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Transfer matrix approach to the three-dimensional Ising model

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Abstract. The {111} plane to {111} plane transfer matrix of the Ising model on a simple cubic lattice is obtained in a simple product form by using a purpose-built matrix product previously defined by this author. As a first application of this theoretical result, the exact analytic expression of the partition function of an Ising model on a $2\times2\times\infty$ lattice is derived.

1. Introduction

To solve exactly a lattice model consists in obtaining an exact analytical expression of its partition function. So far, this goal has only been achieved for two types of three-dimensional Ising models. Firstly, exact solutions for systems of finite size with isotropic interactions have been obtained by computer-assisted counting of spin configurations (Katsura 1954, Ono *et al* 1968, Binder 1972) up to the $4\times4\times4$ size (Pearson 1982, Itzykson *et al* 1983). Secondly, disorder solutions (Stephenson 1970), which benefit from some decoupling of the spin degrees of freedom in the model, have been derived recently (Jaekel and Maillard 1985). On the other hand, the transfer matrix formalism, so successful in solving one- and two-dimensional models, is generally acknowledged not to be feasible in three dimensions. Notwithstanding, it is the purpose of the present paper to show the comparative ability of this method to provide such solutions.

In a previous paper (Audit 1986), we proposed a new method to solve Ising systems and tested it by considering the smallest conceivable three-dimensional lattice ($2\times2\times2$) having anisotropic interactions and non-zero field whose roles in increasing the complexity of the solution were clearly illustrated. Basically the method, which is greatly improved in the present paper, consists in the proper use of a new purpose-built matrix product associated with other classical matrix products to build the transfer matrix; the choice of the [111] transfer direction and suitable periodic boundary conditions for the simple cubic lattice makes the computation far less complicated; and the resulting transfer matrix has a product form which is extremely symmetric and simple, thus suitable for both analytical and computational treatment.

In this paper, we test the method further by deriving exact solutions for two limiting situations, where all dimensions are not kept finite as previously, namely the $\infty\times\infty\times2$ and $2\times2\times\infty$ lattices. Those two simple cubic lattices have, respectively, the shapes of a double layer of {111} infinite planes and an infinite number of {111} planes consisting of four sites. Thus the former is simply related to a planar honeycomb lattice and can be solved trivially, whereas it appears that the latter (a bar with a rhomboid section) is the first genuine three-dimensional Ising model, having at least one dimension in which the system is infinite, to be solved exactly.

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2. The two-layer {111} plane to {111} plane transfer matrix

The partition function of the anisotropic Ising model without field on a simple cubic lattice is defined by

$$Z(K, K', K'') = \sum_{\{\sigma_{lmn}=\pm 1\}} \prod_{lmn} \langle \sigma_{l-1,mn}\sigma_{l,m-1,n}\sigma_{lm,n-1}|P\otimes P'\otimes P''|\sigma_{lmn}\sigma_{lmn}\sigma_{lmn}\rangle$$

$$\times \langle \sigma_{lmn}\sigma_{lmn}\sigma_{lmn}|P\otimes P'\otimes P''|\sigma_{l+1,mn}\sigma_{l,m+1,n}\sigma_{lm,n+1}\rangle \qquad (1)$$

where { } stands for a sum over all configurations of sites σ_{lmn}, $\otimes$ is the direct product of matrices and

$$\boldsymbol{P} = e^{K}\boldsymbol{I} + e^{-K}\boldsymbol{X} \qquad (2)$$

and similarly for $\boldsymbol{P}'$ and $\boldsymbol{P}''$, with $K = J/k_B T$ (J being a coupling constant) and

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \boldsymbol{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \qquad (3)$$

In our method to build the transfer matrix, the natural direction of transfer is the [111] direction. Thus it will be convenient to look at the simple cubic lattice as consisting of $M \times M \times 2N$ sites arranged on {111} planes. Let $2N$ be the number of such planes (consisting of M^2 sites) that will be labelled $i = 0, 1, \ldots, 2N-1$; we assume a periodic boundary condition in the [111] direction by identifying the planes $2N$ and 0. The arrangement of sites in two neighbouring planes i and $i+1$ is shown in figure 1. In each plane, the sites are arranged on a triangular lattice and their positions, by using an oblique coordinate system, are labelled with a pair of indices $j, k = 0, 1, \ldots, M-1$. We impose the periodic boundary condition $(j, k) \equiv (j+M, k) \equiv (j, k+M)$ in the planes {111}. It is important to notice that a spin in a plane {111} interacts only with spins in the two neighbouring {111} planes, whereas spins belonging to the same plane do not interact. In fact, it is the use of the transfer direction [111] which dictated the above choice of periodic boundary conditions in order to ensure that all spin interactions occur between the neighbouring planes only. On the contrary, the usual periodic boundary conditions for a cubic lattice would fit endpoints belonging to different {111} planes.

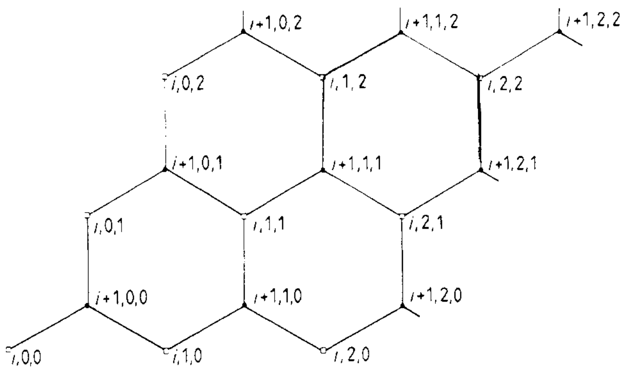

Figure 1. Spins in two adjacent {111} planes.

Relabelling spins with new indices i, j, k the partition function (1) can be conveniently written as

$$Z_{M\times M\times 2N}(K, K', K'')$$
$$= \sum_{\{\sigma_{ijk}=\pm 1\}} \prod_{i=0}^{2N-1} \prod_{j,k=0}^{M-1} \langle \sigma_{i-1,jk}\sigma_{i-1,j-1,k}\sigma_{i-1,j,k-1}|\boldsymbol{P}\otimes\boldsymbol{P}'\otimes\boldsymbol{P}''$$
$$\times|\sigma_{ijk}\sigma_{ijk}\sigma_{ijk}\rangle\langle\sigma_{ijk}\sigma_{ijk}\sigma_{ijk}|\boldsymbol{P}\otimes\boldsymbol{P}'\otimes\boldsymbol{P}''|\sigma_{i+1,jk}\sigma_{i+1,j-1,k}\sigma_{i+1,j,k-1}\rangle. \tag{4}$$

To calculate this expression, we shall use the purpose-built matrix product between direct products of 2×2 matrices, defined in a previous paper (Audit 1986). For the case considered at hand, namely an anisotropic Ising model in zero field, the more general definition of this special product, denoted by $\times$, reduces to the form

$$\langle ii'i''|(\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}'')\times(\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}'')|kk'k''\rangle$$
$$=\sum_j \langle ii'i''|\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}''|jjj\rangle\langle jjj|\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}''|kk'k''\rangle \tag{5}$$

which can be rewritten in terms of the Pauli matrix

$$\boldsymbol{Z}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

as

$$2^2(A\otimes A'\otimes A'')\times(A\otimes A'\otimes A'')=A^2\otimes A'^2\otimes A''^2+A^2\otimes A'ZA'\otimes A''ZA''$$
$$+AZA\otimes A'^2\otimes A''ZA''+AZA\otimes A'ZA'\otimes A''^2 \tag{6}$$

or alternatively in the most convenient form

$$2^3(\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}'')\times(\boldsymbol{A}\otimes\boldsymbol{A}'\otimes\boldsymbol{A}'')$$
$$=\sum_{\varepsilon=\pm 1}(\boldsymbol{A}^2+\varepsilon\boldsymbol{AZA})\otimes(\boldsymbol{A}'^2+\varepsilon\boldsymbol{A}'\boldsymbol{Z}\boldsymbol{A}')\otimes(\boldsymbol{A}''^2+\varepsilon\boldsymbol{A}''\boldsymbol{Z}\boldsymbol{A}''). \tag{7}$$

Now, after a partial summation over spins in every odd plane performed by means of expression (5) in (4), and upon changing the index i of summation, we are left with the following sum over alternate planes:

$$Z_{M\times M\times 2N}(K, K', K'')=\sum_{\{\sigma_{ijk}=\pm 1\}}\prod_{i=0}^{N-1}\prod_{j,k=0}^{M-1}\langle\sigma_{ijk}\sigma_{i,j-1,k}\sigma_{i,j,k-1}|$$
$$\times(\boldsymbol{P}\otimes\boldsymbol{P}'\otimes\boldsymbol{P}'')\times(\boldsymbol{P}\otimes\boldsymbol{P}'\otimes\boldsymbol{P}'')|\sigma_{i+1,jk}\sigma_{i+1,j-1,k}\sigma_{i+1,j,k-1}\rangle \tag{8}$$

or, by using the identity (7), this expression can be reorganised as

$$Z_{M\times M\times 2N}(K, K', K'')=2^{-3NM^2}\sum_{\{\sigma_{ijk}=\pm 1\}}\prod_{i=0}^{N-1}\prod_{j,k=0}^{M-1}\langle\sigma_{ijk}\sigma_{i,j-1,k}\sigma_{ij,k-1}|$$
$$\times\sum_{\varepsilon_{jk}=\pm 1}\boldsymbol{R}_{\varepsilon_{jk}}\otimes\boldsymbol{R}'_{\varepsilon_{jk}}\otimes\boldsymbol{R}''_{\varepsilon_{jk}}|\sigma_{i+1,jk}\sigma_{i+1,j-1,k}\sigma_{i+1,j,k-1}\rangle \tag{9}$$

with

$$\boldsymbol{R}_\varepsilon=\boldsymbol{P}^2+\varepsilon\boldsymbol{PZP} \tag{10}$$

and similarly for $\boldsymbol{R}'_\varepsilon$ and $\boldsymbol{R}''_\varepsilon$. By taking the direct product properties into account we find

$$Z_{M\times M\times 2N}(K, K', K'')$$

$$= 2^{-3NM^2} \sum_{\{\sigma_{ijk}=\pm1\}} \prod_{i=0}^{N-1} \left\langle \prod_{j,k=0}^{M-1} \sigma_{ijk}\sigma_{i,j-1,k}\sigma_{i,j,k-1} \right| \times \sum_{\{\varepsilon_{jk}=\pm1\}} \prod_{j,k=0}^{M-1}{}^{\otimes} (\boldsymbol{R}_{\varepsilon_{jk}} \otimes \boldsymbol{R}'_{\varepsilon_{jk}} \otimes \boldsymbol{R}''_{\varepsilon_{jk}}) \left| \prod_{j,k=0}^{M-1} \sigma_{i+1,jk}\sigma_{i+1,j-1,k}\sigma_{i+1,j,k-1} \right\rangle \tag{11}$$

or, after reordering terms of the multiple direct product $\Pi^{\otimes}$,

$$Z_{M\times M\times 2N}(K, K', K'')$$

$$= 2^{-3NM^2} \sum_{\{\sigma_{ijk}=\pm1\}} \prod_{i=0}^{N-1} \left\langle \prod_{j,k=0}^{M-1} \sigma_{ijk}\sigma_{ijk}\sigma_{ijk} \right| \sum_{\{\varepsilon_{jk}=\pm1\}} \times \prod_{j,k=0}^{M-1}{}^{\otimes} (\boldsymbol{R}_{\varepsilon_{jk}} \otimes \boldsymbol{R}'_{\varepsilon_{j+1,k}} \otimes \boldsymbol{R}''_{\varepsilon_{j,k+1}}) \left| \prod_{j,k=0}^{M-1} \sigma_{i+1,jk}\sigma_{i+1,jk}\sigma_{i+1,jk} \right\rangle. \tag{12}$$

The expression (12) can be further condensed by making use of the Hadamard product, denoted $\odot$, which is simply related to the direct product $\otimes$ by

$$\langle iii|A\otimes B\otimes C|jjj\rangle = \langle i|A\odot B\odot C|j\rangle. \tag{13}$$

Then one obtains

$$Z_{M\times M\times 2N}(K, K', K'')$$

$$= 2^{-3NM^2} \sum_{\{\sigma_{ijk}=\pm1\}} \prod_{i=0}^{N-1} \left\langle \prod_{j,k=0}^{M-1} \sigma_{ijk} \right| \sum_{\{\varepsilon_{jk}=\pm1\}} \prod_{j,k=0}^{M-1}{}^{\otimes} (\boldsymbol{R}_{\varepsilon_{jk}} \odot \boldsymbol{R}'_{\varepsilon_{j+1,k}} \odot \boldsymbol{R}''_{\varepsilon_{j,k+1}}) \times \left| \prod_{j,k=0}^{M-1} \sigma_{i+1,jk} \right\rangle \tag{14}$$

and a summation over the remaining spins yields the result

$$Z_{M\times M\times 2N}(K, K', K'') = 2^{-3NM^2}\,\mathrm{Tr}\,\boldsymbol{\theta}^N_{M,M} \tag{15}$$

where

$$\boldsymbol{\theta}_{M,M} = \sum_{\{\varepsilon_{jk}=\pm1\}} \prod_{j,k=0}^{M-1}{}^{\otimes} (\boldsymbol{R}_{\varepsilon_{jk}} \odot \boldsymbol{R}'_{\varepsilon_{j+1,k}} \odot \boldsymbol{R}''_{\varepsilon_{j,k+1}}) \tag{16}$$

is the two-layer transfer matrix in the [111] direction. Then, by using the relation

$$(\boldsymbol{A}\odot\boldsymbol{B})\otimes(\boldsymbol{C}\odot\boldsymbol{D}) = (\boldsymbol{A}\otimes\boldsymbol{C})\odot(\boldsymbol{B}\otimes\boldsymbol{D}) \tag{17}$$

(which links the Hadamard and direct products) an alternative expression of the two-layer transfer matrix can be obtained from (16) in the form of a multiple Hadamard product $\Pi^{\odot}$, namely

$$\boldsymbol{\theta}_{M,M} = \prod_{j,k=0}^{M-1}{}^{\odot} (\boldsymbol{S}_{jk} + \bar{\boldsymbol{S}}_{jk}) \tag{18}$$

where

$$\boldsymbol{S}_{jk} = \boldsymbol{U}^{\otimes M} \otimes \ldots \otimes \underbrace{(\boldsymbol{U} \otimes \ldots \otimes \overbrace{\boldsymbol{R}''}^{j} \otimes \ldots \otimes \boldsymbol{U})}_{k-1} \otimes \underbrace{(\boldsymbol{U} \otimes \ldots \otimes \overbrace{\boldsymbol{R}'}^{j-1} \otimes \overbrace{\boldsymbol{R}}^{j} \otimes \ldots \otimes \boldsymbol{U})}_{k} \otimes \ldots \otimes \boldsymbol{U}^{\otimes M} \tag{19}$$

with

$$\boldsymbol{U}^{\otimes M} = \boldsymbol{U} \otimes \boldsymbol{U} \otimes \boldsymbol{U} \otimes \ldots \qquad (M \text{ times})$$
$$\boldsymbol{U} = \boldsymbol{I} + \boldsymbol{X} \tag{20}$$

and

$$\boldsymbol{R} = 2\begin{pmatrix} \mathrm{e}^{2K} & 1 \\ 1 & \mathrm{e}^{-2K} \end{pmatrix} \tag{21}$$

and similarly for $\boldsymbol{R}'$ and $\boldsymbol{R}''$. Likewise, we have

$$\bar{\boldsymbol{S}}_{jk}(K, K', K'') = \boldsymbol{S}_{jk}(-K, -K', -K''). \tag{22}$$

It is convenient for writing the elements of the $2^{M^2} \times 2^{M^2}$ matrices that we consider in this paper, to label their rows and columns, respectively, by the vectors

$$\boldsymbol{\mu} = (\mu_{00}, \ldots, \mu_{0,M-1}, \mu_{10}, \ldots, \mu_{1,M-1}, \ldots, \mu_{M-1,0}, \ldots, \mu_{M-1,M-1}) \tag{23}$$

$$\boldsymbol{\nu} = (\nu_{00}, \ldots, \nu_{0,M-1}, \nu_{10}, \ldots, \nu_{1,M-1}, \ldots, \nu_{M-1,0}, \ldots, \nu_{M-1,M-1}) \tag{24}$$

whose components can take the values $+1$ and -1, and can be thought of as the spins in two $\{111\}$ planes. Thus, the elements of the matrix (19) can be written in the form

$$\langle \boldsymbol{\mu} | \boldsymbol{S}_{jk} | \boldsymbol{\nu} \rangle = 2^3 \exp[K(\mu_{jk} + \nu_{jk}) + K'(\mu_{j-1,k} + \nu_{j-1,k}) + K''(\mu_{j,k-1} + \nu_{j,k-1})] \tag{25}$$

and (18) yields the expression

$$\langle \boldsymbol{\mu} | \boldsymbol{\theta}_{M,M} | \boldsymbol{\nu} \rangle = 2^{4M^2} \prod_{j,k=0}^{M-1} \cosh[K(\mu_{jk} + \nu_{jk}) + K'(\mu_{j-1,k} + \nu_{j-1,k}) + K''(\mu_{j,k-1} + \nu_{j,k-1})] \tag{26}$$

for the elements of the two-layer transfer matrix.

3. The partition function of an $\infty \times \infty \times 2$ Ising model

Now, we consider the simple case of an isotropic Ising model on a couple of $\{111\}$ planes, with periodic boundary conditions in the [111] direction. Despite its genuine three-dimensional geometry, this model is in fact equivalent to a planar honeycomb model, having an interaction constant $2K$, because each spin interacts twice with its three neighbours located in the other plane.

The partition function of the honeycomb Ising model being already known (Houtappel 1950), we thus have the opportunity to check the validity of our previous theoretical results and to obtain at little cost the solution of an infinite two-layer Ising model.

The partition function (15) is in this case

$$Z_{M \times M \times 2} = 2^{-3M^2} \operatorname{Tr} \boldsymbol{\theta}_{M,M}. \tag{27}$$

Making use of the diagonal elements of the transfer matrix, obtained from (26), follows the expression

$$Z_{M\times M\times 2}=\sum_{\{\mu_{jk}=\pm 1\}}\prod_{j,k=0}^{M-1}2\cosh[2K(\mu_{jk}+\mu_{j-1,k}+\mu_{j,k-1})] \tag{28}$$

which is just the partition function of a M^2 sites isotropic Ising model on a honeycomb lattice, with a coupling constant $2K$ (Baxter 1982, see (6.4.4)) as was expected.

Now making use of Houtappel's result, the partition function per spin of the $\infty\times\infty\times 2$ Ising model is given by

$$\ln(\tfrac{1}{2}\tilde{Z}_{\infty\times\infty\times 2})=(4\pi)^{-2}\int_0^{2\pi}\int_0^{2\pi}\ln\tfrac{1}{2}\{\cosh^3 4K+1 - \sinh^2 4K[\cos\omega_1+\cos\omega_2+\cos(\omega_1+\omega_2)]\}\,d\omega_1\,d\omega_2. \tag{29}$$

The critical point is obtained, from (29), when the coupling constant satisfies the relation

$$\cosh 4K_c=2. \tag{30}$$

Hence the critical constant of the $\infty\times\infty\times 2$ Ising model is

$$K_c=\tfrac{1}{4}\ln(2+\sqrt{3})=0.3292 \tag{31}$$

a value which happens to be halfway between the exact value $\frac{1}{2}\ln(1+\sqrt{2})=0.4407$ of the $\infty\times\infty$ square model and the numerically estimated value 0.221 66 for the $\infty\times\infty\times\infty$ cubic model (Pawley *et al* 1984). Thus the quite strong three-dimensional behaviour of the double layer model is clearly demonstrated.

4. The factorisation of the transfer matrix

The calculation in § 2 yielded directly the two-layer transfer matrix $\boldsymbol{\theta}_{M,M}$, yet it could sometimes be more convenient to use a one-layer transfer matrix having a simpler expression that is derived below.

Let a $2^{M^2}\times 1$ matrix be defined as

$$\boldsymbol{s}_{jk}=\boldsymbol{u}^{\otimes M}\otimes\ldots\otimes\underbrace{(\boldsymbol{u}\otimes\ldots\otimes\overset{j}{\boldsymbol{r}''}\otimes\ldots\otimes\boldsymbol{u})}_{k-1}\otimes\underbrace{(\boldsymbol{u}\otimes\ldots\otimes\overset{j-1}{\boldsymbol{r}'}\otimes\overset{j}{\boldsymbol{r}}\otimes\ldots\otimes\boldsymbol{u})}_{k}\otimes\ldots\otimes\boldsymbol{u}^{\otimes M} \tag{32}$$

with

$$\boldsymbol{u}=\begin{pmatrix}1\\1\end{pmatrix}\qquad \boldsymbol{r}=\sqrt{2}\begin{pmatrix}e^{K}\\e^{-K}\end{pmatrix}\qquad \text{(and similarly for } \boldsymbol{r}' \text{ and } \boldsymbol{r}''). \tag{33}$$

Likewise, we define the matrix

$$\bar{\boldsymbol{s}}_{jk}(K,K',K'')=\boldsymbol{s}_{jk}(-K,-K',-K''). \tag{34}$$

Clearly we have, from definitions (21) and (33),

$$\boldsymbol{R}=\boldsymbol{r}\boldsymbol{r}^{t} \tag{35}$$

where ^{t} denotes the transpose. It follows that

$$\boldsymbol{S}_{jk}=\boldsymbol{s}_{jk}\boldsymbol{s}_{jk}^{t}. \tag{36}$$

Then the expression (18) of the two-layer transfer matrix can be rewritten in the form

$$\theta_{M,M} = \prod_{j,k=0}^{M-1}{}^{\odot} (s_{jk}s^{t}_{jk} + \bar{s}_{jk}\bar{s}^{t}_{jk}). \tag{37}$$

Taking into account the simple relation

$$s_1 s_1^{t} \odot s_2 s_2^{t} \odot \ldots = (s_1 \odot s_2 \odot \ldots)(s_1^{t} \odot s_2^{t} \odot \ldots) \tag{38}$$

which holds true provided that s_i $(i = 1, 2, \ldots)$ are column matrices; it turns out that the matrix (37) factorises in the form of the product

$$\theta_{M,M} = T_{M,M} T^{t}_{M,M} \tag{39}$$

where the $M^2 \times M^2$ matrix $T_{M,M}$ is given by a multiple Hadamard product of M^2 multiple direct products as

$$T_{M,M} = \{[s_{00}\bar{s}_{00}] \otimes u^{t} \otimes u^{t} \otimes \ldots \otimes u^{t}\} \odot \{u^{t} \otimes [s_{01}\bar{s}_{01}] \otimes u^{t} \otimes \ldots \otimes u^{t}\} \odot \ldots$$
$$\odot \{u^{t} \otimes \ldots \otimes [s_{M-1,M-1}\bar{s}_{M-1,M-1}]\} \tag{40}$$

or in condensed form as

$$T_{M,M} = \prod_{j,k=0}^{M-1}{}^{\odot} \tau_{jk} \tag{41}$$

where the $2^{M^2} \times 2^{M^2}$ matrix τ_{jk} is

$$\tau_{jk} = u^{t^{\otimes M}} \otimes \ldots \otimes (u^{t} \otimes \ldots \otimes [s_{jk}\bar{s}_{jk}] \otimes \ldots \otimes u^{t}) \otimes \ldots \otimes u^{t^{\otimes M}} \tag{42}$$

in which the $2^{M^2} \times 2$ matrix $[s_{jk}\bar{s}_{jk}]$ occupies the kth position in the jth factor of the multiple direct product.

Consideration of (32)-(34), (41) and (42) yields, for the matrix elements, the following expressions:

$$\langle \mu | \tau_{jk} | \nu \rangle = 2^{3/2} \exp[(K\mu_{jk} + K'\mu_{j-1,k} + K''\mu_{j,k-1})\nu_{jk}] \tag{43}$$

$$\langle \mu | T_{M,M} | \nu \rangle = 2^{3M^2/2} \prod_{j,k=0}^{M-1} \exp[(K\mu_{jk} + K'\mu_{j-1,k} + K''\mu_{j,k-1})\nu_{jk}] \tag{44}$$

$$\langle \mu | T^{t}_{M,M} | \nu \rangle = 2^{3M^2/2} \prod_{j,k=0}^{M-1} \exp[(K\nu_{jk} + K'\nu_{j-1,k} + K''\nu_{j,k-1})\mu_{jk}] \tag{45}$$

$$= 2^{3M^2/2} \prod_{j,k=0}^{M-1} \exp[(K\mu_{jk} + K'\mu_{j+1,k} + K''\mu_{j,k+1})\nu_{jk}]. \tag{46}$$

Using the $M \times M$ unit matrix $\mathbf{1}$ and the $M \times M$ cyclic matrices m_1 and m_{-1}, whose entries are respectively (Audit 1985a, b)

$$\langle i | m_1 | j \rangle = \delta_{i+1,j} \tag{47}$$

$$\langle i | m_{-1} | j \rangle = \delta_{i-1,j}. \tag{48}$$

The elements (44), (46) of the transfer matrix can be put in a more condensed form as

$$\langle \mu | T_{M,M} | \nu \rangle = 2^{3M^2/2} \exp\{\langle \mu | K\mathbf{1} \otimes \mathbf{1} + K'm_1 \otimes \mathbf{1} + K''\mathbf{1} \otimes m_1 | \nu \rangle\} \tag{49}$$

$$\langle \mu | T^{t}_{M,M} | \nu \rangle = 2^{3M^2/2} \exp\{\langle \mu | K\mathbf{1} \otimes \mathbf{1} + K'm_{-1} \otimes \mathbf{1} + K''\mathbf{1} \otimes m_{-1} | \nu \rangle\}. \tag{50}$$

Moreover, (44) can be rewritten in terms of the matrices (2) as

$$\langle \mu | T_{M,M} | \nu \rangle = 2^{3M^2/2} \prod_{j,k=0}^{M-1} \langle \mu_{jk} | P | \nu_{jk} \rangle \langle \mu_{j-1,k} | P' | \nu_{jk} \rangle \langle \mu_{j,k-1} | P'' | \nu_{jk} \rangle \tag{51}$$

or in condensed form as

$$\langle\boldsymbol{\mu}|\boldsymbol{T}_{M,M}|\boldsymbol{\nu}\rangle=2^{3M^2/2}\langle\boldsymbol{\mu}|\boldsymbol{P}^{\otimes M^2}|\boldsymbol{\nu}\rangle\langle\boldsymbol{\mu}(\boldsymbol{m}_1\otimes 1)|\boldsymbol{P}'^{\otimes M^2}|\boldsymbol{\nu}\rangle\langle\boldsymbol{\mu}(1\otimes\boldsymbol{m}_1)|\boldsymbol{P}''^{\otimes M^2}|\boldsymbol{\nu}\rangle. \tag{52}$$

A global expression of the transfer matrix follows, of the form

$$\boldsymbol{T}_{M,M}=2^{3M^2/2}(\boldsymbol{P}^{\otimes M^2}\odot \boldsymbol{G}\boldsymbol{P}'^{\otimes M^2}\odot \boldsymbol{H}\boldsymbol{P}''^{\otimes M^2}) \tag{53}$$

where G and H are row permutation matrices corresponding to the transformations $\langle\boldsymbol{\mu}|\rightarrow\langle\boldsymbol{\mu}(\boldsymbol{m}_1\otimes 1)|$ and $\langle\boldsymbol{\mu}|\rightarrow\langle\boldsymbol{\mu}(1\otimes\boldsymbol{m}_1)|$, respectively.

Thus the two-layer transfer matrix (39) factorises in the simple form

$$\boldsymbol{\theta}_{M,M}=2^{3M^2}(\boldsymbol{P}^{\otimes M^2}\odot \boldsymbol{G}\boldsymbol{P}'^{\otimes M^2}\odot \boldsymbol{H}\boldsymbol{P}''^{\otimes M^2})(\boldsymbol{P}^{\otimes M^2}\odot \boldsymbol{P}'^{\otimes M^2}\boldsymbol{G}^{\mathrm{t}}\odot \boldsymbol{P}''^{\otimes M^2}\boldsymbol{H}^{\mathrm{t}}) \tag{54}$$

where it appears to be straightforward to build it up from the simple matrices P, P', P''.

5. The partition function of the $2\times 2\times\infty$ Ising model

It could be instructive to illustrate the results obtained in § 4 by considering the simple case of a simple cubic lattice consisting of $2N$ {111} planes made up of four sites each, as illustrated in figure 2(a). Because of the periodic boundary condition in {111} planes, this lattice is in fact equivalent to the lattice shown in figure 2(b), whose shape is a bar limited by two rhomboid end planes.

Comparing (44) and (46) and taking into account the periodic boundary conditions, we notice that $\boldsymbol{T}_{2,2}=\boldsymbol{T}^{\mathrm{t}}_{2,2}$; the partition function (15) in this case is

$$Z_{2\times 2\times 2N}=2^{-12N}\,\mathrm{Tr}\,\boldsymbol{T}_{2,2}^{2N} \tag{55}$$

and the 16×16 one-layer transfer matrix is obtained from (44) or (53) in the following form:

$$\boldsymbol{T}_{2,2}=2^6\begin{pmatrix}
\mathrm{e}^{12K} & \mathrm{e}^{6K} & \mathrm{e}^{6K} & 1 & \mathrm{e}^{6K} & 1 & 1 & \mathrm{e}^{-6K} & \mathrm{e}^{6K} & 1 & 1 & \mathrm{e}^{-6K} & 1 & \mathrm{e}^{-6K} & \mathrm{e}^{-6K} & \mathrm{e}^{-12K}\\
\mathrm{e}^{6K} & \mathrm{e}^{4K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{2K} & 1 & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-6K}\\
\mathrm{e}^{6K} & \mathrm{e}^{4K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-6K}\\
1 & \mathrm{e}^{2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & 1 & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1 & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & 1\\
\mathrm{e}^{6K} & \mathrm{e}^{4K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{-4K} & \mathrm{e}^{-6K}\\
1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{4K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1\\
1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & 1 & \mathrm{e}^{2K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & 1\\
\mathrm{e}^{-6K} & 1 & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & 1 & \mathrm{e}^{6K}\\
\mathrm{e}^{6K} & 1 & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & 1 & \mathrm{e}^{-6K}\\
1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{2K} & 1 & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & 1 & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1\\
1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{4K} & \mathrm{e}^{2K} & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1\\
\mathrm{e}^{-6K} & \mathrm{e}^{-4K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{4K} & \mathrm{e}^{6K}\\
1 & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{2K} & 1 & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{2K} & 1 & 1 & \mathrm{e}^{-2K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{2K} & 1\\
\mathrm{e}^{-6K} & \mathrm{e}^{-4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & 1 & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{4K} & \mathrm{e}^{6K}\\
\mathrm{e}^{-6K} & \mathrm{e}^{-4K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{-4K} & \mathrm{e}^{-2K} & \mathrm{e}^{-2K} & 1 & 1 & \mathrm{e}^{2K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{2K} & \mathrm{e}^{4K} & \mathrm{e}^{4K} & \mathrm{e}^{6K}\\
\mathrm{e}^{-12K} & \mathrm{e}^{-6K} & \mathrm{e}^{-6K} & 1 & \mathrm{e}^{-6K} & 1 & 1 & \mathrm{e}^{6K} & \mathrm{e}^{-6K} & 1 & 1 & \mathrm{e}^{6K} & 1 & \mathrm{e}^{6K} & \mathrm{e}^{6K} & \mathrm{e}^{12K}
\end{pmatrix}. \tag{56}$$

The matrix $\boldsymbol{T}_{2,2}$ reduces to a block diagonal form by the similarity transformation

$$\boldsymbol{T}'_{2,2}=2^{-1}(\boldsymbol{Z}\otimes\boldsymbol{I}\otimes\boldsymbol{I}\otimes\boldsymbol{I}+\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X})\boldsymbol{T}_{2,2}(\boldsymbol{Z}\otimes\boldsymbol{I}\otimes\boldsymbol{I}\otimes\boldsymbol{I}+\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X}\otimes\boldsymbol{X}) \tag{57}$$

$$=2^7\begin{pmatrix}\boldsymbol{\Gamma} & 0\\ 0 & \boldsymbol{\Sigma}\end{pmatrix} \tag{58}$$

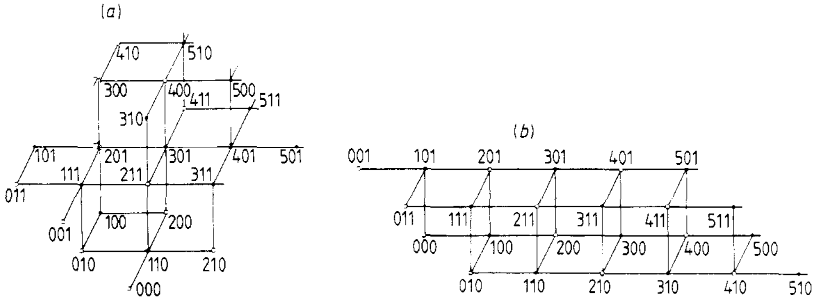

Figure 2. Two equivalent representations of the $2\times2\times2N$ simple cubic lattice.

where

$$\Gamma = \begin{pmatrix} c_{12} & c_6 & c_6 & 1 & c_6 & 1 & 1 & c_6 \\ c_6 & c_4 & c_4 & c_2 & c_4 & c_2 & c_2 & 1 \\ c_6 & c_4 & c_4 & c_2 & 1 & c_2 & c_2 & c_4 \\ 1 & c_2 & c_2 & c_4 & c_2 & 1 & 1 & c_2 \\ c_6 & c_4 & 1 & c_2 & c_4 & c_2 & c_2 & c_4 \\ 1 & c_2 & c_2 & 1 & c_2 & c_4 & 1 & c_2 \\ 1 & c_2 & c_2 & 1 & c_2 & 1 & c_4 & c_2 \\ c_6 & 1 & c_4 & c_2 & c_4 & c_2 & c_2 & c_4 \end{pmatrix} \tag{59}$$

with

$$c_\alpha = \cosh(\alpha K)$$

and

$$\Sigma = \begin{pmatrix} s_4 & -s_2 & s_2 & -s_4 & s_2 & -s_4 & 0 & -s_6 \\ -s_2 & -s_4 & 0 & -s_2 & 0 & -s_2 & s_2 & 0 \\ s_2 & 0 & s_4 & s_2 & 0 & -s_2 & s_2 & 0 \\ -s_4 & -s_2 & s_2 & s_4 & -s_2 & 0 & s_4 & s_6 \\ s_2 & 0 & 0 & -s_2 & s_4 & s_2 & s_2 & 0 \\ -s_4 & -s_2 & -s_2 & 0 & s_2 & s_4 & s_4 & s_6 \\ 0 & s_2 & s_2 & s_4 & s_2 & s_4 & s_4 & s_6 \\ -s_6 & 0 & 0 & s_6 & 0 & s_6 & s_6 & s_{12} \end{pmatrix} \tag{60}$$

with

$$s_\alpha = \sinh(\alpha K).$$

The determination of the eigenvalues is trivial if $K=0$, we find in this case: $\lambda_1 = 8$, $\lambda_2 = \ldots = \lambda_8 = 0$ for the matrix Γ and $\lambda_9 = \ldots = \lambda_{16} = 0$ for the matrix Σ; hence the largest and unique non-zero eigenvalue of $T_{2,2}(0)$ is 2^{10}.

Thus, the block Γ contains the largest eigenvalue λ_m of the $T_{2,2}$ matrix, and in the limit $N\to\infty$, according to Perron's theorem, (55) reduces to

$$Z_{2\times2\times2N} = (2\lambda_m)^{2N}. \tag{61}$$

Further similarity transformations yield the following block diagonal form for the $\mathbf{\Gamma}$ matrix:

$$\begin{pmatrix} c_{12} & 2c_6 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 \\ 2c_6 & 3c_4+1 & 2\sqrt{3}c_2 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{3} & 2\sqrt{3}c_2 & c_4+2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_4-1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & c_4-1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1-c_4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c_4-1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & c_4-1 \end{pmatrix} \tag{62}$$

from which we infer that the largest eigenvalue λ_m of the matrix $\mathbf{\Gamma}$ is just the largest root of the polynomial of degree 3

$$\lambda^3+a_2\lambda^2+a_1\lambda+a_0=0 \tag{63}$$

where

$$a_0=c_{12}(-3c_4^2-7c_4+12c_2^2-2)+4c_6^2(c_4+2)-24c_6c_2+9c_4+3$$
$$a_1=c_{12}(4c_4+3)-4c_6^2+c_4(3c_4+7)-12c_2^2-1$$
$$a_2=-c_{12}-4c_4-3.$$

To write out the solution of (63), by means of Cardan's formula, let us define the quantities

$$\begin{aligned} u&=-\tfrac{1}{3}a_2 \\ p&=3u^2+2a_2u+a_1 \\ q&=u^3+a_2u^2+a_1u+a_0. \end{aligned} \tag{64}$$

The discriminant

$$\Delta=-4p^3-27q^2$$

is found to be positive $\forall K$. Thus the three roots of (63) are real and the largest one is in the form

$$\lambda_m=u+2^{2/3}(q^2+\Delta/27)^{1/6}\cos\left[\tfrac{1}{3}\tan^{-1}\left(\frac{\Delta^{1/2}}{\sqrt{27}q}\right)\right]. \tag{65}$$

Finally by substituting (65) in (61) the partition function of the $2\times2\times\infty$ Ising model follows and its free energy per spin is given by

$$F_{2\times2\times\infty}=-\tfrac{1}{4}kT\ln(2\lambda_m). \tag{66}$$

Differentiation of (66) to obtain other thermodynamic functions is indeed possible, but results in huge formulae that will not be given here. But it is interesting to note that the cosine in (65) has a minimum at $K\simeq0.258$.

6. Conclusion

Thus, by looking at the simple cubic lattice as layers of interacting hexagonal lattices whose interactions are best described by using our special matrix product, the transfer matrix of the three-dimensional Ising model on a simple cubic lattice has been obtained in a very simple factorised form, which exhibits a great symmetry that could remain hidden by following a different approach. This symmetry is indeed actually more pronounced in the considered case of the $2\times 2\times\infty$ model, where it drastically reduces the effective dimensionality of the transfer matrix from 16×16 to 3×3, but it also seems to remain available, when moving up to larger sized lattices, that will be treated analytically or numerically in the near future by using the present theoretical results. The importance of such studies has been clearly demonstrated recently by Martin (1986).

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