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On the ISING model of ferromagnetism

by

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1. Introduction

One of the order-disorder problems in quantum statistics concerns the model of ferromagnetism originally proposed by E. ISING (1925). For detailed discussions of this model and the results obtained with it we refer to the paper of G.F. NEWELL and E.W. MONTROLL (1953). Only the relevant features will be reproduced here.

Let be given a lattice with n lattice sites, each site being occupied by a spin. The spins are assumed to be numbered $1,\dots,n$. Each spin is capable of two orientations which characterize it as a +spin or a -spin. Let there be r_1 +spins and $(n-r_1)$ -spins and assume they are distributed over the lattice in a given way.

In the absence of an outside magnetic field the free energy of the system is assumed to be the sum of the interaction energies of each pair of spins. Let the interaction energy between spin i and j be $-m_{ij}$ $(i,j=1,\dots,n;\ i\neq j)$, and take $m_{ii}=0$ $(i=1,\dots,n)$.

Define quantities x_{ij}^{+}, x_{ij}^{-}, y_{ij}, v_{ij} as follows. For $i\neq j$, $i,j=1,\dots,n$,

$$x_{ij}^{+} = \begin{cases} 1 \text{ if spins } i \text{ and } j \text{ are both +spins,} \\ 0 \text{ if not,} \end{cases}$$

$$x_{ij}^{-} = \begin{cases} 1 \text{ if spins } i \text{ and } j \text{ are both -spins,} \\ 0 \text{ if not,} \end{cases}$$

$$y_{ij} = \begin{cases} 1 \text{ if spins } i \text{ and } j \text{ have unequal signs,} \\ 0 \text{ if not,} \end{cases}$$

for $i=1,\dots,n$ $\quad x_{ii}^{+}=x_{ii}^{-}=y_{ii}=0,$

for $i,j=1,\dots,n$

$$v_{ij} = x_{ij}^{+}+x_{ij}^{-}-y_{ij}. \tag{1.1}$$

Next put

$$x_{+} = \sum_{i,j} m_{ij}x_{ij}^{+},$$

$$x_{-} = \sum_{i,j} m_{ij}x_{ij}^{-},$$

$$y = \sum_{i,j} m_{ij}y_{ij},$$

$$v = \sum_{i,j} m_{ij}v_{ij},$$

thus

$$v = x_{+}+x_{-}-y. \tag{1.2}$$

From the assumptions it then follows that the free energy of the system of spins is equal to $-\frac{v}{2}$. The problem concerned with this model centers around the calculation of the partitionfunction

$$Z = \sum_{r=0}^{n} \sum_{v} g(r,v) \exp\left(\frac{v}{2kT}\right), \tag{1.3}$$

where $g(r,v)$ is the number of ways in which r +spins and $n-r$ -spins can be distributed over the lattice such that the free energy due to spin interactions is equal to $-\frac{v}{2}$, k is BOLTZMANN's constant and T the absolute temperature.

In papers on this problem usually the assumption is introduced that the lattice-ends are joined in a cyclic way, or that the lattice is wrapped around a torus. In our case a similar assumption will be made, viz. that for $i=1,\ldots,n$

$$\sum_j m_{ij} = m, \quad \text{independent of } i. \tag{1.4}$$

Let the +spins have the numbers $\nu_1,\ldots\nu_r$. Then in

$$2\sum_{\mu=1}^{r} \sum_{j=1}^{n} m_{\nu_\mu,j}$$

every contribution m_{ij} between a pair of ++spins is included twice, and the contribution between each pair of spins with unequal sign is included once. Thus

$$2\sum_{\mu=1}^{r} \sum_{j=1}^{n} m_{\nu_\mu,j} = 2\sum_{ij} m_{ij} x_{ij}^{+} + \sum_{ij} m_{ij} y_{ij},$$

and by (1.4)

$$2rm = 2x_+ + y.$$

In the same way

$$2(n-r)m = 2x_- + y,$$

and from (1.2) then follows that

$$v = 4x_+ + nm - 4rm. \tag{1.5}$$

We now rephrase the problem in statistical terminology. Given the value of r, the quantity v can take only a finite number of values, say $v_1,\ldots,v_Q$. Then

$$\frac{g(r,v_h)}{\sum_j g(r,v_j)} \tag{1.6}$$

can be interpreted as a probability, viz. the probability that in distributing r + and $n-r$ -spins at random over the lattice sites, the interaction takes the value $-v_h$ $(h=1,\ldots,Q)$. In distributing the spins at random the quantities x_{ij}^{+}, x_{ij}^{-}, y_{ij}, v_{ij}, x_{+}, x_{-}, y and v become random variables. In order to distinguish clearly between symbols of random variables and values taken on by them, the symbols of the random variables will be underlined. Thus

$$P[\underline{v} = v_h | r] = \frac{g(r, v_h)}{\sum_j g(r, v_j)} .$$

Next observe that $\sum_j g(r, v_j)$ is the number of ways in which r +spins and $n-r$-spins can be distributed over n sites, which is $\binom{n}{r}$. Thus

$$Z = \sum_{r=0}^{n} \sum_{h=1}^{\alpha} \binom{n}{r} P[\underline{v} = v_h | r] \exp\left\{ \frac{v_h}{2kT} \right\} . \tag{1.7}$$

Denoting the mathematical expectation of a function $f(\underline{v})$ of $\underline{v}$, given the value of r, by $E_r f(\underline{v})$, then by definition (1.7) is equal to (writing $\beta = \frac{1}{2kT}$),

$$Z = \sum_{r=0}^{n} \binom{n}{r} E_r \exp(\beta \underline{v}), \tag{1.8}$$

or as (1.5) holds a.c. for the random variables $\underline{v}$ and $\underline{x}_{+}$

$$Z = \sum_{r=0}^{n} \binom{n}{r} \exp\{\beta m(n-4r)\} E_r \exp(4\beta \underline{x}_{+}). \tag{1.9}$$

The properties of the random variables $\underline{x}_{+}$, $\underline{x}_{-}$ and $\underline{y}$ have been the subject of a study which will be presented in a forthcoming thesis. Some results have been given in A.R. BLOEMENA (1960).

2.

In dealing with the moments of the random variables like $\underline{x}$, one can profitable use some concepts from the theory of graphs. For our purpose a (k,l)-graph consists of k oriented joins, labelled $1,\ldots,k$, between l points, such that no points are isolated and no loops occur. Two (k,l)-graphs are equivalent if they can be mapped on one another without changing the labelling of the joins. This gives a classification of graphs in equivalence classes. For our purpose a class of equivalent graphs will be considered as one graph. Two distinct (that is: non-equivalent) (k,l)-graphs have the same (k,l)-configuration if they can be made equivalent by permuting the join-labels and (or) changing the orientation of some joins of one of the graphs. This gives a classification of distinct graphs in configuration classes. By a "configuration of a graph" is meant the configuration class to which it belongs.

A graph is connected if from every point every other one can be reached by travelling along the joins, neglecting their orientations. Each graph consists of one or more connected components. Permutation of the components does not affect either the graph or the configuration of the graph. The components may of course be labelled, but such a labelling is not to be considered as part of the labelling of the graph.

For a connected (k,l)-graph we have $2 \leqslant l \leqslant k+1$, and there are a finite number, say $q_{k,l}$, of different connected (k,l)-configurations. Let $C_{k,l}^{(\alpha)}$ be the α-th one $(\alpha = 1, \ldots, q_{k,l})$.

The configuration of a graph with h connected components can be indicated symbolically by $\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}$, if $C_{k_i,l_i}^{(\alpha_i)}$ is the configuration of the i-th component. Two alternative ways of indicating a configuration are also used, viz. $\sum_{j=1}^{s} g_j C_{k_j,l_j}^{(\alpha_j)}$, if g_j components have the same configuration $C_{k_j,l_j}^{(\alpha_j)}$, and sometimes the configuration is indicated by a graph having this configuration, e.g. $\square$.

Let $\mathcal{N}(C)$ be the number of distinct graphs having the configuration C . A combinatorial argument leads in a simple way to the relation

$$\mathcal{N}\Big(\sum_{j=1}^{s} g_j C_{k_j,l_j}^{(\alpha_j)}\Big) = k! \prod_{j}^{s} \frac{1}{g_j!} \Big\{ \frac{\mathcal{N}(C_{k_j,l_j}^{(\alpha_j)})}{k_j!} \Big\}^{g_j} ; \qquad \Big(\sum_j k_j g_j = k\Big), \qquad (2.1)$$

while for $\mathcal{N}(C_{k,l}^{(\alpha)})$ a recurrence relation can be found. We have e.g.

$\mathcal{N}(\cdot\!\!-\!\!\!-\!\!\cdot) = 1$

$\mathcal{N}(:\!=\!=\!:) = 1$

$\mathcal{N}(\cdot\!-\!\cdot\!-\!\cdot) = 4$

$\mathcal{N}(\cdot\!\!\subset\!\!\supset\!\!\cdot) = 2.$

For 3, 4, 5, 6 joins there are 8, 23, 66, 212 distinct configurations (cf. R.J. RIDELL and G.E. UHLENBECK (1953)).

In the following we shall be interested especially in configurations which in every point an even number of joins meet. These configurations will be called <u>even joined</u>.

Let be given numbers w_{ij} $(i,j = 1, \ldots, n)$ satisfying $w_{ii} = 0$ and $w_{ij} = w_{ji}$. Consider from $(\sum_{ij} w_{ij})^k$ one term

$$t = w_{\tau_1,\tau_2} \ldots . w_{\tau_{2k-1},\tau_{2k}} \qquad (\tau_{2j-1} \neq \tau_{2j},\ j = 1, \ldots, k).$$

Amongst the subscripts $\tau_1,\ldots,\tau_{2k}$, say l unequal numbers from $1,\ldots,n$ occur. Let these numbers be $\lambda_1,\ldots,\lambda_l$ with $\lambda_1<\ldots<\lambda_l$. Each of the τ's is equal to one of the λ's. Let

$$\tau_{2j-1}=\lambda_{\mu_j},\ \tau_{2j}=\lambda_{\nu_j}$$

then

$$t=w_{\lambda_{\mu_1},\lambda_{\nu_1}}\cdots w_{\lambda_{\mu_k},\lambda_{\nu_k}}\quad(\mu_j\neq\nu_j,\ j=1,\ldots,k).$$

To each set of numbers $\mu_1,\ldots\mu_k,\nu_1,\ldots,\nu_k$ - and therefore to t - there corresponds a graph in the following way. Take l points numbered $1,\ldots,l$. The j-th join connects the points numbered μ_j and ν_j, and is directed from μ_j to ν_j. Omit the labels of the points. As the numbering of the points does not enter in the classifications of the graphs, it follows that the two terms

$$w_{\lambda_{\mu_1},\lambda_{\nu_1}}\cdots w_{\lambda_{\mu_k},\lambda_{\nu_k}}\quad\text{and}\quad w_{\theta_{\mu_1},\theta_{\nu_1}}\cdots w_{\theta_{\mu_k},\theta_{\nu_k}},$$

where $\theta_1,\ldots,\theta_l$ is a permutation of $\lambda_1,\ldots,\lambda_l$, have equivalent graphs. Further considerations show that all $l!$ terms of $(\sum_{ij}w_{ij})^k$, having the same (k,l) graph corresponding to the numbers $\mu_1,\ldots\mu_k,\nu_1,\ldots,\nu_k$, can be written as

$$\sum_{\substack{\theta_1=1\\(\theta_1,\ldots,\theta_l)\neq}}^{h}\cdots\sum_{\theta_l=1}^{n} w_{\theta_{\mu_1},\theta_{\mu_2}}\cdots w_{\theta_{\mu_k},\theta_{\nu_k}},\tag{2.2}$$

while all $l!$ terms corresponding to a distinct (k,l)-graph having the same configuration have the same value as (2.2). As there are $\mathcal{N}(\ )$ distinct graphs with the same configuration, the value of the terms in $(\sum_{ij}w_{ij})^k$ corresponding to graphs having a given configuration $\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}$ is

$$\mathcal{N}\Big(\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}\Big)\sum_{\substack{\theta_1=1\\(\theta_1,\ldots,\theta_l)\neq}}^{n}\cdots\sum_{\theta_l=1}^{n} w_{\theta_{\mu_1},\theta_{\nu_1}}\cdots w_{\theta_{\mu_k},\theta_{\nu_k}},\tag{2.3}$$

where to the numbers $\mu_1,\ldots,\mu_k,\nu_1,\ldots,\nu_k$ a graph corresponds with configuration $\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}$. (2.3) will be denoted symbolically by

$$\mathcal{N}\Big(\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}\Big)\Sigma^*\Big\{w^{(1)}\ldots w^{(k)}\Big|\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}\Big\}.$$

Let $\Sigma^*_{\lfloor k,l,h\rfloor}$ mean a summation over all configurations with h connected component ,with in all k joins and l points, then

$$(\sum_{ij}w_{ij})^k=\sum_{l=2}^{2k}\sum_{h=1}^{[\frac{l}{2}]}\Sigma^*_{\lfloor k,l,h\rfloor}\mathcal{N}\Big(\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}\Big)\Sigma^*\Big\{w^{(1)}\ldots w^{(k)}\Big|\sum_{i=1}^{h}C_{k_i,l_i}^{(\alpha_i)}\Big\}.\tag{2.4}$$

While $\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} w_{ij}w_{jk}w_{kl}w_{li}$ is indicated symbolically by $\Sigma^*\{m^{(1)}\cdots m^{(4)}|\square\}^{(ijkl)\neq}$, we also need symbols for the same type of sums but without the inequality restriction on the sum, thus for e.g. $\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} w_{ij}w_{jk}w_{kl}w_{li}$. For this sum we use the notation $\Sigma\{w^{(1)}\cdots w^{(4)}|\square\}$, though not to all terms of the sum there corresponds a graph with configuration $\square$. In general $\Sigma\{w^{(1)}\cdots w^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\}$ indicates the same sum as $\Sigma^*\{w^{(1)}\cdots w^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\}$, but without the inequality restrictions imposed on the latter sum. The sums $\Sigma^*\{\ldots\}$ can be expressed in terms of $\Sigma\{\ldots\}$, thus e.g.

$$\Sigma^*\{w^{(1)}\cdots w^{(4)}|\square\} = \Sigma\{w^{(1)}\cdots w^{(4)}|\square\} - 2\Sigma\{w^{(1)}\cdots w^{(4)}|\infty\} + \\ + \Sigma\{w^{(1)}\cdots w^{(4)}|\ominus\}, \tag{2.5}$$

and in general

$$\Sigma^*\{w^{(1)}\cdots w^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\} = \sum_{l'=2}^{l}\sum_{h'=1}^{[\frac{l'}{2}]}\Sigma^*_{\lfloor k,l',h'\rfloor}\, \mathcal{A}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)};\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)}) \cdot \\ \cdot\Sigma\{w^{(1)}\cdots w^{(k)}|\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)}\}. \tag{2.6}$$

Of course (2.4) does not change if instead of numbers w_{ij} are random variables satisfying $\underline{w}_{ii}=0$ a.c., and $\underline{w}_{ij}=\underline{w}_{ji}$.

The random variable $\underline{v}_{ij}$ has the following property. The mathematical expectation of a product of v_{ij}'s, e.g.

$$\underline{v}_{\tau_1,\tau_2}\cdots\underline{v}_{\tau_{2k-1},\tau_{2k}} \tag{2.7}$$

does not depend on the actual values of $\tau_1,\ldots,\tau_{2k}$, but only on the configuration of the graph corresponding to the product. If this configuration is $\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}$, we indicate the expectation of (2.7) by

$$E(\underline{v}^{(1)}\cdots\underline{v}^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}).$$

From this property it follows that if in (2.4) w_{ij} is replaced by $m_{ij}\underline{v}_{ij}$, and expectations are taken, that

$$E\underline{v}^k = \sum_{l=2}^{2k}\sum_{h=1}^{[\frac{l}{2}]}\Sigma^*_{\lfloor k,l,h\rfloor}\, \mathcal{N}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)})\, E(\underline{v}^{(1)}\cdots\underline{v}^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}) \cdot \\ \cdot\Sigma^*\{m^{(1)}\cdots m^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\}. \tag{2.8}$$

From the properties of the distribution of $\underline{x}_+$, $\underline{x}_-$ and $\underline{y}$, (cf. A.R. BLOEMENA (1960)) one can derive that

$$\sum_{r=0}^{n}\binom{n}{r} E(\underline{v}^{(1)}\cdots\underline{v}^{(k)}|\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}) = \begin{cases} 0 & \text{if either } \sum_{i=1}^{h} l_i > n \text{ or } \sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \\ & \text{is not even joined, or both,} \\ 2^n & \text{if } \sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \text{ is even joined and } \\ & \sum_{i=1}^{h} l_i \le n. \end{cases} \tag{2.9}$$

3. The expansion of Z for high temperatures

Assume that there exists a positive constant β_1, such that for $0 \le \beta < \beta_1$, $E\exp(\beta \underline{v})$ converges. Small values of β correspond to high values of the temperature. From (1.8)

$$Z = \sum_{r=0}^{n}\binom{n}{r}\sum_{k=0}^{\infty}\frac{\beta^k}{k!}E\underline{v}^k = 2^n + \sum_{k=1}^{\infty}\frac{\beta^k}{k!}\sum_{r=0}^{n}\binom{n}{r}E\underline{v}^k =$$

$$= 2^n + \sum_{k=1}^{\infty}\frac{\beta^k}{k!}\cdot\sum_{l=2}^{2k}\sum_{h=1}^{[\frac{l}{2}]}\sum{}^{*}_{\lfloor k,l,h\rfloor}\mathcal{N}\Big(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i}\Big)\cdot$$

$$\cdot\sum{}^{*}\{m^{(1)}\ldots m^{(k)}\mid \sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i}\}\sum_{r=0}^{n}\binom{n}{r}E(v^{(1)}\ldots v^{(k)}\mid \sum C^{(\alpha_i)}_{k_i,l_i}).$$

Let $\sum^{*''}_{\lfloor k,l,h\rfloor}$ mean a summation over all even joined configurations with h connected components, l points and k joins, then by (2.9)

$$Z = 2^n\Big[1 + \sum_{k=2}^{\infty}\frac{\beta^k}{k!}\sum_{l=2}^{\min(n,k)}\sum_{h=1}^{[\frac{l}{2}]}\sum{}^{*''}_{\lfloor k,l,h\rfloor}\mathcal{N}\Big(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i}\Big)\sum{}^{*}\{m^{(1)}\ldots m^{(k)}\mid\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i}\}\Big] \quad (3.1)$$

where in the upper summation limit for l $2k$ has been changed into k, as even joined configurations have at least as many joins as they have points, and as for $k=1$ no even joined configuration exists the lower summation limit of k becomes 2.

(3.1) is usually called the high temperature expansion of Z. Assuming n to be large we shall write down in a more explicit way the terms with $\beta^2,\ldots,\beta^6$. In order to simplify the notation we write e.g.

$\sum^{*}(\circ\,\circ)$ instead of $\sum^{*}\{m^{(1)}\ldots m^{(4)}\mid \circ\,\circ\}$

and

$\sum(\circ\,\circ)$ instead of $\sum\{m^{(1)}\ldots m^{(4)}\mid \circ\,\circ\}$.

Of course

$$\sum(\circ\,\circ) = \big(\sum(\circ)\big)^2.$$

Tables 3.1, 3.2, 3.3 list the configurations involved for $k = 4$, 5 and 6, together with the quantity $\mathcal{N}(\;)$, and the coefficients $\mathcal{A}(\ldots;\ldots)$. (cf. (2.6)).

Tables 3.1 - 3.3 $\mathcal{A}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\,;\,\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)})$ and $\mathcal{N}(\sum_{i=1}^{k} C_{k_i,l_i}^{(\alpha_i)})$ for even joined configurations with $\sum k_i = \sum k'_i = k$, $k=4$, 5 and 6.

Table 3.1; k=4

$\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)} \rightarrow$ / $\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \downarrow$					$\mathcal{N}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)})$
	+1		-4	+2	12
		+1	-2	+1	48
			+1	-1	48
				+1	8

Table 3.2; k=5

$\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)} \rightarrow$ / $\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \downarrow$					$\mathcal{N}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)})$
	+1		-6	+6	160
		+1	-5	+5	384
			+1	-2	960
				+1	320

Table 3.3; k=6

$\sum_{i=1}^{h'} C_{k'_i,l'_i}^{(\alpha'_i)} \rightarrow$ / $\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \downarrow$																$\mathcal{N}(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)})$
	+1				-12			+6	+24		+16		-48	-8	+16	120
		+1				-9				+18				-6		640
			+1		-2		-8	+1	+8	+4	+8	+8	-24	-4	+8	1440
				+1		-3	-6		+3	+9	+4	+6	-12	-4	+3	3840
					+1			-1	-4		-2		+10	+2	-4	1440
						+1				-4				+2		5760
							+1		-1	-1	-1	-2	+5	+1	-2	11520
								+1					-4		+2	240
									+1				-2	-1	+1	2880
										+1				-1		960
											+1		-3		+2	3840
												+1	-2		+1	5760
													+1		-1	960
														+1		960
															+1	32

For $k=2$ there is one even joined configuration, viz. $\bigcirc$, while $\mathcal{N}(\bigcirc)=2$, and $\Sigma^*(\bigcirc)=\Sigma(\bigcirc)$. For $k=3$ there is also one even joined configuration, viz. $\triangle$, with $\mathcal{N}(\triangle)=8$, and $\Sigma^*(\triangle)=\Sigma(\triangle)$.

Using (2.6) we obtain for (3.1)

$$
\begin{aligned}
Z = {} & 2^n[1+\beta^2\Sigma(\bigcirc)+\tfrac{4}{3}\beta^3\Sigma(\triangle)+\beta^4\{\tfrac{1}{2}(\Sigma(\bigcirc))^2+2\Sigma(\square)+\\
& -4\Sigma(\infty)+\tfrac{4}{3}\Sigma(\ominus)\}+\beta^5\{\tfrac{4}{3}\Sigma(\triangle)\cdot\Sigma(\bigcirc)-16\Sigma(\triangle\bigcirc)+\tfrac{16}{5}\Sigma(\pentagon)+\\
& +10\tfrac{2}{3}\Sigma(\triangle)\}+\beta^6\{\tfrac{1}{6}(\Sigma(\bigcirc))^3+\tfrac{8}{9}(\Sigma(\triangle))^2-4\Sigma(\infty)\Sigma(\bigcirc)+\\
& +2\Sigma(\square).\Sigma(\bigcirc)+\tfrac{4}{3}\Sigma(\ominus)\cdot\Sigma(\bigcirc)+\tfrac{16}{3}\Sigma(\hexagon)-16\Sigma(\bowtie)+\\
& -32\Sigma(\square\bigcirc)+32\Sigma(\triangleleft\bigcirc\triangleright)+21\tfrac{1}{3}\Sigma(\cdots)+21\tfrac{1}{3}\Sigma(\cdots)+\\
& -42\tfrac{2}{3}\Sigma(\ominus\bigcirc)-10\tfrac{2}{3}\Sigma(\triangle)+6\tfrac{2}{45}\Sigma(\ominus)\}+\ldots\ldots],
\end{aligned}
$$

which suggests for the "partition function per spin", which is the n-th root of the partition function

$$
\begin{aligned}
[Z''']^{\frac{1}{n}} = {} & 2[1+\beta^2\tfrac{1}{n}\Sigma(\bigcirc)+\tfrac{4}{3}\beta^3\tfrac{1}{n}\Sigma(\triangle)+\beta^4\{\tfrac{1}{2}(\tfrac{1}{n}\Sigma(\bigcirc))^2+\tfrac{2}{n}\Sigma(\square)+\\
& -\tfrac{4}{n}\Sigma(\infty)+\tfrac{4}{3n}\Sigma(\ominus)\}+\beta^5\{\tfrac{4}{3}(\tfrac{1}{n}\Sigma(\triangle))(\tfrac{1}{n}\Sigma(\bigcirc))-\tfrac{16}{n}\Sigma(\triangle\bigcirc)+\\
& +\tfrac{16}{5n}\Sigma(\pentagon)+10\tfrac{2}{3}\cdot\tfrac{1}{n}\Sigma(\triangle)\}+\beta^6\{\tfrac{1}{6}(\tfrac{1}{n}\Sigma(\bigcirc))^3+\tfrac{8}{9}(\tfrac{1}{n}\Sigma(\triangle))^2+\\
& -4(\tfrac{1}{n}\Sigma(\infty))(\tfrac{1}{n}\Sigma\bigcirc)+2(\tfrac{1}{n}\Sigma(\square))(\tfrac{1}{n}\Sigma(\bigcirc))+\tfrac{4}{3}(\tfrac{1}{n}\Sigma(\ominus))(\tfrac{1}{n}\Sigma(\bigcirc))+\\
& +\tfrac{16}{3n}\Sigma(\hexagon)-\tfrac{16}{n}\Sigma(\bowtie)+\ldots\ldots+6\tfrac{2}{45}\cdot\tfrac{1}{n}\Sigma(\ominus)\}+\ldots]=\\
= {} & 2[1+\sum_{k=2}^{\infty}\frac{\beta^k}{k!}\sum_{l=2}^{k}\sum_{h=1}^{[\frac{l}{2}]}\Sigma^{*''}{}_{\lfloor k,l,h\rfloor}\,\mathcal{N}(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i}).\sum_{l'=2}^{l}\sum_{h'=1}^{h}\Sigma^{*''}{}_{\lfloor k,l',h'\rfloor}\cdot\\
& .\mathcal{A}(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i};\sum_{i=1}^{h'}C^{(\alpha_i')}_{k_i',l_i'})n^{-h'}\Sigma\{m^{(1)}\ldots m^{(k)}\mid\sum_{i=1}^{h'}C^{(\alpha_i')}_{k_i',l_i'}\}]
\end{aligned}
$$

and for the logarithm of the partition function per spin

$$
\begin{aligned}
\tfrac{1}{n}\ln Z'' = {} & \ln 2+\beta^2\tfrac{1}{n}\cdot\Sigma(\bigcirc)+\beta^3\tfrac{4}{3n}\Sigma(\triangle)+\beta^4\{\tfrac{2}{n}\Sigma(\square)+\\
& -\tfrac{4}{n}\Sigma(\infty)+\tfrac{4}{3n}\Sigma(\ominus)\}+\beta^5\{-\tfrac{16}{n}\Sigma(\triangle\bigcirc)+\tfrac{16}{5n}\Sigma(\pentagon)+\\
& +10\tfrac{2}{3}\cdot\tfrac{1}{n}\Sigma(\triangle)\}+\beta^6\{\tfrac{16}{3n}\Sigma(\hexagon)-\tfrac{16}{n}\Sigma(\bowtie)+\ldots\ldots+6\tfrac{2}{45}\cdot\tfrac{1}{n}\Sigma(\ominus)\}+\\
& +\ldots = \ln 2+\sum_{k=2}^{\infty}\frac{\beta^k}{k!}\sum_{l=2}^{k}\Sigma^{*''}{}_{\lfloor k,l,l\rfloor}\sum_{l'=l}^{k}\sum_{h=1}^{[\frac{l}{2}]}\Sigma^{*''}{}_{\lfloor k,l',h\rfloor}\cdot\\
& .\mathcal{N}(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i})\,\mathcal{A}(\sum_{i=1}^{h}C^{(\alpha_i)}_{k_i,l_i};C^{(\alpha)}_{k,l})\tfrac{1}{n}\Sigma\{m^{(1)}\ldots m^{(k)}\mid C^{(\alpha)}_{k,l}\}.
\end{aligned}
$$

No proof which is formally correct in all respects has been found to show that $Z'' = Z'''$, but if $Z'' = Z'''$, then $Z' = Z'' = Z'''$, where Z' is given by

$$Z' = 2^n \Big[1 + \sum_{k=2}^{\infty} \frac{\beta^k}{k!} \sum_{l=2}^{k} \sum_{h=1}^{[\frac{l}{2}]} \Sigma^{*''} \lfloor k,l,h \rfloor \mathcal{N}\Big(\sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)}\Big) \Sigma^{*}\Big\{ m^{(1)} \ldots m^{(k)} \Big| \sum_{i=1}^{h} C_{k_i,l_i}^{(\alpha_i)} \Big\},$$

which differs from Z only with respect to the upper-summation limit of l. The term with the lowest power of β included in Z' but not in Z, is the one with β^{n+1}. With the very large values of n which are relevant and small β, the difference between Z and Z' is negligable. It is felt that approximating Z by Z' corresponds to the usual procedure in the matrix methods for solving Z to neglect all but the largest characteristic value of the matrix.

In order to evaluate the termswith $\beta^2, \ldots, \beta^6$ an easier form of the coefficients may be obtained. The results of tables 3.1, 3.2, 3.3 can be used to give e.g. for the logarithm of the partition function per spin

$$\ln 2 + \beta^2\Big(\frac{1}{n}\Sigma(\bigcirc)\Big) + \beta^3 \frac{4}{3n}\Sigma(\triangle) + \beta^4\Big\{\frac{2}{n}\Sigma^*(\square) - \frac{2}{3n}\Sigma(\ominus)\Big\} +$$
$$+ \beta^5\Big\{\frac{16}{5n}\Sigma^*(\pentagon) - \frac{16}{3n}\Sigma^*(\triangle)\Big\} + \beta^6\Big\{\frac{16}{3n}\Sigma^*(\hexagon) - \frac{16}{n}\Sigma^*(\lhd\!\bigcirc\!\rhd) +$$
$$- 10\tfrac{2}{3} \cdot \frac{1}{n}\Sigma^*(\square) - \frac{16}{3n}\Sigma(\triangle) + \frac{32}{45} \cdot \frac{1}{n}\Sigma(\ominus)\Big\} + \ldots.. \qquad (3.2)$$

(3.2) is now one of the results valid for any lattice (subject to restriction (1.4)) with arbitrary interactions. We have evaluated (3.2) for the case of a cubic lattice. Let the shortest distance between spins be +1, then we suppose the interactionenergy between two spins at distance +1 to be J_1, at distance $\sqrt{2}$ to be J_2, at distances $> \sqrt{2}$ to be zero. Then

$$\frac{1}{n}\Sigma(\bigcirc) = 6J_1^2 + 12J_2^2,$$
$$\frac{1}{n}\Sigma(\triangle) = 72J_1^2J_2 + 48J_2^3,$$
$$\frac{1}{n}\Sigma^*(\square) = 24J_1^4 + 696J_1^2J_2^2 + 264J_2^4,$$
$$\frac{1}{n}\Sigma(\ominus) = 6J_1^4 + 12J_2^4,$$

Putting $2\beta J_1 = k_1$ and $2\beta J_2 = k_2$ the terms up to the one with β^4 of (3.2) are:

$$\ln 2 + \tfrac{3}{2}k_1^2 + 3k_2^2 + 12k_1^2k_2 + 8k_2^3 + \tfrac{11}{4}k_1^4 + 87k_1^2k_2^2 + \tfrac{65}{2}k_2^4.$$

In taking $J_2 = 0$ one obtains the first few terms of the expansion for the simple cubic lattice with only nearest neighbour interactions, taking $J_1 = 0$ one obtains the same for the face-centered cubic lattice (cf. e.g. E. TREFFTZ (1950), C. DOMB and M.F. SYKES (1957)).

In order to write down further terms of (3.2), the calculation of $\Sigma^*(\hexagon), \Sigma^*(\hexagon)$ will be carried out by the Computation Department of the Mathematical Centre on their X-1 computor.

4. The expansion of Z for low temperatures

From (1.9)

$$Z = e^{\beta mn} \sum_{r=0}^{n} \binom{n}{r} \sum_{a} P[\underline{x}_+ = a \mid r] e^{4\beta(a - rm)}.$$

Now
$$P[\underline{x}_+ = 0 \mid r = 0] = 1,$$
$$P[\underline{x}_+ = 0 \mid r = 1] = 1,$$

while for the lattices usually considered in order-disorder problems

$$P[x_+ \geqslant r.m \mid r] = 0 \quad \text{for } r > 0.$$

Thus

$$Z = e^{\beta mn}\left[1 + ne^{-4\beta m} + \sum_{r=2}^{n}\binom{n}{r}\sum_{a} P[\underline{x}_+ = a \mid r]\, e^{4\beta(a - rm)}\right]. \tag{4.1}$$

An elementary reasoning using indicator quantities enables to calculate the probability distribution of $\underline{x}_+$. In detail this has been worked out for $r=3$ and an arbitrary lattice, while m_{ij} can take only three unequal values. Again we apply these results to the case of the cubic lattice with interaction $\pm J_1$ between nearest neighbours and $\pm J_2$ between next nearest neighbours. The probability distribution of $\underline{x}_+$ is given in table 4.1.

Table 4.1 $(n-1)(n-2)\,P[\underline{x}_+ = a \mid r = 3]$ for a cubic lattice, with two types of interactions.

a		a	
0	$n^2 - 57n + 908$	$4J_2$	252
$2J_1$	$18(n-28)$	$4J_1 + 2J_2$	72
$2J_2$	$36(n-30)$	$2J_1 + 4J_2$	0
$2J_1 + 2J_2$	288	$6J_1$	0
$4J_1$	18	$6J_2$	48

Also has been calculated (assuming $J_1 >> J_2$).

$$P[\underline{x}_+ = 8J_1 + 4J_2 \mid r = 4] = \frac{72}{(n-1)(n-2)(n-3)},$$
$$P[\underline{x}_+ = 8J_1 + aJ_2 \mid r = 4] = 0 \quad \text{for } a \neq 4,$$
$$P[\underline{x}_+ > 8J_1 + 4J_2 \mid r = 4] = 0.$$

For the sake of definiteness we take $J_1 \gg J_2$, say $J_1 \backsimeq 50 J_2$. Then

$$Z = e^{n\beta(6J_1+12J_2)} \Big[1 + ne^{-4\beta(6J_1+12J_2)} + 3ne^{-4\beta(10J_1+24J_2)} +$$
$$+ 6ne^{-4\beta(12J_1+22J_2)} + \tfrac{1}{2}n(n-19)e^{-4\beta(12J_1+24J_2)} + 12ne^{-4\beta(14J_1+34J_2)} +$$
$$+ 3ne^{-4\beta(14J_1+36J_2)} + 48ne^{-4\beta(16J_1+34J_2)} + 3n(n-28)e^{-4\beta(16J_1+36J_2)} +$$
$$+ 3ne^{-4\beta(16J_1+44J_2)} + 8ne^{-4\beta(18J_1+30J_2)} + 42ne^{-4\beta(18J_1+32J_2)} +$$
$$+ 6n(n-30)e^{-4\beta(18J_1+34J_2)} + \tfrac{1}{6}n(n^2-57n+908)e^{-4\beta(18J_1+36J_2)} + \ldots . \Big]. \qquad (4.2)$$

The first term after the one with $e^{-4\beta(18J_1+36J_2)}$ is

$$P\left[\underline{X}_+ = 6J_1 + 4J_2 \mid r=4\right] e^{-4\beta(18J_1+44J_2)}.$$

The expansion for the partitionfunction per spin suggested by (4.2) is:

$$e^{\beta(6J_1+12J_2)} \Big[1 + e^{-4\beta(6J_1+12J_2)} + 3e^{-4\beta(10J_1+24J_2)} +$$
$$+ 6e^{-4\beta(12J_1+22J_2)} - 9e^{-4\beta(12J_1+24J_2)} + 12e^{-4\beta(14J_1+34J_2)} +$$
$$+ 3e^{-4\beta(14J_1+36J_2)} + 48e^{-4\beta(16J_1+34J_2)} - 81e^{-4\beta(16J_1+36J_2)} +$$
$$+ 3e^{-4\beta(16J_1+44J_2)} + 8e^{-4\beta(18J_1+30J_2)} + 42e^{-4\beta(18J_1+32J_2)} +$$
$$- 174e^{-4\beta(18J_1+34J_2)} + 142e^{-4\beta(18J_1+36J_2)} + \ldots \Big]. \qquad (4.3)$$

The form insides the square brackets converges rapidly for large values of β, thus for low values of the temperature. Taking $J_2 = 0$ in (4.3) gives

$$e^{6J_1\beta}\left[1 + e^{-24\beta J_1} + 3e^{-40\beta J_1} - 3e^{-48\beta J_1} + 15e^{-56\beta J_1} - 30e^{-64\beta J_1} + \ldots \right],$$

which is the well-known result for the simple cubic lattice with only nearest neighbour interaction (cf. e.g. A.J. WAKEFIELD (1950)). Taking $J_1 = 0$ gives

$$e^{12J_2\beta}\Big[1 + e^{-48\beta J_2} + 6e^{-88\beta J_2} - 6e^{-96\beta J_2} + 8e^{-120\beta J_2} + 42e^{-128\beta J_2} +$$
$$- 114e^{-136\beta J_2} + \ldots \Big],$$
which is the result for the face centered cubic lattice with only nearest neighbour interactions (cf. e.g. G.F. NEWELL and E.W. MONTROLL (1953)).

5. The approximation method of J.G. KIRKWOOD

An approximation method often used in quantum-statistics is to replace a sum over a number of terms by the largest of the terms.

Thus if

$$Z(r) \overset{\text{def}}{=} \binom{n}{r} e^{\beta m(n-4r)} E_r e^{4\beta \underline{x}_+} \tag{5.1}$$

then an approximation to Z is obtained by taking

$$Z = Z(\hat{r}),$$

in which $\hat{r}$ is the value of r maximizing (5.1), or what amounts to the same maximizing

$$\ln Z(r) = \ln \binom{n}{r} + \beta m(n-4r) + \ln E_r e^{4\beta \underline{x}_+} . \tag{5.2}$$

Assuming all cumulants of $\underline{x}_+$, defined by

$$\ln E_r e^{4\beta \underline{x}_+} = \sum_{i=0}^{\infty} \frac{\varkappa_i t^i}{i!}$$

to exist, (5.2) can be written

$$\ln Z(r) = \ln \binom{n}{r} + \beta m(n-4r) + \sum_{i=0}^{\infty} \frac{\varkappa_i (4\beta)^i}{i!} . \tag{5.3}$$

If β is sufficiently small one may expect that from the equations obtained from (5.3) by neglecting all but the first few terms of the infinite series $\hat{r}$ can be approximated with a reasonable degree of accuracy.

The first four cumulants for a general lattice and with arbitrary, but given, interactions can be calculated from the first four moments of $\underline{x}_+$ cf. A.R. BLOEMENA (1960). Asymptotic expressions (for r and w large) for $\varkappa_1, \ldots, \varkappa_4$ are

$$\begin{aligned}
\varkappa_1 &= m \frac{r^2}{n}, \\
\varkappa_2 &= 2 \frac{r^2(n-r)^2}{n^4} \sum_{ij} m_{ij}^2, \\
\varkappa_3 &= 4 \frac{r^2(n-r)^2(n-2r)^2}{n^6} \sum_{ij} m_{ij}^3 + 8 \frac{r^3(n-r)^3}{n^6} \sum_{ijk} m_{ij} m_{ik} m_{jk}, \\
\varkappa_4 &= 8 \frac{r^2(n-r)^2}{n^4} \left\{ 1 - 6 \frac{r(n-r)}{n^2} \frac{2n^2 - 5nr + 5r^2}{n^2} \right\} \sum_{ij} m_{ij}^4 + \\
&+ 48 \frac{r^4(n-r)^4}{n^8} \sum_{(ijkl)\neq} m_{ij} m_{jk} m_{kl} m_{li} + \\
&+ 12 \frac{r^3(n-r)^3(n-2r)}{n^7} m \cdot \sum_{ijk} m_{ij} m_{ik} m_{jk} + \\
&+ 6 \frac{r^3(n-r)^3(n-2r)^2}{n^8} \sum_{ijk} m_{ij}^2 m_{ik} m_{jk} .
\end{aligned} \tag{5.4}$$

For special cases these cumulants have been given by J.G. KIRKWOOD (1938), H.A. BETHE and J.G. KIRKWOOD (1939) and T.C. CHANG (1941).

We shall now maximize

$$\ln Z_1(r) = \ln\binom{n}{r} + \beta m(n-4r) + 1 + 4\varkappa_1\beta + 8\varkappa_2\beta^2 + \tfrac{32}{3}\varkappa_3\beta^3 + \tfrac{32}{3}\varkappa_4\beta^4, \quad (5.5)$$

using (5.4) and the approximation

$$\ln\binom{n}{r} + 1 \approx n\ln n - (n-r)\ln(n-r) - r\ln r.$$

As for $t = 1,2,\ldots$

$$\frac{d}{dr}\, r^t(n-r)^t = t r^{t-1}(n-r)^{t-1}(n-2r)$$

the equation obtained by differentiation of (5.5) has a root at $r = \frac{n}{2}$. If

$$\left[\frac{d^2\ln Z_1(r)}{dr^2}\right]_{r=\frac{n}{2}} < 0,$$

$\ln Z_1(r)$ has a maximum at $r = \frac{n}{2}$; if it is >0, it has a minimum. Thus the equation in β

$$\left[\frac{d^2\ln Z_1(r)}{dr^2}\right]_{r=\frac{n}{2}} = 0 \quad (5.6)$$

marks a transition. If (5.6) has a positive and real solution $\beta = \beta_c$, then the temperature T_c corresponding to β_c is the KIRKWOOD approximation to the CURIE-temperature. Equation (5.6) is

$$(4\beta)^4\left\{\tfrac{1}{32}\cdot\tfrac{1}{n}\sum_{ijk} m_{ij}^2 m_{ik} m_{jk} - \tfrac{1}{4}\cdot\tfrac{1}{n}\sum_{(ijkl)\neq} m_{ij}m_{jk}m_{kl}m_{li} - \tfrac{1}{12}\cdot\tfrac{1}{n}\sum_{ij} m_{ij}^4\right\} +$$
$$+ (4\beta)^3\left\{\tfrac{1}{3}\cdot\tfrac{1}{n}\sum_{ij} m_{ij}^3 - \tfrac{1}{2}\cdot\tfrac{1}{n}\sum_{ijk} m_{ij}m_{ik}m_{jk}\right\} - (4\beta)^2\tfrac{1}{n}\sum_{ij} m_{ij}^2 +$$
$$+ (4\beta)\,\tfrac{2}{n}\sum_{ij} m_{ij} - 4 = 0. \quad (5.7)$$

For $r = \frac{n}{2}$,

$$\tfrac{1}{n}\ln Z_1(r) = \ln 2 + \beta^2\cdot\tfrac{1}{n}\sum m_{ij}^2 + \tfrac{4}{3}\beta^3\tfrac{1}{n}\sum_{ijk} m_{ij}m_{ik}m_{jk} +$$
$$+ 2\beta^4\tfrac{1}{n}\sum_{(ijkl)\neq} m_{ij}m_{jk}m_{kl}m_{li} - \tfrac{2}{3}\beta^4\tfrac{1}{n}\sum_{ij} m_{ij}^4,$$

which checks exactly with the first terms of (3.2).

As an example we consider the case of the cubic lattice with nearest neighbour interaction $\pm J_1$, and next nearest neighbour interaction $\pm J_2$ (cf. sections 3 and 4). Here

$$m = \tfrac{1}{n}\sum_{ij} m_{ij} = 6J_1 + 12J_2,$$
$$\tfrac{1}{n}\sum_{ij} m_{ij}^2 = 6J_1^2 + 12J_2^2,$$
$$\tfrac{1}{n}\sum_{ij} m_{ij}^3 = 6J_1^3 + 12J_2^4,$$
$$\tfrac{1}{n}\sum_{ij} m_{ij}^4 = 6J_1^4 + 12J_2^4,$$
$$\tfrac{1}{n}\sum_{ijk} m_{ij}m_{ik}m_{jk} = 72J_1^2J_2 + 48J_2^3,$$
$$\tfrac{1}{n}\sum_{ijk} m_{ij}^2 m_{ik}m_{jk} = 48J_1^3J_2 + 24J_1^2J_2^2 + 48J_2^4,$$
$$\tfrac{1}{n}\sum_{(ijkl)\neq} m_{ij}m_{jk}m_{kl}m_{li} = 24J_1^4 + 696J_1^2J_2^2 + 264J_2^4.$$

Then for this case the solution of (5.7) is

a) for $J_2 = o$ (which is the solution for the simple cubic lattice with only nearest neighbour interactions)

$$T_c = 4.62 \frac{J_1}{k},$$

which compares very well with the value 4.58 as given by M.E. FISHER and M.F. SYKES (1959),

b) for $J_1 = 50 J_2$

$$T_c = 4.90 \frac{J_1}{k},$$

c) for $J_1 = o$ (which is the solution for the face centered cubic lattice with only nearest neighbour interactions)

$$T_c = 10.18 \frac{J_1}{k},$$

which compares rather well with the value 9.816 given by M.E. FISCHER and M.F. SYKES (1959).

In neglecting the terms with $\beta^2, \beta^3, \beta^4$ in (5.7) one obtains a first approximation for T_c, being the well known BRAGG and WILLIAMS-approximation. Neglecting terms with β^3, β^4 or with β^4 gives a second and third approximation. In case a) these three approximations to T_c are 6.0, 4.76 and 4.95 $\frac{J_1}{k}$ respectively, in case c) 12.0, 10.9, 10.4 $\frac{J_2}{k}$.

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