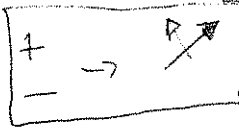


Perspectives:

- see TD for generalization to higher dimensions
- ~~#~~ A similar argument is not known for hard spheres in 2 or 3 dimensions.

* Spin waves: Absence of order if

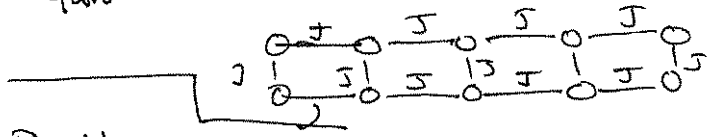


Transfer matrix for 2xM

Ising model without periodic boundary conditions in y-direction ($L=0$)

Schulz, Mattis, Lieb

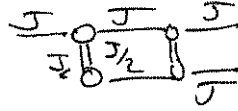
856-862, 863-871
thesis biblio



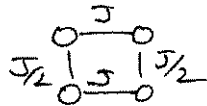
Flischke

184-189, 190-199
thesis biblio

→



→



Onsager, 1944

$$1 = \langle - \rangle$$

$$2 = \langle + \rangle$$

$$3 = \langle - \rangle$$

$$4 = \langle + \rangle$$

4 states

$$1 = \langle - \rangle$$

$$2 = \langle + \rangle$$

$$3 = \langle - \rangle$$

$$4 = \langle + \rangle$$

$$T(1,1) = \begin{matrix} - & - \\ - & - \end{matrix} = \dots 3J. \frac{e^{-3\beta J}}{e^{3K}} \quad \text{with } -\beta J = K$$

$$T(1,2) = \begin{matrix} - & + \\ - & - \end{matrix} = e^0 = 1$$

$$T(1,3) = \begin{matrix} - & - \\ - & + \end{matrix} = e^0 = 1$$

$$T(1,4) = \begin{matrix} - & + \\ - & + \end{matrix} = e^{-K}$$

$T(2,2) = T(1,2)$ as the matrix is symmetric.

$$T(2,2) = \langle + | + \rangle = e^K$$

$$T(2,3) = \langle + | - \rangle = e^{-3K}$$

$$T(2,4) = \langle + | + \rangle = 1$$

$$T(3,1) = T_{13}$$

$$T(3,2) = T(4,3)$$

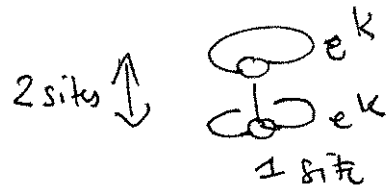
$$T(3,3) = \langle - | - \rangle = e^K$$

$$T(3,4) = \langle - | + \rangle = 1$$

$$T(4,4) = \begin{matrix} + & + \\ + & + \end{matrix} = e^{3K}$$

$$\Rightarrow T = \begin{bmatrix} e^{3K} & 1 & 1 & e^{-K} \\ 1 & e^K & e^{-3K} & 1 \\ 1 & e^{-3K} & e^K & 1 \\ e^{-K} & 1 & 1 & e^{3K} \end{bmatrix}$$

a) Testing this result for $M=1$



Partition Function, The vertical link $\pm K$
The two horizontal links $+K$

$$\langle = | \rangle e^{3K}$$

$\langle \frac{1}{4} \frac{1}{4} \rangle \quad c_{3k}$

$$\langle \pm \pm \rangle e^k$$

$$\langle \tau, \tau \rangle e^k$$

$$Z = 2e^{3K} + 2e^K$$

Note that this equals the trace of the transfer matrix.

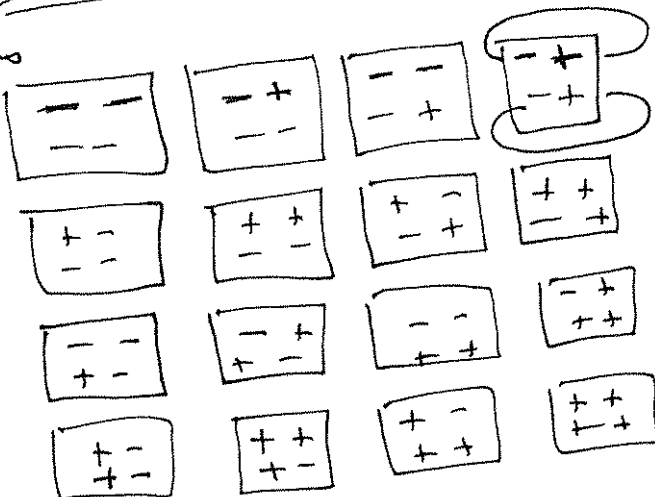
b) Testing the trans for matrix for $\pi=2$.

$$Z = \text{Tr}(T \cdot T) \quad (\text{Mathematica}).$$

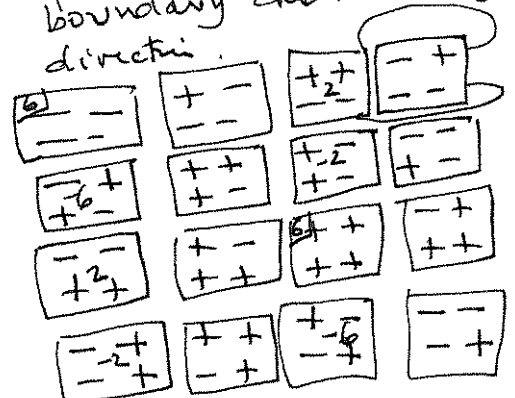
$$= 2 + e^{-2K} + e^{6K} + 2 + e^{-6K} + e^{2K} + 2 + e^{-6K} + e^{2K} + 2 + e^{-2K} + e^{6K}$$

$$= 8 + 2e^{-2K} + 2e^{2K} + 2e^{-6K} + 2e^{6K}$$

8 configurations
with
one spw
different
from the
three
others



but no periodic boundary conditions in y.



Transfer Matrix for the 2 x M Ising model (stripe of height 2 without periodic boundary conditions in the y-direction).

Material for the 5th ENS-ICFP lecture on Statistical Physics, 5 October 2016 (Werner Krauth).

```

T = {{Exp[3 K], 1, 1, Exp[-K]}, {1, Exp[K], Exp[-3 K], 1},
      {1, Exp[-3 K], Exp[K], 1}, {Exp[-K], 1, 1, Exp[3 K]}}
{{e^3 K, 1, 1, e^-K}, {1, e^K, e^-3 K, 1}, {1, e^-3 K, e^K, 1}, {e^-K, 1, 1, e^3 K}}

T.T
{{2 + e^-2 K + e^6 K, e^-3 K + e^-K + e^K + e^3 K, e^-3 K + e^-K + e^K + e^3 K, 2 + 2 e^2 K},
 {e^-3 K + e^-K + e^K + e^3 K, 2 + e^-6 K + e^2 K, 2 + 2 e^-2 K, e^-3 K + e^-K + e^K + e^3 K},
 {e^-3 K + e^-K + e^K + e^3 K, 2 + 2 e^-2 K, 2 + e^-6 K + e^2 K, e^-3 K + e^-K + e^K + e^3 K},
 {2 + 2 e^2 K, e^-3 K + e^-K + e^K + e^3 K, e^-3 K + e^-K + e^K + e^3 K, 2 + e^-2 K + e^6 K}}

Eigenvalues[T]
{e^-3 K (-1 + e^4 K), e^-K (-1 + e^4 K),
 1/2 e^-3 K (1 + e^2 K + e^4 K + e^6 K - (1 + e^2 K) sqrt[1 - 4 e^2 K + 10 e^4 K - 4 e^6 K + e^8 K]),
 1/2 e^-3 K (1 + e^2 K + e^4 K + e^6 K + (1 + e^2 K) sqrt[1 - 4 e^2 K + 10 e^4 K - 4 e^6 K + e^8 K])}

V2 = {{Exp[2 K], 1, 1, Exp[-2 K]}, {1, Exp[2 K], Exp[-2 K], 1},
      {1, Exp[-2 K], Exp[2 K], 1}, {Exp[-2 K], 1, 1, Exp[2 K]}}
{{e^2 K, 1, 1, e^-2 K}, {1, e^2 K, e^-2 K, 1}, {1, e^-2 K, e^2 K, 1}, {e^-2 K, 1, 1, e^2 K}}

V1sq = {{Exp[K/2], 0, 0, 0},
        {0, Exp[-K/2], 0, 0}, {0, 0, Exp[-K/2], 0}, {0, 0, 0, Exp[K/2]}}
{{e^K/2, 0, 0, 0}, {0, e^-K/2, 0, 0}, {0, 0, e^-K/2, 0}, {0, 0, 0, e^K/2}}

V1sq.V2.V1sq
{{e^3 K, 1, 1, e^-K}, {1, e^K, e^-3 K, 1}, {1, e^-3 K, e^K, 1}, {e^-K, 1, 1, e^3 K}}

```

Using the Transfer matrix,
we know the partition function of
equilibrium states of ~~elements~~ of ~~width~~ width 2.

compute 2×2 .

Let us do the Transfer matrix with less
lebar

$$\left[\begin{array}{c|c|c} \begin{array}{c} \text{---} K \text{---} \\ \text{---} 0 \text{---} \\ \text{---} 0 \text{---} \end{array} & \begin{array}{c} \text{---} K \text{---} \\ \text{---} 0 \text{---} \\ \text{---} K \text{---} \end{array} & \begin{array}{c} \text{---} K/2 \text{---} \\ \text{---} 0 \text{---} \\ \text{---} 0 \text{---} \end{array} \end{array} \right]$$

$V_2^{1/2} \quad V_2 \quad V_1^{1/2}$

$$V_1 = \begin{bmatrix} \exp K & 0 & 0 & 0 \\ 0 & \exp -K & 0 & 0 \\ 0 & 0 & \exp -K & 0 \\ 0 & 0 & 0 & \exp K \end{bmatrix} \quad \boxed{V_1^{1/2} \xrightarrow{0} K \rightarrow K/2}$$

$$V_2 = \begin{bmatrix} \exp 2K & 1 & 1 & \exp(-2K) \\ 1 & \exp(2K) & \exp(-2K) & 1 \\ 1 & \exp(-2K) & \exp(2K) & 1 \\ \exp(-2K) & 1 & 1 & \exp(2K) \end{bmatrix}$$

Mathematica allows us
to see that

$$V_1^{1/2} V_2 V_1^{1/2} = \overline{1}$$

Analysis of V_2 :

$$* V_2(k, r) = \exp((M-2n)K)$$

where n is the # of different spins.

* V_2 describes the interactions in the horizontal direction

* V_1 describes the vertical interactions

V_1 is a diagonal matrix

$$V_1(k, k) = \exp K((\# \text{ equal links}) - (\# \text{ unequal links})).$$

→ Periodic boundary conditions are easily integrated
the matrix is easily generalized to larger values of M .

→ * If we use $V_2 V_1$, instead of $V_1^{1/2} V_2 V_1^{1/2}$, we have a non-symmetric matrix, but it has the same trace.

This allows us now to compute the transfer matrix for arbitrary values of M .

Let

Let us now introduce the

Pauli matrices:

$$\begin{aligned}\sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & \sigma_x &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ \sigma^+ &= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & \sigma_y &= -i \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \\ \sigma^- &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\end{aligned}$$

$$\Rightarrow V_1 = \exp \left(K \sum_{j=1}^M \sigma_{j,z} \sigma_{(j+1),z} \right)$$

M ← if periodic boundary conditions sum up to M-1 otherwise.

$s_{ik1} \rightarrow + \rangle$
 $s_{ik2} \rightarrow + \rangle$

$$\sigma_j \begin{pmatrix} + \\ + \end{pmatrix} = \begin{pmatrix} + \\ + \end{pmatrix}$$

$$\sigma_z \begin{pmatrix} + \\ + \end{pmatrix} = + \begin{pmatrix} + \\ + \end{pmatrix}$$

$$\sigma_1 \begin{pmatrix} - \\ + \end{pmatrix} = -1 \begin{pmatrix} - \\ + \end{pmatrix}$$

$$\sigma_2 \begin{pmatrix} - \\ + \end{pmatrix} = +1 \begin{pmatrix} - \\ + \end{pmatrix}$$

The Pauli Matrices commute on different sites

$\sigma_{j,z} \sigma_{j+1,z} = \sigma_{j+1,z} \sigma_{j,z}$

Same, for the V_2 matrix, we can write it as

$$\langle \{ \mu \} | V_2 | \{ \mu' \} \rangle = \langle \{ \mu \} | \prod_{j=1}^M e^{K \cdot 1 + e^{-K} \sigma_{j,x}} | \{ \mu' \} \rangle$$

$$\begin{aligned}|- \rangle &= \sigma_x^+ | + \rangle \\ | + \rangle &= \sigma_x^- | - \rangle\end{aligned}$$

$$\prod_j \left[e^{K \cdot 1_j} + e^{-K} \sigma_{j,x} \right]$$

$$V_2 = (2 \sinh 2K)^{M/2} \exp \left(K^* \sum_{j=1}^M \sigma_{j,x} \right)$$

~~if periodic boundary~~

$$\begin{aligned}e^{K \cdot 1} + e^{-K} \sigma_x &= A(K) \cdot \exp(K^* \sigma_x) \\ &= A(K) \left[1 + K^* \sigma_x + \frac{(K^*)^2}{2!} \sigma_x^2 + \frac{(K^*)^3}{3!} \sigma_x^3 + \dots \right] \\ &= A \cdot \cosh(K^*) + A \sinh(K^*) \sigma_x\end{aligned}$$

$A \cosh K^* = e^K$
 $A \sinh K^* = e^{-K}$
 or $\tanh K^* = \frac{e^{-2K}}{e^K + e^{-K}}$
 $A = \sqrt{2 \sinh 2K}$

(6)

We arrive at the expression of the transfer matrix as

$$V = V_1^{1/2} V_2 V_1^{1/2} = \underbrace{V_2^{1/2} V_1 V_2^{1/2}}_{\text{this is the formulation that people use}}$$

$$V = (2 \sinh 2K)^{N/2} \exp \left(\frac{K^*}{2} \sum_{j=1}^N \sigma_{j,x} \right) \exp \left(K \sum \sigma_{j,z} \sigma_{j+1,z} \right) \exp \left(\frac{K^*}{2} \sum_{j=1}^N \sigma_{j,x} \right)$$

This is a quantum spin problem (the Pauli Matrices have commutation relations, or in other words, we are working on matrices!).

We can rewrite $\sigma_z \rightarrow -\sigma_x$ (Right-Hand rule)
 $\sigma_x \rightarrow \sigma_z$

$$V_1 = \exp \left\{ K \sum_{j=1}^N (\sigma_j^+ + \sigma_j^-) (\sigma_{j+1}^+ + \sigma_{j+1}^-) \right\}$$

$$V_2 = (2 \sinh 2K)^{N/2} \exp \left\{ 2K^* \sum_{j=1}^N \sigma_j^+ \sigma_j^- - \frac{1}{2} \cdot 1 \right\}$$

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\sigma^- \sigma^+ = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\sigma^- \sigma^+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sigma^+ \sigma^- = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$2\sigma^+ \sigma^- - 1 = \sigma_z$$

$\sigma_x = \sigma_j^+ + \sigma_j^-$
on the same site

$$\sigma^+ \sigma^- + \sigma^- \sigma^+ = [\sigma^+, \sigma^-]_+ = 1$$

on the other hand, on different sites

$$[\sigma_j^+ \sigma_k^-]_- = 0.$$

The mixed Bosonic, Fermionic commutation relations is what poses problems for the diagonalization of the matrix. Dixit Schultz Mattis Lieb

Jordan-Wigner transform \rightarrow

$$\sigma_j^+ = \exp\left(\pi i \sum_{m=1}^{j-1} c_m^+ c_m\right) c_j^+$$

$$\sigma_j^- = \exp\left(\pi i \sum_{m=1}^{j-1} c_m^+ c_m\right) c_j$$

$$(c_j^+ c_m^+)_{+} = c_j c_m^+ + c_m^+ c_j = \delta_{jm}$$

$$[c_j c_m]_{+} = [c_j^+ c_m^+]_{+} = 0.$$

$$V_2 = (2\pi\hbar 2\pi)^{N/2} \exp\left\{2\pi^* \left(c_j^+ c_j - \frac{1}{2}\right)\right\} \quad \text{c dagger}$$

$$V_1 = \exp\left\{K \sum_{j=1}^M (c_j^+ - c_j)(c_{j+1}^+ + c_{j+1})\right\}$$

Introduce ~~Bosons~~ Plane Waves: $q = \frac{j \cdot \pi}{M}$

$j = \pm 1, \pm 3, \dots, \pm(M-1)$ for n even
 $j = 0, \pm 2, \pm 4, \dots, M$ for n odd.

$$V_2 = (2 \sinh 2K)^{M/2} \exp \left\{ 2K^* \sum_{q>0} (a_q^\dagger a_{-q} + a_{-q}^\dagger a_{-q} - 1) \right\}$$

$$= (2 \sinh 2K)^{M/2} \prod_{q>0} V_{2q} \quad \begin{matrix} 4 \times 4 \\ \text{matrices} \end{matrix}$$

$$V_1 = \exp \left\{ 2K \sum_{q>0} \cos q (a_q^\dagger a_q + a_{-q}^\dagger a_{-q} - \dots) \right\}$$

$$= \prod_{q>0} V_{1q} \quad \begin{matrix} 4 \times 4 \text{ matrices} \end{matrix}$$

$$T_c: \sinh 2K \sinh 2K^* = 1$$

$$\beta F(0, T)$$

$$C_v \sim \ln \left| 1 - \frac{T}{T_c} \right|$$

$$M(T) \sim (T_c - T)^{\beta} \quad \beta = \frac{1}{8}$$

$$\chi(0, T) \sim (T - T_c)^{-7/4}$$



Further developments

Kaufman (1949)
Ferdinand & Fisher (1969)
Beale (1996)

Lecture 7

Two-dimensional Ising model: Solution through high-temperature expansions)

in this lecture, we introduce, on the one hand, to the concept of duality in the Ising model[?, 20] On the other hand, we present the graphical method for the solution of the Ising model, due to Kac and Ward. Our discussion relies on a few pages of the SMAC book[5, 236-247], and on the original papers [?, 20]. A modern echo (among many others) can be found in the work by Saul and Kardar (1992).

7.1 High-temperature expansion of the 2D Ising model

The word “enumeration” has two meanings: it refers to listing items (configurations), but it also applies to simply counting them. The difference between the two is of more than semantic interest: in the list generated by Alg. `enumerate-ising.py`, we were able to pick out any information we wanted, for example the number of configurations of energy E and magnetization M , that is, the density of states $\mathcal{N}(E, M)$. In this subsection we discuss an alternative enumeration for the two-dimensional Ising model. It does not list the spin configurations, but rather all the loop configurations which appear in the high-temperature expansion of the Ising model. This program will then turn, in Section ??, into an enumeration of the second kind (the counting), as pioneered by Kac and Ward[?]. It counts configurations and obtains $Z(\beta)$ for a two-dimensional Ising system of any size (Kaufman, 1949)[21], and even for the infinite system (Onsager, 1944)[17]. However, it then counts without listing. For example, it finds the number $\mathcal{N}(E)$ of configurations with energy E but does not tell us how many of them have a magnetization M .

Van der Waerden, in 1941 [?], noticed that the Ising-model partition function,

$$\begin{aligned} Z &= \sum_{\sigma} \exp \left(J\beta \sum_{\langle k,l \rangle} \sigma_k \sigma_l \right) \\ &= \sum_{\sigma} \prod_{\langle k,l \rangle} e^{J\beta \sigma_k \sigma_l}, \end{aligned} \quad (7.1)$$

allows each term $e^{J\beta \sigma_k \sigma_l}$ to be expanded and rearranged into just two terms, one independent of the spins and the other proportional to $\sigma_k \sigma_l$:

$$\begin{aligned} e^{\beta \sigma_k \sigma_l} &= 1 + \beta \sigma_k \sigma_l + \frac{\beta^2}{2!} \underbrace{(\sigma_k \sigma_l)^2}_{=1} + \frac{\beta^3}{3!} \underbrace{(\sigma_k \sigma_l)^3}_{=\sigma_k \sigma_l} + \dots - \dots \\ &= \underbrace{\left(1 + \frac{\beta^2}{2!} + \frac{\beta^4}{4!} + \dots \right)}_{\cosh \beta} + \sigma_k \sigma_l \underbrace{\left(\beta + \frac{\beta^3}{3!} + \frac{\beta^5}{5!} + \dots \right)}_{\sinh \beta} \\ &= (\cosh \beta) (1 + \sigma_k \sigma_l \tanh \beta) \end{aligned}$$

Inserted into eq. (7.1), with $J = +1$, this yields

$$Z(\beta) = \sum_s \prod_{\langle k,l \rangle} ((\cosh \beta) (1 + \sigma_k \sigma_l \tanh \beta)). \quad (7.2)$$

For concreteness, we continue with a 4×4 square lattice without periodic boundary conditions (with $J = 1$). This lattice has 24 edges and 16 sites, so that, by virtue of eq. (7.2), its partition function $Z_{4 \times 4}(\beta)$ is the product of 24 parentheses, one for each edge:

$$\begin{aligned} Z_{4 \times 4}(\beta) &= \sum_{\{\sigma_1, \dots, \sigma_{16}\}} \cosh^{24} \beta \overbrace{(1 + \sigma_1 \sigma_2 \tanh \beta)}^{\text{edge 1}} \overbrace{(1 + \sigma_1 \sigma_5 \tanh \beta)}^{\text{edge 2}} \\ &\quad \times \dots (1 + \sigma_{14} \sigma_{15} \tanh \beta) \underbrace{(1 + \sigma_{15} \sigma_{16} \tanh \beta)}_{\text{edge 24}}. \end{aligned} \quad (7.3)$$

We multiply out this product: for each edge (parenthesis) k , we have a choice between a “one” and a “tanh” term. This is much like the option of a spin-up or a spin-down in the original Ising-model enumeration, and can likewise be expressed through a binary variable n_k :

$$n_k = \begin{cases} 0 & (\equiv \text{edge } k \text{ in eq. (7.3) contributes } 1) \\ 1 & (\equiv \text{edge } k \text{ contributes } (\sigma_{s_k} \sigma_{s'_k} \tanh(\beta))) \end{cases},$$

where s_k and s'_k indicate the sites at the two ends of edge k . Edge $k = 1$ has $\{s_1, s'_1\} = \{1, 2\}$, and edge $k = 24$ has, from eq. (7.3), $\{s_{24}, s'_{24}\} = \{15, 16\}$. Each factored term can be identified by variables

$$\{n_1, \dots, n_{24}\} = \{\{0, 1\}, \dots, \{0, 1\}\}.$$

For $\{n_1, \dots, n_{24}\} = \{0, \dots, 0\}$, each parenthesis picks a “one”. Summed over all spin configurations, this gives 2^{16} . Most choices of $\{n_1, \dots, n_{24}\}$ average to zero when summed over spin configurations because the same term is generated with $\sigma_k = +1$ and $\sigma_k = -1$. Only choices leading to spin products $\sigma_s^0, \sigma_s^2, \sigma_s^4$ at each lattice site s remain finite after summing over all spin configurations. The edges of these terms form loop configurations, such as those shown for the 4×4 lattice in Fig. 7.1.

The list of all loop configurations may be generated by Alg. `edge-ising.py`, a recycled version of the Gray code for 24 digits, coupled to an incremental calculation of the number of spins on each site. The $\{o_1, \dots, o_{16}\}$ count the number of times the sites $\{1, \dots, 16\}$ are present. The numbers in this vector must all be even for a loop configuration, and for a nonzero contribution to the sum in eq. (7.3).

Table 7.1: Numbers of loop configurations in Fig. 7.1 with given numbers of edges (the figure contains one configuration with 0 edges, 9 with 4 edges, etc). (From Alg. `edge-ising.py`).

# Edges	# Configs
0	1
4	9
6	12
8	50
10	92
12	158
14	116
16	69
18	4
20	1

For the thermodynamics of the 4×4 Ising model, we only need to keep track of the number of edges in each configuration, not the configurations themselves. Table 7.1, which shows the number of loop configurations for any given number of edges, thus yields the exact partition function for the 4×4 lattice without periodic boundary conditions:

$$Z_{4 \times 4}(\beta) = (2^{16} \cosh^{24}(\beta))(1 + 9 \tanh^4 \beta + 12 \tanh^6 \beta + \dots + 4 \tanh^{18} \beta + 1 \tanh^{20} \beta). \quad (7.4)$$

Partition functions obtained from this expression are easily checked against the Gray-code enumeration that we had before.

7.2 Counting (not listing) loops in two dimensions

Following Kac and Ward[?], we now construct a matrix whose determinant counts the number of loop configurations in Fig. 7.1. This is possible because the determinant of a matrix $U = (u_{kl})$ is defined by a sum of permutations P (with signs and weights). Each permutation can be written as a collection of cycles, a “cycle configuration”. Our

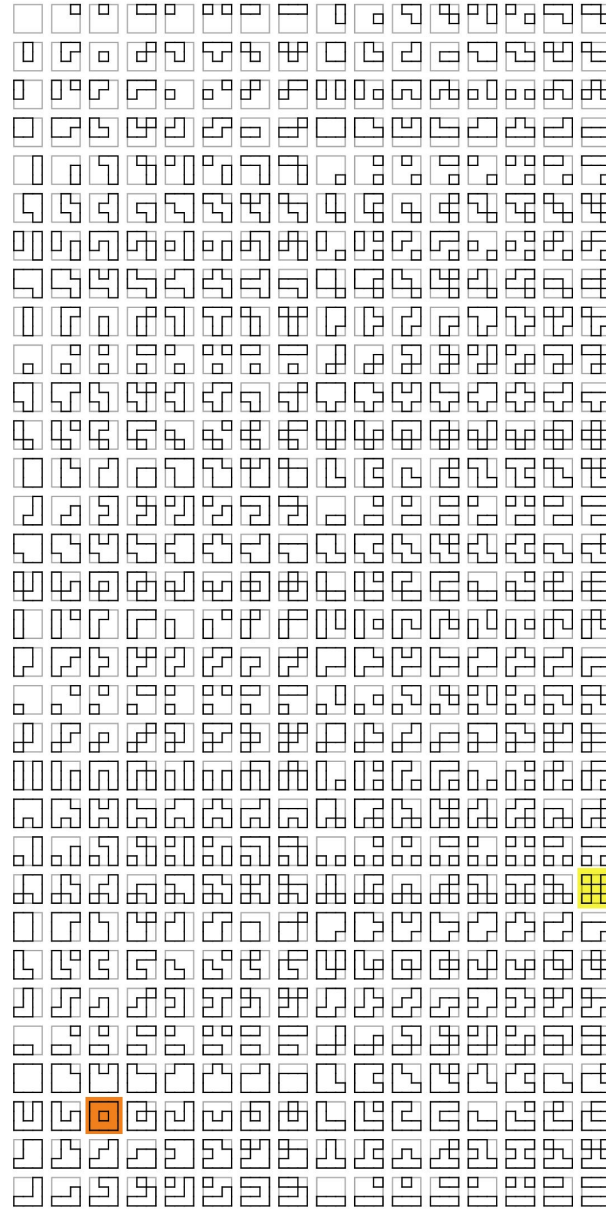


Figure 7.1: The list of all 512 loop configurations for the 4×4 Ising model without periodic boundary conditions. The “golden” configuration is the only one with 20 edges. It gives rise to the $1 \tanh^{20} \beta$ term in eq. (7.4). The “red” configuration represents a “loop within a loop”.

task will consist in choosing the elements u_{kl} of the matrix U in such a way that the signs and weights of each cycle configurations correspond to the loop configurations in the two-dimensional Ising model. We shall finally arrive at a computer program which implements the correspondence, and effectively solves the enumeration problem for large two-dimensional lattices. For simplicity, we restrict ourselves to square lattices without periodic boundary conditions, and consider the definition of the determinant of a matrix U ,

$$\det U = \sum_{\text{permutations}} (\text{sign } P) u_{1P_1} u_{2P_2} \dots u_{NP_N}.$$

We now represent P in terms of cycles. The sign of a permutation P of N elements with n cycles is $\text{sign } P = (-1)^{N+n}$ (an example may be found in the SMAC 1.2.2). In the following, we shall consider only matrices with even N , for which $\text{sign } P = (-1)^{\# \text{ of cycles}}$. The determinant is thus

$$\begin{aligned} \det U &= \sum_{\text{cycle configs}} (-1)^{\# \text{ of cycles}} \underbrace{u_{P_1 P_2} u_{P_2 P_3} \dots u_{P_M P_1}}_{\text{weight of first cycle}} \underbrace{u_{P'_1 P'_2} \dots}_{\text{other cycles}} \\ &= \sum_{\text{cycle configs}} \left(\left\{ \begin{array}{c} (-1) \cdot \text{weight of} \\ \text{first cycle} \end{array} \right\} \right) \times \dots \times \left(\left\{ \begin{array}{c} (-1) \cdot \text{weight of} \\ \text{last cycle} \end{array} \right\} \right). \end{aligned}$$

It follows from this representation of a determinant in terms of cycle configurations that we should choose the matrix elements u_{kl} such that each cycle corresponding to a loop on the lattice (for example (P_1, \dots, P_M)) gets a negative sign (this means that the sign of $u_{P_1 P_2} u_{P_2 P_3} \dots u_{P_M P_1}$ should be negative). All cycles not corresponding to loops should get zero weight.

We must also address the problem that cycles in the representation of the determinant are directed. The cycle $(P_1, P_2, \dots, P_{M-1}, P_M)$ is different from the cycle $(P_M, P_{M-1}, \dots, P_2, P_1)$, whereas the loop configurations in Fig. 7.1 have no sense of direction.

7.2.1 2x2 lattice, naive 4×4 matrix

For concreteness, we start with a 2×2 lattice without periodic boundary conditions, for which the partition function is

$$Z_{2 \times 2} = (2^4 \cosh^4 \beta) (1 + \tanh^4 \beta). \quad (7.5)$$

The prefactor in this expression (2^N multiplied by one factor of $\cosh \beta$ per edge) was already encountered in eq. (7.4). We can find naively a 4×4 matrix $\hat{U}_{2 \times 2}$ whose determinant generates cycle configurations which agree with the loop configurations. Although this matrix cannot be generalized to larger lattices, it illustrates the problems which must be overcome. This matrix is given by

$$\hat{U}_{2 \times 2} = \begin{bmatrix} 1 & \gamma \tanh(\beta) & \cdot & \cdot \\ \cdot & 1 & \cdot & \gamma \tanh \beta \\ \gamma \tanh(\beta) & \cdot & 1 & \cdot \\ \cdot & \cdot & \gamma \tanh(\beta) & 1 \end{bmatrix}.$$

(In the following, zero entries in matrices are represented by dots.) The matrix must satisfy

$$Z_{2 \times 2} = (2^4 \cosh^4 \beta) \det \hat{U}_{2 \times 2},$$

and because of

$$\det \hat{U}_{2 \times 2} = 1 - \gamma^4 \tanh^4 \beta,$$

we have to choose $\gamma = \exp i\pi/4 = \sqrt[4]{-1}$. The value of the determinant is easily verified by expanding with respect to the first row, or by naively going through all the 24 permutations of 4 elements. Only two permutations have nonzero contributions: the unit permutation $\begin{pmatrix} 1234 \\ 1234 \end{pmatrix}$, which has weight 1 and sign 1 (it has four cycles), and the permutation, $\begin{pmatrix} 2413 \\ 1234 \end{pmatrix} = (1, 2, 4, 3)$, which has weight $\gamma^4 \tanh^4 \beta = -\tanh^4 \beta$. The sign of this permutation is -1 , because it consists of a single cycle.

The matrix $\hat{U}_{2 \times 2}$ cannot be generalized directly to larger lattices. This is because it sets u_{21} equal to zero because $u_{12} \neq 0$, and sets $u_{13} = 0$ because $u_{31} \neq 0$; in short it sets $u_{kl} = 0$ if u_{lk} is nonzero (for $k \neq l$). In this way, no cycles with hairpin turns are retained (which go from site k to site l and immediately back to site k). It is also guaranteed that between a permutation and its inverse (in our case, between the permutation $\begin{pmatrix} 2413 \\ 1134 \end{pmatrix}$ and $\begin{pmatrix} 3142 \\ 1234 \end{pmatrix}$), at most one has nonzero weight.

Table 7.2: Correspondence between lattice sites and directions, and the indices of the Kac–Ward matrix U

Site	Direction	Index
1	\rightarrow	1
	\uparrow	2
	\leftarrow	3
	\downarrow	4
2	\rightarrow	5
	\uparrow	6
	\leftarrow	7
	\downarrow	8
\vdots	\vdots	\vdots
k	\rightarrow	$4k - 3$
	\uparrow	$4k - 2$
	\leftarrow	$4k - 1$
	\downarrow	$4k$

For larger lattices, this strategy is too restrictive. We cannot generate all loop configurations from directed cycle configurations if the direction in which the edges are gone through is fixed. We would thus have to allow both weights u_{kl} and u_{lk} different from zero, but this would reintroduce the hairpin problem. For larger N , there is no $N \times N$ matrix whose determinant yields all the loop configurations.

7.2. Counting (not listing) loops in two dimensions

Kac and Ward's solution to this problem associates a matrix index, not with each lattice site, but with each of the four directions on each lattice site (see Table 7.2), and a matrix element with each pair of directions and lattice sites. Matrix elements are nonzero only for neighboring sites, and only for special pairs of directions (see Fig. 7.2), and hairpin turns can be suppressed.

For concreteness, we continue with the 2×2 lattice, and its 16×16 matrix $U_{2 \times 2}$. We retain from the preliminary matrix $\hat{U}_{2 \times 2}$ that the nonzero matrix element must essentially correspond to terms $\tanh \beta$, but that there are phase factors. This phase factor is 1 for a straight move (case *a* in Fig. 7.2); it is $\exp(i\pi/4)$ for a left turn, and $\exp(-i\pi/4)$ for a right turn.

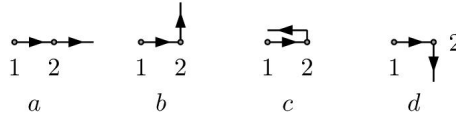


Figure 7.2: Graphical representation of the matrix elements in the first row of the Kac-Ward matrix $U_{2 \times 2}$

Table 7.3: The matrix elements of Fig. 7.2 that make up the first row of the Kac-Ward matrix $U_{2 \times 2}$ (see eq. (7.6)).

Case	Matrix element	value	type
<i>a</i>	$u_{1,5}$	$\nu = \tanh \beta$	(straight move)
<i>b</i>	$u_{1,6}$	$\alpha = e^{i\pi/4} \tanh \beta$	(left turn)
<i>c</i>	$u_{1,7}$	0	(hairpin turn)
<i>d</i>	$u_{1,8}$	$\bar{\alpha} = e^{-i\pi/4} \tanh \beta$	(right turn)

The nonzero elements in the first row of $U_{2 \times 2}$ are shown in Fig. 7.2, and taken up in Table 7.3. We arrive at the matrix

$$U_{2 \times 2} = \begin{bmatrix} 1 & \cdot & \cdot & \cdot & \nu & \alpha & \cdot & \bar{\alpha} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \bar{\alpha} & \nu & \alpha & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \bar{\alpha} & \nu & \alpha & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \bar{\alpha} & \nu & \alpha & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \alpha & \cdot & \bar{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \alpha & \cdot & \bar{\alpha} & \nu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{bmatrix}. \quad (7.6)$$

The matrix $U_{2 \times 2}$ contains four nonzero permutations, which we can generate with a naive program (in each row of the matrix, we pick one term out of $\{1, \nu, \alpha, \bar{\alpha}\}$, and then check that each column index appears exactly once). We concentrate in the following on the nontrivial cycles in each permutation (that are not part of the identity). The identity permutation, $P^1 = \begin{pmatrix} 1 & \dots & 16 \\ 1 & \dots & 16 \end{pmatrix}$, one of the four nonzero permutations, has

only trivial cycles. It is characterized by an empty nontrivial cycle configuration c_1 . Other permutations with nonzero weights are

$$c_2 \equiv \begin{pmatrix} \text{site} & 1 & 2 & 4 & 3 \\ \text{dir.} & \rightarrow & \uparrow & \leftarrow & \downarrow \\ \text{index} & 1 & 6 & 15 & 12 \end{pmatrix}$$

and

$$c_3 \equiv \begin{pmatrix} \text{site} & 1 & 3 & 4 & 2 \\ \text{dir.} & \uparrow & \rightarrow & \downarrow & \leftarrow \\ \text{index} & 2 & 9 & 16 & 7 \end{pmatrix}.$$

Finally, the permutation c_4 is put together from the permutations c_2 and c_3 , so that we obtain

$$\begin{aligned} c_1 &\equiv 1, \\ c_2 &\equiv u_{1,6}u_{6,15}u_{15,12}u_{12,1} = \alpha^4 = -\tanh^4(\beta), \\ c_3 &\equiv u_{2,9}u_{9,16}u_{16,7}u_{7,2} = \bar{\alpha}^4 = -\tanh^4(\beta), \\ c_4 &\equiv c_2c_3 = \alpha^4\bar{\alpha}^4 = \tanh^8(\beta). \end{aligned}$$

We thus arrive at

$$\det U_{2 \times 2} = 1 + 2 \tanh^4 \beta + \tanh^8 \beta = \underbrace{(1 + \tanh^4 \beta)^2}_{\text{see eq. (7.5)}}, \quad (7.7)$$

and this is proportional to the square of the partition function in the 2×2 lattice (rather than the partition function itself).

The cycles in the expansion of the determinant are oriented: c_2 runs anticlockwise around the pad, and c_3 clockwise. However, both types of cycles may appear simultaneously, in the cycle c_4 . This is handled by drawing two lattices, one for the clockwise, and one for the anticlockwise cycles (see Fig. 7.3). The cycles $\{c_1, \dots, c_4\}$ correspond to all the loop configurations that can be drawn simultaneously in both lattices. It is thus natural that the determinant in eq. (7.7) is related to the partition function in two independent lattices, the square of the partition function of the individual systems.

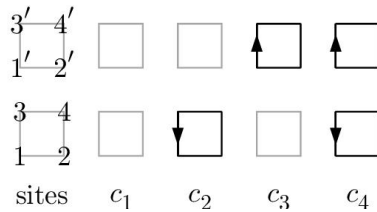


Figure 7.3: Neighbor scheme and cycle configurations in two independent 2×2 Ising models.

Before moving to larger lattices, we note that the matrix $U_{2 \times 2}$ can be written in

more compact form, as a matrix of matrices:

$$U_{2 \times 2} = \begin{bmatrix} 1 & u_{\rightarrow} & u_{\uparrow} & \cdot \\ u_{\leftarrow} & 1 & \cdot & u_{\uparrow} \\ u_{\downarrow} & \cdot & 1 & u_{\rightarrow} \\ \cdot & u_{\downarrow} & u_{\leftarrow} & 1 \end{bmatrix} \quad \left(\begin{array}{l} \text{a } 16 \times 16 \text{ matrix,} \\ \text{see eq. (7.9)} \end{array} \right), \quad (7.8)$$

where 1 is the 4×4 unit matrix, and furthermore, the 4×4 matrices u_{\rightarrow} , u_{\uparrow} , u_{\leftarrow} , and u_{\downarrow} are given by

$$\begin{aligned} u_{\rightarrow} &= \begin{bmatrix} \nu & \alpha & \cdot & \bar{\alpha} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, & u_{\uparrow} &= \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \bar{\alpha} & \nu & \alpha & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, \\ u_{\leftarrow} &= \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \bar{\alpha} & \nu & \alpha \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}, & u_{\downarrow} &= \begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \alpha & \cdot & \bar{\alpha} & \nu \end{bmatrix}. \end{aligned} \quad (7.9)$$

The difference between eq. (7.6) and eq. (7.8) is purely notational.

The 2×2 lattice is less complex than larger lattices. For example, one cannot draw loops in this lattice which sometimes turn left, and sometimes right. (On the level of the 2×2 lattice it is unclear why left turns come with a factor α and right turns with a factor $\bar{\alpha}$.) This is what we shall study now, in a larger matrix. Cycle configurations will come up that do not correspond to loop configurations. We shall see that they sum up to zero.

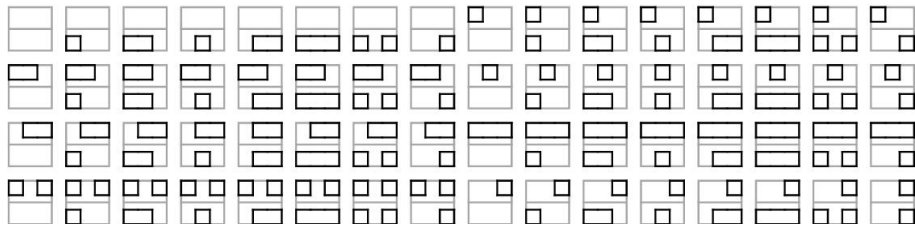


Figure 7.4: All 64 loop configurations for two uncoupled 4×2 Ising models without periodic boundary conditions (a subset of Fig. 7.1).

For concreteness, we consider the 4×2 lattice (without periodic boundary conditions), for which the Kac–Ward matrix can still be written down conveniently. We understand by now that the matrix and the determinant describe pairs of lattices, one for each sense of orientation, so that the pair of 4×2 lattices corresponds to a single 4×4 lattice with a central row of links eliminated. The 64 loop configurations for this

The cycle c_2 makes four left and four right turns (so that the weight is proportional to $\bar{\alpha}^4 \alpha^4 \propto +1$) whereas the cycle c_1 turns six times to the left and twice to the right, with weight $\bar{\alpha}^6 \alpha^2 \propto -1$, canceling c_2 .

A naive program easily generates all of the nontrivial cycles in $U_{4 \times 2}$ (in each row of the matrix, we pick one term out of $\{1, \nu, \alpha, \bar{\alpha}\}$, and then check that each column index appears exactly once). This reproduces the loop list, with 64 contributions, shown in Fig. 7.4. There are in addition 80 more cycle configurations, which are either not present in the figure, or are equivalent to cycle configurations already taken into account. Some examples are the cycles c_1 and c_2 in Fig. 7.5. It was the good fortune of Kac and Ward that they all add up to zero.

On larger than 4×2 lattices, there are more elaborate loops. They can, for example, have crossings (see, for example, the loop in Fig. 7.6). There, the cycle configurations c_1 and c_2 correspond to loops in the generalization of Fig. 7.4 to larger lattices, whereas the cycles c_3 and c_4 are superfluous. However, c_3 makes six left turns and two right turns, so that the overall weight is $\alpha^4 = -1$, whereas the cycle c_4 makes three left turns and three right turns, so that the weight is $+1$, the opposite of that of c_3 . The weights of c_3 and c_4 thus cancel.

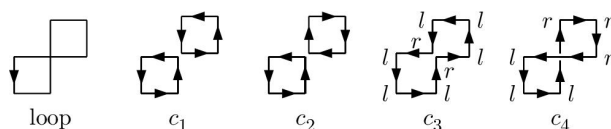


Figure 7.6: Loop and cycle configurations. The weights of c_3 and c_4 cancel.

For larger lattices, it becomes difficult to establish that the sum of cycle configurations in the determinant indeed agrees with the sum of loop configurations of the high-temperature expansion, although rigorous proofs exist to that effect. However, at our introductory level, it is more rewarding to proceed heuristically. We can, for example, write down the 144×144 matrix $U_{6 \times 6}$ of the 6×6 lattice for various temperatures (using Alg. combinatorial-ising.py), and evaluate the determinant $\det U_{6 \times 6}$ with a standard linear-algebra routine. Partition functions thus obtained are equivalent to those resulting from Gray-code enumeration, even though the determinant is evaluated in on the order of $144^3 \simeq 3 \times 10^6$ operations, while the Gray code goes over $2^{35} \simeq 3 \times 10^{10}$ configurations. The point is that the determinant can be evaluated for lattices that are much too large to go through the list of all configurations.

The matrix $U_{L \times L}$ for the $L \times L$ lattice contains the key to the analytic solution of the two-dimensional Ising model first obtained, in the thermodynamic limit, by Onsager (1944). To recover Onsager's solution, we would have to compute the determinant of U , not numerically as we did, but analytically, as a product over all the eigenvalues. Analytic expressions for the partition functions for Ising models can also be obtained for finite lattices with periodic boundary conditions. To adapt for the changed boundary conditions, one needs four matrices, generalizing the matrix U (compare with the analogous situation for dimers in chapter xx. Remarkably, evaluating $Z(\beta)$ on a finite lattice reduces to evaluating an explicit function (see the classical papers by Kaufman (1949) [21] and Ferdinand and Fisher (1969) [22]).

Lecture 7. Two-dimensional Ising model: Solution through high-temperature expansions)

The analytic solutions of the Ising model have not been generalized to higher dimensions, where only Monte Carlo simulations, high-temperature expansions, and renormalization-group calculations allow to compute to high precision the properties of the phase transition. These properties, as mentioned, are universal, that is, they are the same for a wide class of systems, called the Ising universality class.

Lecture 8

The three pillars of mean-field theory (Transitions and order parameters 1/2)

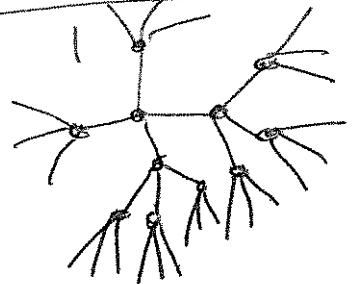
Saxton 1982:
Exactly solved models
in Statistical
mechanics
limit

What we will discuss,
Mean-field theory

→ Infinite-dimensional model
of a physical model

→ Self consistency,

(TD: Bethe lattice).



absence of fluctuations

Pierre-ERNEST WEISS
1865 → 1940

Interpretation as a
Landau theory,

Free energy as a function
of an order parameter
(and possibly of its
derivatives)

Bragg-Williams theory.

Introduction

Weiss
magnetic
field

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i$$

$$\sigma_i = \pm 1$$

$\langle ij \rangle$: nearest neighbors

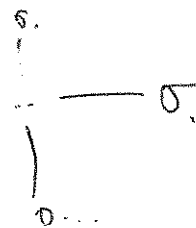
References: 1)

2)

3) ---

4) ---

5) ---



$$\langle \sigma_j(t) \rangle = m$$

introduce an

$$E|_{\sigma_0} = -J \sigma_0 \sum_{j \in \text{neighbors of } 0} \sigma_j - h \sigma_0$$

$$= -\sigma_0 \left[J \sum_j \sigma_j + h \right]$$

\approx Weiss \propto constant

$\sum \sigma_j = \text{const}$
2) Neglecting fluctuations

Weiss $\langle \sigma_j \rangle = m$
1) Self consistency
(each site at
any moment
identical with
each or
every other site)

$$m_0 = -$$

σ_0	E	$e^{-\beta H}$
1	$J - h_{\text{Weiss}}$	$e^{\beta h_{\text{Weiss}}}$

σ_0	E	$e^{-\beta H}$
1	- h_{weiss}	$e^{\beta H_{weiss}}$
-1	+ h_{weiss}	$e^{-\beta H_{weiss}}$

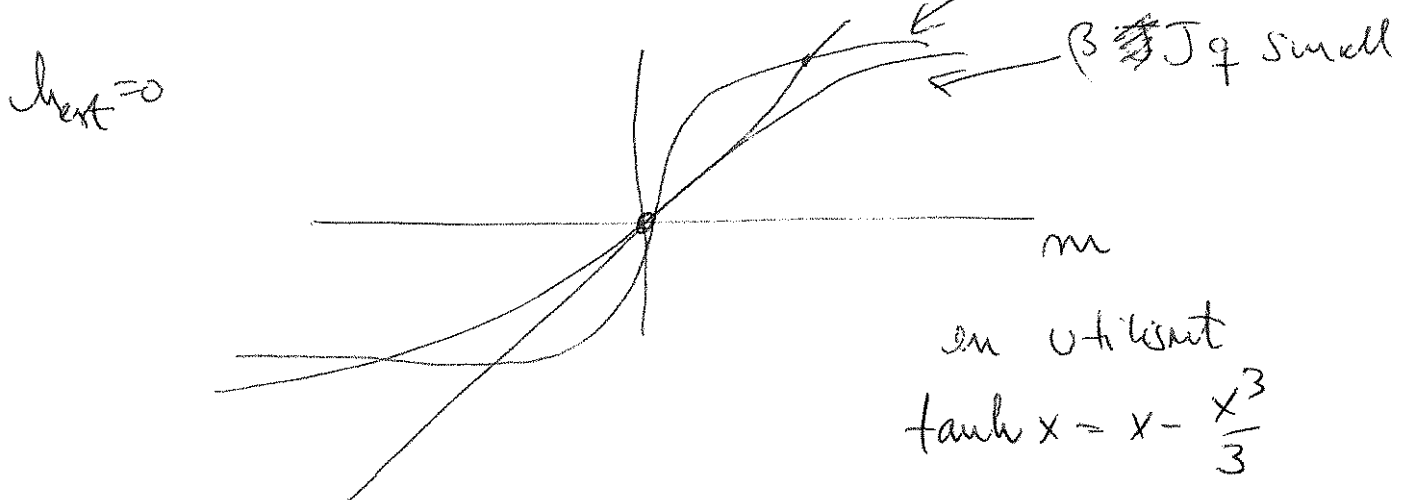
$$m_0 = \frac{e^{\beta H_{weiss}} - e^{-\beta H_{weiss}}}{e^{\beta H_{weiss}} + e^{-\beta H_{weiss}}} = \tanh(\beta H_{weiss})$$

$$m_0 = \tanh(\beta h_{weiss})$$

$$= \tanh \beta [J q m + h_{ext}]$$

Self consistency ($m_0 = m$)

$$m = \tanh \beta [J q m + h_{ext}]$$



$$m = \beta J q m - \frac{[\beta J q m]^3}{3}$$

$$m = \alpha m - \frac{\alpha^3 m^3}{3}$$

$$1 = \alpha - \frac{\alpha^3 m^2}{3}$$

$$\frac{\alpha^3 m^2}{3} = \alpha - 1$$

$$m = \sqrt{\frac{3(\alpha - 1)}{\alpha^3}}$$

$$\beta J q = \alpha$$

$$\beta J q = 1 \quad \alpha = 1: \text{critical point}$$

$$\boxed{k_B T = q J}$$

$m = 0$ is a solution

$$\alpha \rightarrow 1 = \varepsilon$$

$$\alpha^2 = [\varepsilon + 1]^2 = 1 + 2\varepsilon$$

$$m = \pm \sqrt{\frac{3\varepsilon}{1+2\varepsilon}} = \pm \sqrt{3} \sqrt{\varepsilon}$$

$$\beta_c =$$

$$m(T) = \pm \sqrt{3} \left(\frac{T}{T_c} \right)^{3/2} \left(\frac{T_c}{T} - 1 \right)^{1/2}$$

$$m(T) \sim \left(\frac{T_c}{T} - 1 \right)^\beta \quad \text{Critical exponent } \beta_{MF} = \frac{1}{2}$$

CRITICAL EXPONENT (exact solution $\beta = \frac{1}{2}$).

~~Some authors~~ A less well-known example.

One-dimensional Ising chain. ($J=1$). $\beta_c = 2 = \frac{1}{2}$
 $\beta_c \sim \frac{1}{2}$
 $T_c \sim 2$

$m_0 = 1$, setting any spin at site k equal to its mean value.

$$m_k = \tanh(J\beta(m_{k-1} + m_{k+1}))$$

let us linearize the equation

$$m_0 = 1$$

$$m_k = \beta(m_{k-1} + m_{k+1}) \quad \forall k \geq 0$$

This is a linear difference equation (see Bender & Orszag)

$$m_k = r^k$$

$$r^k = \beta(r^{k-1} + r^{k+1})$$

$$\frac{1}{\beta} = \frac{1}{r} + r \quad r = \frac{1}{2\beta} \pm \sqrt{\frac{1}{4\beta^2} - 1}$$

$$r = \frac{1}{2\beta} \pm \sqrt{\frac{1}{4\beta^2} - 1}$$

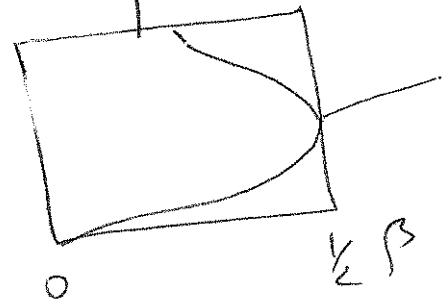
Bifurcation

$$1 = \frac{1}{2\beta}$$

$$\beta = \frac{1}{2}$$

This checks with the previous self-consistency equation.

$$r = \frac{\beta_c}{\beta} \pm \frac{\beta_c}{\beta} \sqrt{1 - \left(\frac{\beta}{\beta_c}\right)^2}$$



We analyze behavior of the lower branch for small positive values of $t = \frac{(T - T_c)}{T_c}$.

$$t > 0$$

$T > T_c$
PARA

$$r = \beta_c T - \beta_c T \sqrt{1 - \left(\frac{1}{\beta_c T}\right)^2} \quad \left| \begin{array}{l} t = \frac{T}{T_c} - 1 \\ \frac{T}{T_c} = 1 + t \\ r = 1 + t - \sqrt{t^2 + 2t} \end{array} \right.$$

$$= t + 1 - \sqrt{t^2 + 2t}$$

$$\boxed{m_k} \sim (1 - \sqrt{2t})^k \sim e^{-k \sqrt{2t}} \sim 1 + t - \sqrt{2t} \sim \boxed{1 - \sqrt{2t}}$$

$$m_k \sim \exp(-k \xi) \quad \xi \sim \frac{1}{t^{1/2}}$$

This means that the correlation length in 4d mean field theory is $\nu = \frac{1}{2}$. One can also do a limited Taylor expansion around $t = 0$ and find $\nu' = \frac{1}{2}$.

The correlation length as a scale \Rightarrow Scaling (next week).

Mean-field

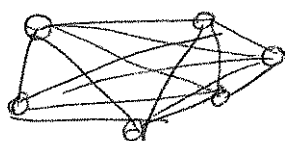
~~Infinite dimensional~~ Ising model

(Baxter 1982)

The approximation $\sum_j \sigma_j = q \cdot m$ is exact if we consider a d -dimensional lattice in the limit $d = q/2 \rightarrow \infty$. (5)

~~We then solve this model~~

RATHER Than considering this model, we solve exactly the fully connected cluster



The total field on a site

$$h + (N-1)^{-1} q J \sum_{j \neq i} \sigma_j$$

Scaling of Interaction with N

$$J \rightarrow \frac{J}{N-1}$$

$$E(\vec{\sigma}) = - \left[\frac{q J}{N-1} \right] \sum_{(i,j)} \sigma_i \sigma_j - h \sum_{i=1}^N \sigma_i$$

For a given configuration of spins

$$M = \sum_{i=1}^N \sigma_i$$

This sum is over the $\frac{1}{2} N(N-1)$ distinct pairs of i and j .

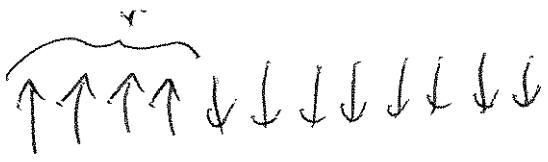
$$E(\vec{\sigma}) = - \frac{1}{2} q J \frac{(M^2 - N)}{N-1} - h M$$

$$E(\vec{\sigma}) = E(M)$$

which is amazing, and not

In finite dimensions

$$\begin{array}{c} E(\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow) \\ \# \\ E(\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow) \end{array}$$



There are $\frac{N}{2}$ arrangements of spins

r up
 $N-r$ down
 $C_N^r = \frac{N!}{r!(N-r)!}$

$$Z = \sum_{r=0}^N C_r$$

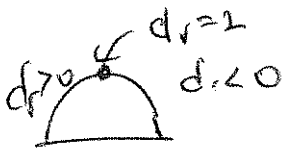
$$C_r = \frac{N!}{r!(N-r)!} \exp \left\{ \frac{1}{2} \beta g J \left[(N-2r)^2 - N \right] / (N-1) + \beta H (N-2r) \right\}$$

$$M = \frac{1}{N} \langle \sum \mu_i \rangle = \left(1 - \frac{2r}{N} \right)$$

$$= \frac{1}{Z} \sum_{r=0}^N (1 - 2r/N) C_r$$

but in practice
One needs only the
peaking electron

$$d_r = \frac{C_{r+1}}{C_r} = \frac{N-r}{r+1} \exp \left\{ -2\beta g J \left(\frac{N-2r-1}{N-1} \right) - 2\beta H \right\}$$



$$\frac{C_{r+1}}{C_r} = 1 \Rightarrow M = \tanh [g J H + H] \beta$$

Mean field exponent

Sp

definition 1.7.9.

free energy
internal energy ~ continuous
specific heat ~ jump

$$1.7.10 \rightarrow \boxed{\alpha = 0}$$

$$\langle E \rangle = -T \frac{\partial}{\partial T} \ln Z$$

$$\boxed{\beta = \frac{1}{T}}$$

$$C = \frac{\partial}{\partial T} E$$

Susceptibility

$$\chi = (-2g J t)^{-1}$$

$$\gamma = \gamma' = 1.$$

$$Z = C_r = \frac{N!}{r!(N-r)!} \exp \left\{ \frac{1}{2} \beta J \frac{(N-2r)^2 - N}{N-1} \right\} \quad [7]$$

\Downarrow
 $M = N - 2r$

$$Z = C_r = \frac{N!}{r!(N-r)!} \exp \left(\frac{1}{2} \beta J \frac{M^2 - N}{N-1} \right)$$

$$\frac{\log Z}{N} = -\beta f = \underbrace{\frac{1}{2} \beta J M^2}_{\text{term of exponential}} \quad \boxed{m^2 = \frac{M}{N}}$$

log prefactor: $N \log N - r \log r - (N-r) \log (N-r)$

$$\frac{N!}{e^{-N} N^N} \quad \Downarrow$$

$$(N-r) = \frac{1}{2} N(1+M)$$

$$r = \frac{1}{2} N(1-M)$$

$$N \log N - \frac{1}{2} N \log \left[\frac{1}{2} N(1-M) \frac{1}{2} N(1+M) \right] + \frac{1}{2} N M \log \left(\frac{1-M}{1+M} \right)$$

replace $M = \tanh \beta J M$ and

$$\log \left(\frac{1 - \tanh x}{1 + \tanh x} \right) = -2x$$

prefactor $\boxed{\frac{1}{2} N \log \frac{4}{1-M^2} - \beta J N M^2}$

$$-\beta f = \frac{1}{2} \log \frac{4}{1-M^2} - \frac{1}{2} \beta J M^2$$

It is not true that
 $\text{Combi} = \text{Entropy}$
 $\text{expo} = \text{Energy}$

A too simple approximation

18

Each spin interacts with a local field h_{mol}

$$\frac{\sinh^2(ahx)}{\cosh^2(ahx)} = \tanh^2(ahx) = x^2$$

↑ ↑ ↓ ↑
↑

$$Z = [2 \cosh h_{weiss} \beta]^N$$

↑ → h_{mol}
 h_{weiss}

Using $m = \tanh(\beta H_{weiss})$

↑ → $h_{weiss} \beta$

$$H = \frac{1}{\beta} \alpha \tanh M$$

$$Z = [2 \cosh \alpha \tanh M]^N = \left[\frac{1}{1 - M^2} \right]^{N/2}$$

$$\alpha \tanh x = \frac{1}{2} \log \left(\frac{1+x}{1-x} \right)$$

44.

Bragg - Williams theory (Better)

$$E = -J [N_{++} - N_{+-} + N_{--}]$$

$$N_+ = N \frac{(1+m)}{2} \quad N_- = N \frac{(1-m)}{2}$$

$$S = -k_B N \left(\frac{N_+}{N} \log \frac{N_+}{N} + \frac{N_-}{N} \log \frac{N_-}{N} \right)$$

Independent site
each site is (+) with probability $\frac{N_+}{N}$
each site is (-) with probability $\frac{N_-}{N}$

$$p_+ \log p_+ + (1-p_+) \log (1-p_+)$$

$$F = E - TS$$

$$\left[\frac{N_+}{N} \right]$$

9

$$N_{++} = N \frac{q}{2} \left(\frac{N_+}{N} \right) \left(\frac{N_+}{N} \right)$$

$$N_{++} = \left[\frac{q}{2} \frac{N_+^2}{N} \right]$$

$$N_{--} = \frac{q}{2} \frac{N_-^2}{N}$$

$$N_{+-} = \frac{q}{2} \frac{N_+ N_-}{N}$$

$$G = -q \frac{JN}{2} m^2 - N \ln m + N k_B \left(\frac{1+m}{2} \log \frac{1+m}{2} + \frac{1-m}{2} \log \frac{1-m}{2} \right)$$

$$\frac{\partial G}{\partial m} = 0 \Rightarrow m = \tanh \left[\beta (qJm + h) \right]$$

as in the argument with Weiss field

$$E = -\frac{1}{2} N m^2 qJ$$

$$\frac{E}{N} = -\frac{1}{2} \frac{N}{N} m^2 qJ = -\frac{1}{2} m^2 qJ$$

$$-\frac{TS}{N} = -\frac{1}{2\beta} \log \frac{4}{1-m^2} + m^2 qJ$$

$$E - TS = -\frac{1}{2} m^2 qJ - \frac{1}{2\beta} \log \frac{4}{1-m^2} + m^2 qJ$$

per particle

Lecture 9

Landau theory / Ginzburg criterium (Transitions and order parameters 2/2)

Lecture 10 (CFP)

STATISTICAL MECHANICS: CONCEPTS & APPLICATIONS

Mean-field theory 2/2:
(1937)

LANDAU THEORY, GINZBURG CRITERION (1960)

1) Review of last week. (see) Homework 09

(we showed that $\gamma = \frac{1}{2} = \gamma'$).

We did not show that $\gamma = 1 = \delta' / \gamma$

$$\chi = -\frac{\partial m}{\partial H} \Big|_{H=0} = (-2\epsilon + J)^{-1}$$

Exact solution of model on complete graph.

$$-\beta F = \frac{1}{2} \log \frac{4}{1-M^2} - \frac{1}{2} \beta J M^2$$

More importantly, we could write

$$Z \sim C_r = \frac{N!}{r!(N-r)!} \exp \left\{ \frac{1}{2} \beta J \frac{(N-2r)^2 - N}{N-1} \right\}$$

$$M = N - 2r$$

$$-\beta F / \text{prefactor} \quad N \log N - \frac{1}{2} N \log \left(\frac{1}{2} N (1-M) \frac{1}{2} N (1+M) \right)$$

$$N! \sim e^{-N} N^N \quad + \frac{1}{2} N M \log \frac{1-M}{1+M}$$

The $N \log N$ terms:

$$N \log N - \frac{1}{2} N \log \left[\frac{1}{4} N^2 \right] = + \frac{1}{2} N \log 4 = \underline{N \log 2}$$

$$-\beta F / \text{prefactor} = \underbrace{-\frac{1}{2} N \log (1-M^2)}_{-M^2 - \frac{M^4}{2}} + \underbrace{\frac{1}{2} N M \log \left(\frac{1-M}{1+M} \right)}_{-2M - \frac{2M^3}{3}} \quad \underline{N \log 2}$$

$$= -\frac{1}{2} M^2 - \frac{1}{12} M^4$$

$$-\beta F|_{\text{exponential}} \simeq \frac{1}{2} \beta g \pi^2$$

total:

$$-\beta F = \frac{1}{2} \beta g \pi^2 - \frac{1}{2} \pi^2 - \frac{1}{12} \pi^4$$

$$\beta f = \left[-\frac{1}{2} \beta g + \frac{1}{2} \right] \pi^2 + \frac{1}{12} \pi^4$$



$$\beta \frac{\partial f}{\partial \pi} = 0 \quad \left[-\beta g + 1 \right] \pi + \frac{1}{3} \pi^3 = 0 \quad \pi = 0$$

or

$$\boxed{\begin{aligned} \pi^2 &= [\beta g - 1] \cdot 3 \\ \pi &= \sqrt{\beta g - 1} \sqrt{3} \end{aligned}}$$

more general

$$G(m, T) = a(T) + \frac{1}{2} b(T) m^2 + \frac{1}{4} c(T) m^4 + \frac{1}{6} d(T) m^6$$

$$\frac{\partial G}{\partial m} = 0 \Rightarrow m(T)$$

$$S = -\frac{\partial G}{\partial T}, \quad C = + \frac{\partial S}{\partial T}.$$

Landau (1936): Connection between symmetry breaking of free energy and 2nd order phase transitions.

A too simple approximation

13

$$Z = [2 \cosh h_{\text{weiss}} \beta]^N$$

Using $m = \tanh(\beta h_{\text{weiss}})$

$$h_{\text{weiss}} = \frac{1}{\beta} \operatorname{atanh} m$$

$$Z = [2 \cosh \operatorname{atanh} m]^N = \left[\frac{1}{1-m^2} \right]^{N/2}$$

too simple

BRAGG WILLIAMS Theory

$$E = -J [N_{++} - N_{+-} + N_{--}]$$

$$N_+ = N \frac{1+m}{2} \quad N_- = N \frac{1-m}{2}$$

$$N_{++} = N \frac{q}{2} \frac{N_+}{N} \frac{N_+}{N} = \frac{q}{2} \frac{N_+^2}{N}$$

$$N_{--} = \frac{q}{2} \frac{N_-^2}{N}$$

$$N_{+-} = q \frac{N_+ N_-}{N}$$

$$S = -k_B N \left[\frac{N_+}{N} \log \frac{N_+}{N} + \frac{N_-}{N} \log \frac{N_-}{N} \right]$$

$$p_+ \log p_+ + (1-p_+) \log (1-p_+)$$

14

The GINZBURG CRITERIUM.

(V. GINZBURG, 1960)

Ising model.

Approximation of Mean-field theory (naive version)
Neglecting fluctuations

Ansatz of mean field theory (better version)

$$\left[(\delta\pi)_{\Omega} \right]^2 \ll \left[M_{\Omega} \right]^2$$

TRICK: Use this Ansatz below T_c .
In a region Ω of the size of the correlation function length

LHS: $\left\langle \left(\sum_{\Omega} (S_i - \langle S_i \rangle) \right)^2 \right\rangle =$

$$= \left\langle \sum_{\substack{i \in \Omega \\ j \in \Omega}} (S_i - \langle S_i \rangle) (S_j - \langle S_j \rangle) \right\rangle$$

$$= N(\Omega) \cdot \sum_{\Omega} \langle S_0 S_i - \langle S \rangle^2 \rangle$$

$$= N(\Omega) \sum_{\Omega} \left[\langle S_0 S_i \rangle - \langle S \rangle^2 \right]$$

Compare with

M
 \uparrow
tot

Compare with:

Total Magnetization in a big volume V

$$M = \sum_{i \in V} S_i e^{-\beta [E + H \sum_j S_j]}$$

$$\frac{\partial \ln}{\partial H} = \sum_{i \in V} \sum_{j \in V} S_i S_j$$

$$\left. \frac{\partial M}{\partial H} \right|_{H=0} = \sum_{j \in V} \langle S_0 S_j \rangle$$

$$\left. \frac{\partial M}{\partial H} \right|_{H=0} = \chi = \sum_{j \in V} \langle S_0 S_j \rangle$$

It follows that

$$\text{LHS: } N(\Omega) \cdot \chi$$

$$\text{RHS: } (N(\Omega))^2 \cdot m^2$$

$$\chi \ll N(\Omega) \cdot m^2$$

$$t^{-\gamma} \ll t^{-\nu d + 2\beta}$$

$$1 \ll t^{-\underbrace{\nu d + 2\beta + \gamma}_{< 0}}$$

$$-\gamma d + 2\beta + \gamma < 0$$

$$2 = 2\beta + \gamma < \nu d$$

$$\boxed{4 < d}$$

$d=4$: upper
critical
dimension

Lecture 10

Kosterlitz-Thouless physics in two dimensions: The XY model (Transitions without order parameters 1/2)

①

The XY (planar rotor) model.
(aka Coulomb gas).

F. Wegner

Kosterlitz and Thouless
J. Phys C 1973

Kostelich
J. Phys. C 1974

$$H = -J \sum_{\langle i, j \rangle} \vec{S}_i \cdot \vec{S}_j = -J \cos(\varphi_i - \varphi_j)$$

S_i and S_j classical spins in the XY plane with $|S|=1$.

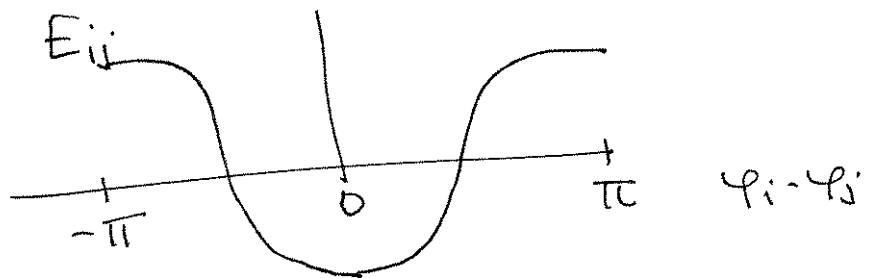
J : Spin stiffness.

Mervin Wagner
Phys. Rev Lett 17, 1133 (1966)

Mermin-Wagner - theorem:
Absence of phase transition

Domany, Schick, Sorensen
Phys. Rev. Lett 52, 1535 (1984)

M. Hasenbusch 5PhA 2005



At high temperature; this model must be disordered for temperatures. This can be shown through standard high-temperature expansion. It can also be shown using GRIFITHS inequality that

using GRIFITHS
inequality that

- Subjects
- Splines
- Vortices
- Exact Results
- Nonanalyticities

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle_{J, 2\beta} \leq \langle \sigma_i \cdot \sigma_j \rangle_{J\beta}.$$

\uparrow \uparrow
 XY model. Ising model

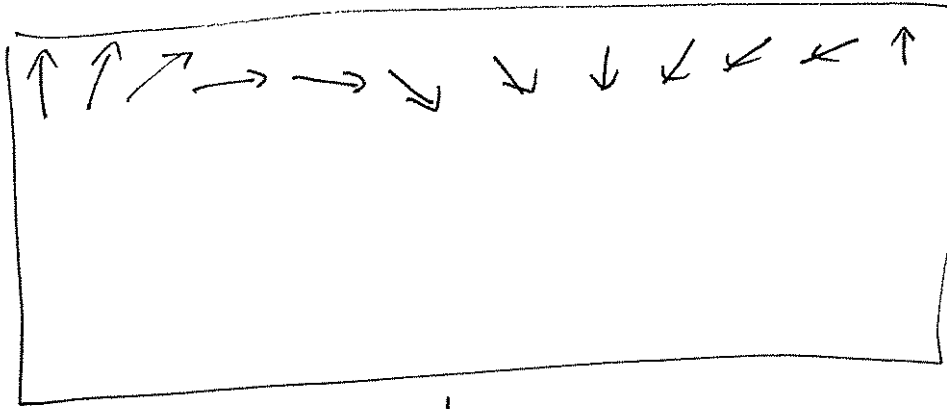
One d: $\int d\theta_1 \dots d\theta_L = 2\pi \prod_{j=2}^L \int_0^{2\pi} d\theta_j e^{i\theta_j}$ BJ was θ

$F = -\frac{1}{2\pi} \log(2\pi I_0(\beta J))$

Spin waves

(2)

L



$$\Delta\phi = \begin{cases} \frac{2\pi}{L} & \text{if horizontal link} \\ 0 & \text{if vertical link} \end{cases}$$

$$\text{total energy} \sim L^2 \cdot \frac{2\pi^2}{L} \sim 4\pi^2 = \text{constant}$$

if you suppose that you have many different types & orientations of spin waves, then you would expect that at low temperature, there is no spontaneous magnetization.

Spin correlation functions:

At high temperature $T \gg 2J$, you would expect that the correlation functions are exponentially decaying.

Let us next study what is going on at low temperature.

Lüscher &
Weisz 1988

vegus 1967

(3)

"We consider a D-dimensional system of classical spins rotating in a plane and interacting via a Heisenberg coupling...."

$$H = -\frac{1}{2} \sum_{\vec{r}, \vec{r}'} I(\vec{r} - \vec{r}') \cos(\varphi_{\vec{r}} - \varphi_{\vec{r}'})$$

in low temperature approximation

$$H = -\frac{N}{2} \sum_{\vec{r}} I(\vec{r}) + \frac{1}{4} \sum_{\vec{r}, \vec{r}'} (\varphi_{\vec{r}} - \varphi_{\vec{r}'})^2$$

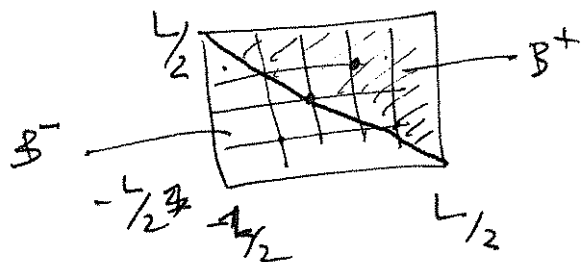
$$\varphi_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_{\vec{r}} e^{-i\vec{k}\cdot\vec{r}} \varphi_{\vec{r}} \quad \varphi_{\vec{r}} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \varphi_{\vec{k}}$$

$$\varepsilon_{\vec{k}} = \sum_{\vec{r}} I(\vec{r}) \cdot (1 - \cos \vec{k} \cdot \vec{r}) = 2 \sum_{\vec{r}} I(\vec{r}) \sin^2\left(\frac{\vec{k} \cdot \vec{r}}{2}\right)$$

$$H = -\frac{N}{2} \sum_{\vec{r}} I(\vec{r}) + \frac{1}{2} \sum_{\vec{k}} \varepsilon_{\vec{k}} \varphi_{\vec{k}} \varphi_{-\vec{k}}$$

where

$$\varphi_{\vec{k}} = \frac{1}{L} \sum_{\vec{r}}$$



$$\varphi_{\vec{k}} = \frac{2\pi i \hbar k}{L}$$

$$k \cdot L =$$

$$\varphi_{\vec{k}} = \frac{1}{\sqrt{2}} (\varphi_{\vec{k}} + \varphi_{-\vec{k}}) \quad \varphi_{-\vec{k}} = \frac{1}{i\sqrt{2}} (\varphi_{\vec{k}} - \varphi_{-\vec{k}})$$

and get $H = -\frac{N}{2} \sum_{\vec{r}} I(\vec{r}) + \frac{1}{2} \sum_{\vec{k}} \varepsilon_{\vec{k}} \varphi_{\vec{k}}^2$

(4)

$$g(\vec{r}) = \langle \cos(\varphi_0 - \varphi_{\vec{r}}) \rangle = \text{Re} \langle \exp(i(\varphi_0 - \varphi_{\vec{r}})) \rangle$$

↑
Spin correlation function

$$\varphi_0 - \varphi_{\vec{r}} = \sqrt{\frac{2}{N}} \sum_{\vec{k} \in B^+} \left(\gamma_{\vec{k}} (1 - \cos \vec{k} \cdot \vec{r}) + \gamma_{-\vec{k}} \sin \vec{k} \cdot \vec{r} \right)$$

It follows

$$g(\vec{r}) = \frac{\int d^N \gamma_{\vec{k}} \exp(-\beta H + i(\varphi_0 - \varphi_{\vec{r}}))}{\int d^N \gamma_{\vec{k}} \exp(-\beta H)}$$

$$= \exp \left(-\frac{2k_B T}{N} \sum_{\vec{k}} \frac{\sin^2 \left(\frac{\vec{k} \cdot \vec{r}}{2} \right)}{\varepsilon_{\vec{k}}} \right)$$

$$\varepsilon_{\vec{k}} = \begin{cases} I & \text{nearest neighbors} \\ 0 & \text{otherwise} \end{cases}$$

$$\varepsilon_{\vec{k}} = 4I \sum_{i=1}^D \sin^2 \frac{k_i}{2}$$

In one dimension $\underline{g_1(r)} = \exp \left(-\frac{k_B T |r|}{2I} \right)$

In two dimensions $\underline{g_2(r)} = \exp \left(-\frac{k_B T}{I} \left(\text{freq} + \text{const} + \frac{1}{2\pi} \ln r \right) \right)$
 $\sim \exp(-k_B T / 2\pi I)$

In three dimensions $\underline{g_3(r)} = \exp(-k_B T f_3(\infty) / I)$

$$f_3(\infty) = \frac{1}{\pi^3} \int_0^\pi d^3 k \frac{I}{\varepsilon_{\vec{k}}}$$

Wegner 1967

On 10/16/2016 08:17 PM, Ze Lei wrote:

Hi Werner,

Here I collected some data:

The core energy: $E_{\text{core}} = E_{\text{total}} - \pi \ln L$ (as $a = 1$)

for $L = 8$, energy = 8.63203435584 , core energy = 2.09927608493
 for $L = 16$, energy = 10.8240288449 , core energy = 2.11368448373
 for $L = 32$, energy = 13.0050815665 , core energy = 2.11715111498
 for $L = 64$, energy = 15.1835264432 , core energy = 2.11800990142
 Then Tommaso helped using C, and run for quite long:
 $L = 1024$, energy = 23.8941552245, core energy = 2.11829432

I think it almost converged.

Vortex pair energy and J_R calculation

As for a **vortex-antivortex pair** (I use core energy = 2.118, $E_{\text{pair}} = E_{\text{total}} - 2E_{\text{core}}$)

$L = 64$ (dst is the horizontal displacement from vortex to antivortex, the real distance should be multiplied by $\sqrt{2}$)

dst = 3, E = 21.263989
 dst = 4, E = 22.971028
 dst = 5, E = 24.207665
 dst = 6, E = 25.137539
 dst = 7, E = 25.845934
 dst = 8, E = 26.383322
 dst = 9, E = 26.782272

$E_{\text{pair}} - \ln(\text{dst})$ or $(E - \ln(\text{dst}))$ is almost linear:

$E = 5.0518 \text{ dst} + \mathbf{15.91729729}$, correlation coefficient: $r = 0.9965$

the rest of the energy is far from twice the core energy. Since the theory treated a quite distance pair, it may be acceptable.

From the thesis, the factor should be $\pi * J_R$, then $J_R(T = 0) \sim 1.137$, quite close to 1, it's almost self-consistent.

This may make a good homework.

--
 Massive open online course

Statistical Mechanics: Algorithms and Computations

3rd edition running (self-paced): <https://www.coursera.org/learn/statistical-mechanics>

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.rtex-homework(cosine models)

Subject: vortex-homework(cosine models)

From: Ze Lei <leizelaser@gmail.com>

Date: 10/16/2016 08:17 PM

To: Werner Krauth <krauth@tournesol.lps.ens.fr>

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(5)

In two dimensions,
the XY model, in harmonic approximation,
shows algebraic order, with correlation function

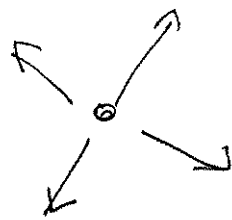
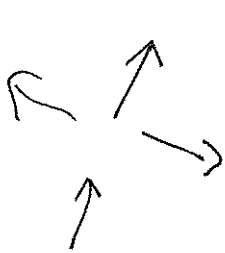
$$\cos(\varphi_0 - \varphi_r) \sim \frac{1}{\sqrt{\text{const} \cdot r}}$$

This connects well with the ground state
of the system, where $\cos(\varphi_0 - \varphi_r) = 1 = \frac{1}{\sqrt{r_0}}$

This calculation, and the calculation of the susceptibility

$$\chi = \frac{\partial m}{\partial h} = \beta \sum_{\vec{r}} \langle \vec{g}(\vec{r}) \rangle,$$

suggest that there must be a phase transition
at some temperature.



$n=+1$



$n=-1$

/// same configuration



$$\oint_C \vec{\nabla} \Theta d\vec{l} = 2\pi g$$

The appearance of vortices can be shown by the famous free-energy argument

$$|\vec{\nabla} \Theta| \sim \frac{1}{r}$$

$$E_{\text{vortex}} = \frac{1}{2} J_R \int_0^L 2\pi r \frac{1}{r^2} dr + E_c$$

$$= \pi J_R \log \frac{L}{a} + E_c$$

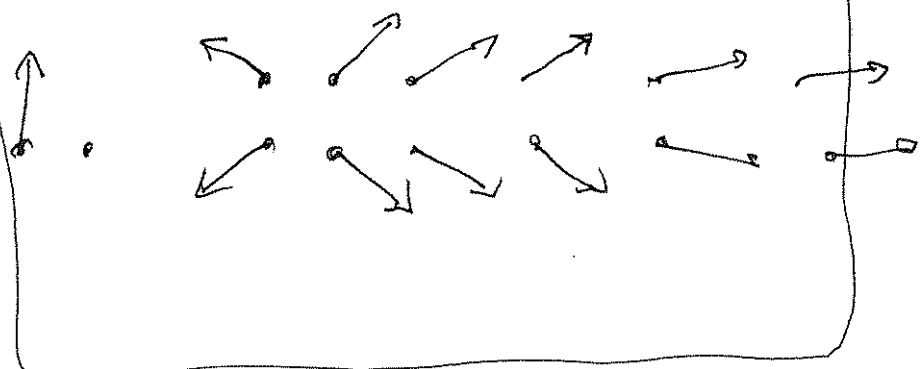
J_R : Renormalized spin stiffness

The vortex energy has a precise ~~best~~ meaning

$L \times L$

Lattice

find local minimum



$$\Delta E_{16-8} = \frac{10.824}{8.632} = 2.192$$

$$E =$$

$$\Delta E_{32-16} = \frac{13.005}{10.824} = 2.181$$

$$\Delta E_{64-32} = \frac{15.18352}{13.00598} = 2.17844$$

$$\pi \cdot J_R \cdot [\log 16 - \log 8]$$

$$2.178 = \pi \cdot J_R \cdot \log 2$$

$$\boxed{J_R = 1.0}$$

$$J_R(T) = J_R(T_k) \left[1 + c \cdot (T_k - T)^{1/2} \right]$$

$$\beta = \frac{2}{\pi} \sim 0.17$$

$$J_R = 1$$

$$\Delta E_{64} = 15.18352 = \pi \cdot \log 64 + E_c$$

$$\boxed{E_c = 2.118}$$

The Famous Kosterlitz-Thouless argument.

8

$$E_v = \pi J_R \log \frac{L}{a} + E_c$$

$$S_v = k_B \cdot \log \frac{L^2}{a^2}$$

$$\pi J_R \log \frac{L}{a} + E_c - \frac{2}{\beta} \log \frac{L}{a}$$

$$F_v = \left[\pi J_R - \frac{2}{\beta} \right] \log \frac{L}{a}$$

$$\boxed{\beta J_R > \frac{2}{\pi}} : F_v \rightarrow \infty$$

Single vortex cannot be supported -

Therefore, a phase transition takes place

at..... $\boxed{\beta_{KT} J_R = \frac{2}{\pi}}$

$$U_{ij}(r_{ij}) \sim -\pi J_R q_i q_j \log \left(\frac{r_{ij}}{a} \right)$$

$$\sim \pi J_R \log \left(\frac{r_{ij}}{a} \right)^{\beta \pi J_R}$$

$$e^{-\log \left[\left(\frac{r_{ij}}{a} \right)^{\beta \pi J_R} \right]}$$

$$\left(\frac{r_{ij}}{a} \right)^{-\beta \pi J_R}$$

$$\sim r_{ij}^{-2} \quad \text{at } T_{KT}$$