16\beta^2 J^2\right]$

$= \pi/2 \,(1 + 4\beta^2 J^2)$

$\tanh 2\beta J \approx 2\beta J \qquad \coth 2\beta J \approx 1/2\beta J$

$\frac{1}{N}\langle E\rangle = -J \,\frac{1}{2\beta J}\left[1 + 2/\pi\left[8\beta^2 J^2 - 1\right]\frac{\pi}{2}(1 + 4\beta^2 J^2)\right]$

$= -J \,\frac{1}{2\beta J}\left[1 - (1 - 8\beta^2 J^2)(1 + 4\beta^2 J^2)\right]$

$= -J \,\frac{1}{2\beta J}\left[1 - (1 - 4\beta^2 J^2)\right]$

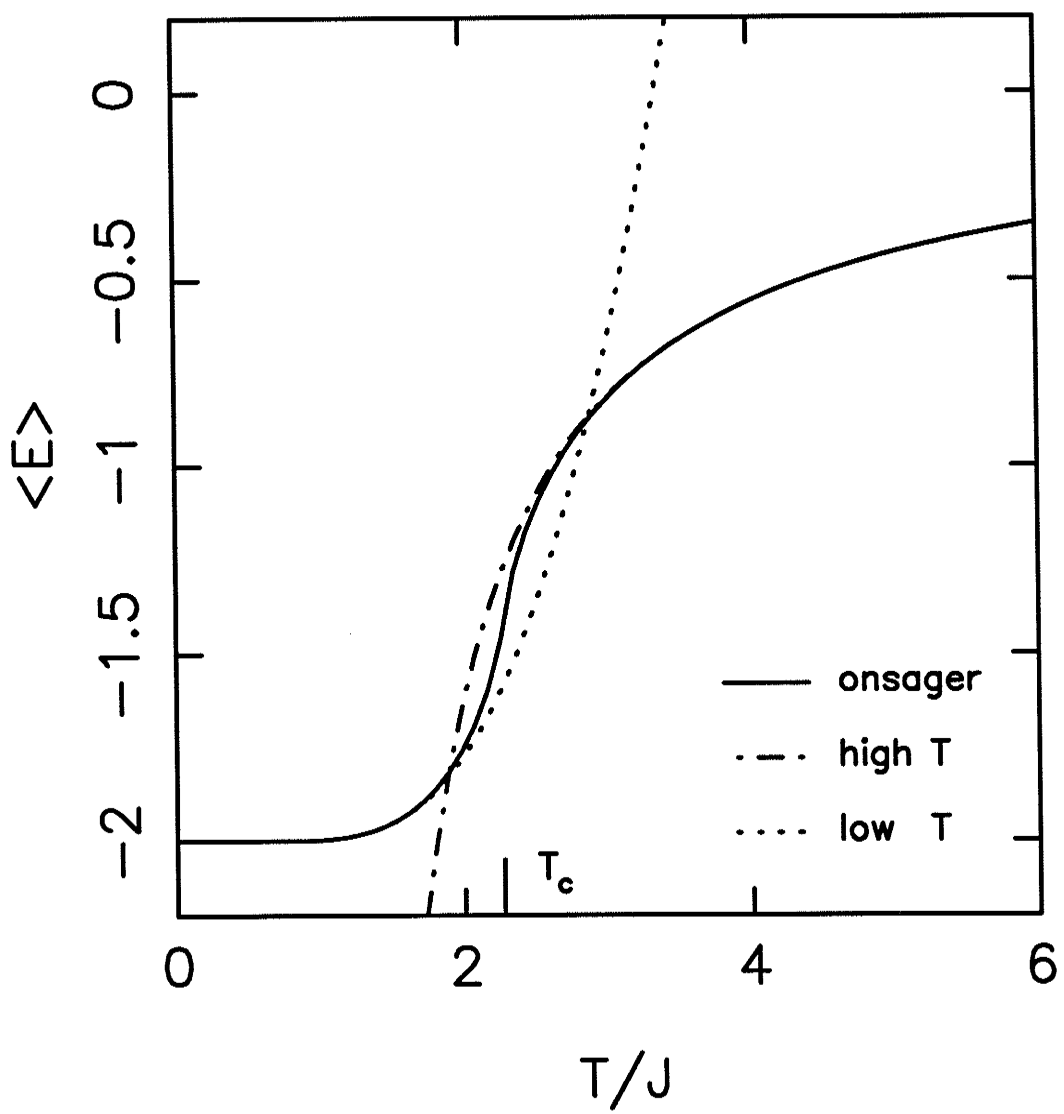
$= -J \,\frac{1}{2\beta J}\left[4\beta^2 J^2\right]$

$= -J \; 2\beta J$

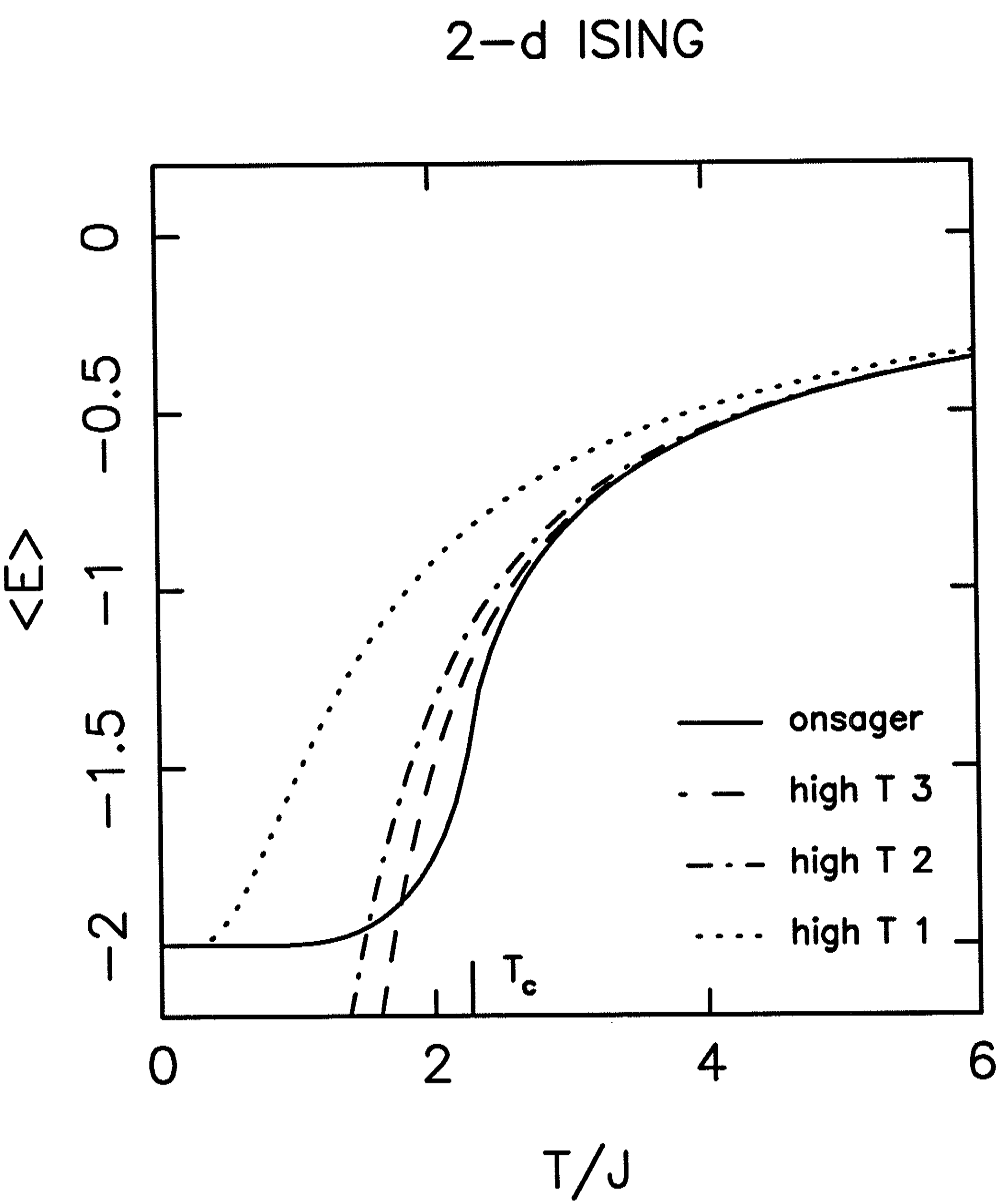
$\approx -2J \tanh\beta J$ ← this is the first term in the high T expansion!

3-3-04-3

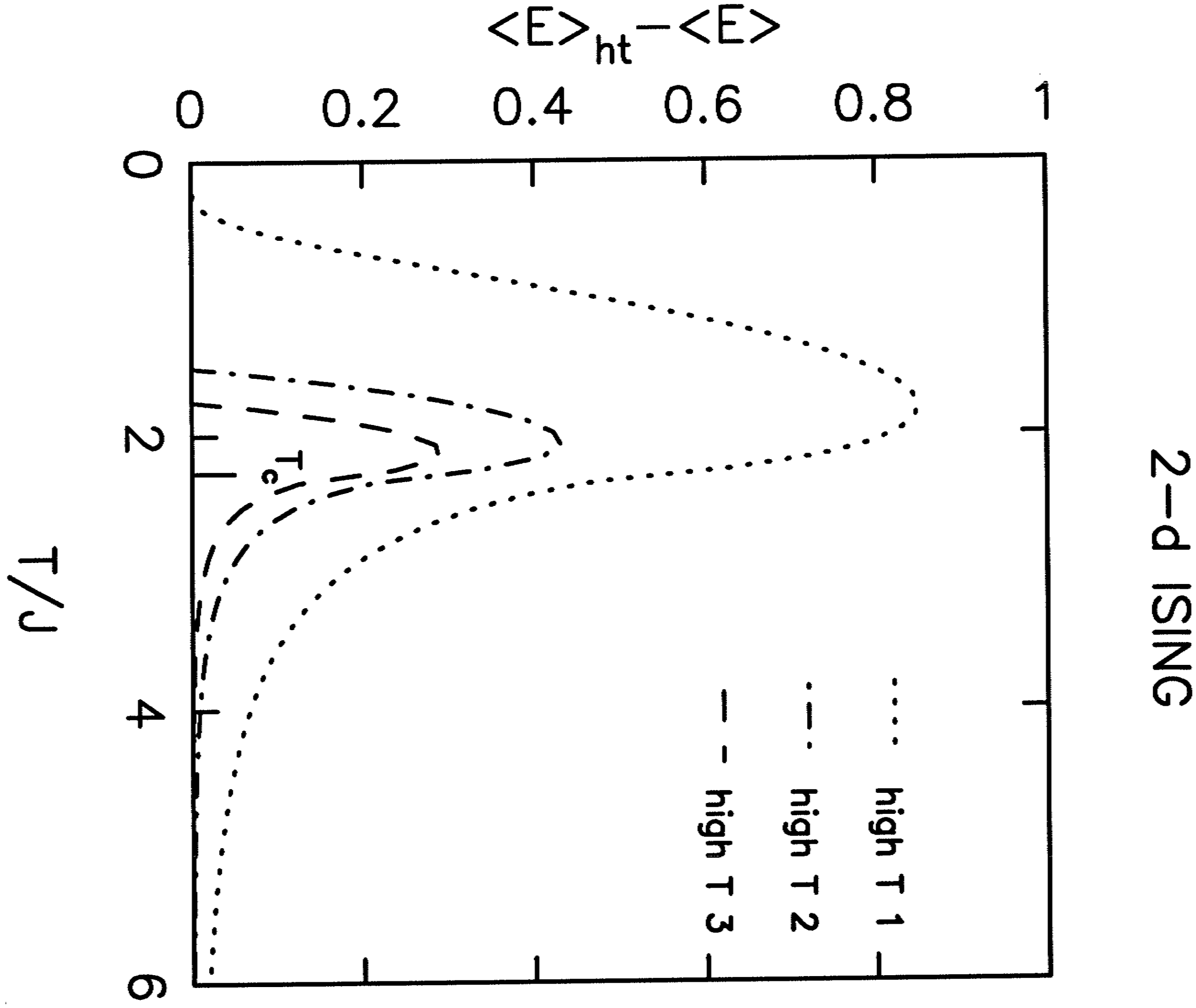
2-d ISING (sq. lattice)



3-4 → 4-4



3-5 → 4-5



2–d ISING
$\langle E \rangle_{ht} - \langle E \rangle$
0
0.2
0.4
0.6
0.8
1
T/J
0
2
4
6
T_c
high T 1
high T 2
high T 3

4-1 → 5-1

As discussed in class,

$$Z = \int d\theta_1 d\theta_2 \ldots d\theta_n \; e^{\beta J \cos(\theta_1 - \theta_2)} e^{\beta J \cos(\theta_2 - \theta_3)} \ldots, e^{\beta J \cos(\theta_N - \theta_1)}$$

pbc term

$$= \mathrm{Tr}\, M^N$$

where $M(\theta, \theta') = e^{\beta J \cos(\theta - \theta')}$ is the transfer matrix.

To compute its eigenvalues, note

$$e^{\beta J \cos(\theta - \theta')} = \sum_{n=-\infty}^{\infty} I_n(\beta J)\, e^{in\theta} e^{-in\theta'}$$

Bessel function.

so $f_\ell(\theta) = e^{i\ell\theta}$ is the eigenfunction:

$$\int d\theta' \, M(\theta, \theta') f_\ell(\theta') = \int d\theta' \sum_n I_n(\beta J) e^{in\theta} e^{-in\theta'} e^{i\ell\theta'}$$

$$= \sum_n I_n(\beta J)\, e^{in\theta}\, 2\pi \delta_{\ell n}$$

$$= 2\pi I_\ell(\beta J)\, e^{i\ell\theta} = \lambda_\ell f_\ell(\theta)$$

with eigenvalue $\lambda_\ell = 2\pi I_\ell(\beta J)$.

For a finite chain $Z = \sum_{n=-\infty}^{\infty} \lambda_\ell^N$. In the thermodynamic limit ($N \to \infty$) we just need λ_{max}, in this case it is I_0, so $Z = \lambda_0^N$.