

Three-Dimensional Ising Model and Transfer Matrices

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The use of a transfer matrix method to solve the 3D Ising model is straightforwardly generalized from the 2D case. We follow B. Kaufman's approach. No approximation is made; however the largest eigenvalue cannot be identified. This problem comes from the fact that we follow the choice of directions of 2-dimensional rotations in the direct product space of the 2D Ising model such that all eigenvalue equations reduce miraculously to only one equation. Other choices of directions of 2-dimensional rotations for finding the largest eigenvalue may lose this fascinating feature. Comparing the series expansion of internal energy per site at the high temperature limit with the series obtained from the computer graphic method, we find these two series have very similar structures. A possible correcting factor $\Phi(x)$ is suggested to fit the result of the graphic method.

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I. Introduction

Although over a half-century has passed, solving the 3D Ising model exactly is still an open problem. Anyone who claims to solve this model exactly should, at least, evaluate its partition function, internal energy per site, critical temperature and the critical exponents α and β calculated from the relevant heat capacity and magnetization per site individually. In addition, a crucial test, similar to one L. Onsager [1] did in 1944, to check whether the results are right or wrong, is that one should compare the series expansion coefficients of the internal energy per site at the high temperature limit with the series obtained from some other methods, [9] e.g., the computer graphic method, at least up to the first three or four nonvanishing terms [2, 4-8].

Among the many various methods for deriving the partition function of 2D the Ising model, the transfer matrix method is the oldest and original method. However, the generalization of this method to the 3D case has had relatively little discussion. In this paper, we have no ambition to solve this 3D Ising model the satisfying all of the requirements mentioned above. Instead, B. Kaufman's approach [3] in the 3D Ising model is carried out step by step. Any approximation is avoided if we possibly can. In the following, it is shown that, when a transfer matrix formalism is set up, a spinor representation can work. 2-dimensional rotations in the direct product space and the feature that all of the eigenvalue equations reduce miraculously to only one equation also appear in the 3D Ising model. Even though the final high-temperature expansion series of internal energy per site is not exactly the same as the computer graphic method's, these two series do have the same structures. This discrepancy may be related to a dilemma between the choice of

the directions of the 2-dimensional rotations in order to find the largest eigenvalue and losing the fascinating feature that all of the eigenvalue equations reduce to only one equation. Be it ever not so perfect, we hope this generalization may lay the foundations for further study.

II. Transfer matrices

Let us consider a simple cubic lattice with l layers, each has m rows and n sites per row. So there are N points on the lattice, $N=mnl$. Periodic boundary conditions are used. To each lattice point, with integral coordinates τ, ρ, ζ , we assign a spin variable $s(\tau, \rho, \zeta)$ which takes two values ± 1 . The energy of the configuration is given by

$$E(s) = -J \sum_{\tau=1}^n \sum_{\rho=1}^m \sum_{\zeta=1}^l \{s(\tau, \rho, \zeta)s(\tau + 1, \rho, \zeta) + s(\tau, \rho, \zeta)s(\tau, \rho + 1, \zeta) + s(\tau, \rho, \zeta)s(\tau, \rho, \zeta + 1)\}. \quad (1)$$

$J(> 0)$ is the coupling of a pair of neighboring spins. The partition function

$$\mathcal{Z} = \sum_{(s)} e^{-E(s)/T} \quad (2)$$

$$= \sum_{(s)} \prod_{\tau=1}^n \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho+1, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho, \zeta+1)}, \quad (3)$$

is taken over all the 2^N possible configurations. Here $K \equiv J/T$. Now we factor the partition function into terms each involving only two neighboring spins, giving

$$\mathcal{Z} = \sum_{s(1, \cdot, \cdot)} \cdots \sum_{s(n, \cdot, \cdot)} \langle s(1, \cdot, \cdot) | \mathcal{V} | s(2, \cdot, \cdot) \rangle s(2, \cdot, \cdot) | \mathcal{V} | s(3, \cdot, \cdot) \rangle \cdots \langle s(n, \cdot, \cdot) | \mathcal{V} | s(1, \cdot, \cdot) \rangle \quad (4)$$

$$= Tr \mathcal{V}^n, \quad (5)$$

where the matrix elements of the transfer matrix \mathcal{V} are

$$\langle s(\tau, \cdot, \cdot) | \mathcal{V} | s(\tau + 1, \cdot, \cdot) \rangle = \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho+1, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho, \zeta+1)}. \quad (6)$$

\mathcal{V} can be put into a more convenient form by factoring it into the product of simpler matrices,

$$\mathcal{V} = \mathcal{V}_3 \mathcal{V}_2 \mathcal{V}_1, \tag{7}$$

$$\langle s(\tau, \cdot, \cdot) | \mathcal{V}_1 | s(\tau + 1, \cdot, \cdot) \rangle = \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)}, \tag{8}$$

$$\langle s(\tau, \cdot, \cdot) | \mathcal{V}_2 | s(\tau + 1, \cdot, \cdot) \rangle = \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau, \rho+1, \zeta)} \delta_{s(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)}, \tag{9}$$

$$\langle s(\tau, \cdot, \cdot) | \mathcal{V}_3 | s(\tau + 1, \cdot, \cdot) \rangle = \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau, \rho, \zeta+1)} \delta_{s(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)}. \tag{10}$$

The above decomposition may be checked as follows:

$$\langle s(\tau, \cdot, \cdot) | \mathcal{V}_3 \mathcal{V}_2 \mathcal{V}_1 | s(\tau + 1, \cdot, \cdot) \rangle \tag{11}$$

$$\begin{aligned} &= \sum_{s(\tau+1, \cdot, \cdot)} \sum_{s'(\tau, \cdot, \cdot)} \sum_{s''(\tau+1, \cdot, \cdot)} \sum_{s''(\tau, \cdot, \cdot)} \sum_{s''(\tau+1, \cdot, \cdot)} \langle s(\tau, \cdot, \cdot) | \mathcal{V}_3 | s(\tau + 1, \cdot, \cdot) \rangle \\ &\quad \langle s(\tau + 1, \cdot, \cdot) | s'(\tau, \cdot, \cdot) \rangle \langle s'(\tau, \cdot, \cdot) | \mathcal{V}_2 | s'(\tau + 1, \cdot, \cdot) \rangle \\ &\quad \langle s'(\tau + 1, \cdot, \cdot) | s''(\tau, \cdot, \cdot) \rangle \langle s''(\tau, \cdot, \cdot) | \mathcal{V}_1 | s''(\tau + 1, \cdot, \cdot) \rangle \\ &\quad \langle s''(\tau + 1, \cdot, \cdot) | s(\tau + 1, \cdot, \cdot) \rangle \end{aligned} \tag{12}$$

$$\begin{aligned} &= \prod_{\rho=1}^m \prod_{\zeta=1}^l \left\{ \sum_{s(\tau+1, \rho, \zeta)} \sum_{s'(\tau, \rho, \zeta)} \sum_{s'(\tau+1, \rho, \zeta)} \sum_{s''(\tau, \rho, \zeta)} \sum_{s''(\tau+1, \rho, \zeta)} \right. \\ &\quad (e^{Ks(\tau, \rho, \zeta)s(\tau, \rho, \zeta+1)} \delta_{s(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)}) (\delta_{s(\tau+1, \rho, \zeta)s'(\tau, \rho, \zeta)}) \\ &\quad (e^{Ks'(\tau, \rho, \zeta)s'(\tau, \rho+1, \zeta)} \delta_{s'(\tau, \rho, \zeta)s'(\tau+1, \rho, \zeta)}) (\delta_{s'(\tau+1, \rho, \zeta)s''(\tau, \rho, \zeta)}) \\ &\quad \left. (e^{Ks''(\tau, \rho, \zeta)s''(\tau+1, \rho, \zeta)}) (\delta_{s''(\tau+1, \rho, \zeta)s(\tau+1, \rho, \zeta)}) \right\} \end{aligned} \tag{13}$$

$$= \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{Ks(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho+1, \zeta)} e^{Ks(\tau, \rho, \zeta)s(\tau, \rho, \zeta+1)}. \tag{14}$$

In the above equation, due to periodic boundary conditions, the identity

$$\prod_{\rho=1}^m \prod_{\zeta=1}^l \delta_{s(\tau, \rho, \zeta)s'(\tau, \rho, \zeta)} = \prod_{\rho=1}^m \prod_{\zeta=1}^l \delta_{s(\tau, \rho+1, \zeta)s'(\tau, \rho+1, \zeta)} \tag{15}$$

is used. Furthermore, $\mathcal{V}_1, \mathcal{V}_2, \mathcal{V}_3$ can be rewritten as matrices in the direct product space. Observing from (8), let us define a matrix a with matrix elements

$$\langle s(\tau, \rho, \zeta) | a | s(\tau + 1, \rho, \zeta) \rangle = e^{Ks(\tau, \rho, \zeta)s(\tau+1, \rho, \zeta)}. \tag{16}$$

$$a = \begin{pmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{pmatrix} \quad (17)$$

$$= e^K (I + e^{-2K} \sigma_x) \quad (18)$$

$$= (2 \sinh 2K)^{1/2} e^{K^* \sigma_x}. \quad (19)$$

I is a 2×2 unit matrix. $\tanh K^* = e^{-2K}$, $\tanh K = e^{-2K^*}$, $\sinh 2K \sinh 2K^* = 1$. To simplify the matrices $\mathcal{V}_1, \mathcal{V}_2, \mathcal{V}_3$, we define

$$X_{i,j} = \underbrace{\left(\begin{array}{cccc} I & I & \cdots & I \end{array} \right)}_{\zeta=1} \cdots \underbrace{\left(\begin{array}{cccc} I & \cdots & \overbrace{\sigma_x}^{\rho=i} & \cdots & I \end{array} \right)}_{\zeta=j} \cdots \underbrace{\left(\begin{array}{cccc} I & I & \cdots & I \end{array} \right)}_{\zeta=l}. \quad (20)$$

$Y_{i,j}$ and $Z_{i,j}$ are also defined similarly by replacing the Pauli matrix σ_x with σ_y and σ_z respectively.

$$\mathcal{V}_1 = \overbrace{a \quad a \quad \cdots \quad a}^{ml \text{ times}} \quad (21)$$

$$= (2 \sinh 2K)^{ml/2} \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{K^* X_{\rho,\zeta}}. \quad (22)$$

As for \mathcal{V}_2 , we introduce another matrix b with matrix elements

$$\langle s(\tau, \rho, \zeta) | b | s(\tau + 1, \rho, \zeta) \rangle = \delta_{s(\tau, \rho, \zeta) s(\tau + 1, \rho, \zeta)} e^{K s(\tau, \rho, \zeta) s(\tau + 1, \rho, \zeta)}, \quad (23)$$

$$b = \begin{pmatrix} e^K & 0 & 0 & 0 \\ 0 & e^{-K} & 0 & 0 \\ 0 & 0 & e^K & 0 \\ 0 & 0 & 0 & e^{-K} \end{pmatrix} = e^{K \sigma_z} \sigma_z = e^{K(\sigma_z - I)(I + \sigma_z)}, \quad (24)$$

$$\mathcal{V}_2 = \overbrace{b \quad b \quad \cdots \quad b}^{ml \text{ times}} \quad (25)$$

$$= \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{K Z_{\rho+1, \zeta} Z_{\rho, \zeta}}. \quad (26)$$

Similarly, \mathcal{V}_\ni is obtained from a matrix c ,

$$c = e^{K(\sigma_z \overbrace{I \cdots I}^{m \text{ times}}) (\overbrace{I \cdots I}^{m \text{ times}} \sigma_z)}. \quad (27)$$

$$\mathcal{V}_3 = \overbrace{c \cdots c}^{ml \text{ times}} \quad (28)$$

$$= \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{KZ_{\rho,\zeta}Z_{\rho,\zeta+1}}. \quad (29)$$

III. Spinor representation

$\mathcal{V}_1, \mathcal{V}_2, \mathcal{V}_3$ in 2^{ml} -space can be related to matrices in $2ml$ -spaces via Dirac Γ matrices. The process of reducing the dimensions of \mathcal{V} had been used in 2D the Ising model. Define a set of matrix $\Gamma_{\mu,\zeta}$ satisfying anticommutation relations

$$\Gamma_{\mu,\zeta}\Gamma_{\mu',\zeta'} + \Gamma_{\mu',\zeta'}\Gamma_{\mu,\zeta} = 2\delta_{\mu\mu'}\delta_{\zeta\zeta'}, \quad (30)$$

$$(\mu, \mu' = 1, 2 \cdots 2m; \zeta, \zeta' = 1, 2 \cdots l). \quad (31)$$

Every $\Gamma_{\mu,\zeta}$ is a $2^{ml} \times 2^{ml}$ matrix. A possible representation of $\Gamma_{\mu,\zeta}$ is

$$\Gamma_{1,1} = Z_{1,1} \quad (32)$$

$$\Gamma_{2,1} = Y_{1,1} \quad (33)$$

$$\Gamma_{3,1} = X_{1,1}Z_{2,1} \quad (34)$$

$$\Gamma_{4,1} = X_{1,1}Y_{2,1} \quad (35)$$

\vdots

$$\Gamma_{2m-1,1} = X_{1,1}X_{2,1} \cdots X_{m-1,1}Z_{m,1} \quad (36)$$

$$\Gamma_{2m,1} = X_{1,1}X_{2,1} \cdots X_{m-1,1}Y_{m,1} \quad (37)$$

$$\Gamma_{1,2} = (X_{1,1}X_{2,1} \cdots X_{m,1}) Z_{1,2} = U_1 Z_{1,2} \quad (38)$$

$$\Gamma_{2,2} = (X_{1,1}X_{2,1} \cdots X_{m,1}) Y_{1,2} = U_1 Y_{1,2} \quad (39)$$

\vdots

$$\Gamma_{1,\zeta} = U_1 U_2 \cdots U_{\zeta-1} Z_{1,\zeta} \quad (40)$$

$$\Gamma_{2,\zeta} = U_1 U_2 \cdots U_{\zeta-1} Y_{1,\zeta} \quad (41)$$

\vdots

$$\Gamma_{2m-1,l} = U_1 U_2 \cdots U_{l-1} Z_{m,l} \quad (42)$$

$$\Gamma_{2m,l} = U_1 U_2 \cdots U_{l-1} Y_{m,l} \quad (43)$$

where

$$U_\zeta \equiv (I \ \cdots \ I) \ \cdots \ \underbrace{(\sigma_x \ \sigma_x \ \cdots \ \sigma_x)}_{\zeta^{\text{th}} \text{ block}} \ (I \ \cdots \ I) \cdots (I \ \cdots \ I). \quad (44)$$

The total number of the Γ matrix is $2ml$. A special $2^{ml} \times 2^{ml}$ matrix U is defined as

$$U = \underbrace{\sigma_x \ \sigma_x \ \cdots \ \sigma_x}_{ml \text{ times}} \quad (45)$$

$$= i^{ml} \prod_{\zeta=1}^l \left(\prod_{\mu=1}^{2m} \Gamma_{\mu,\zeta} \right). \quad (46)$$

U and U_ζ have the following relations:

$$U^2 = I, \quad U_\zeta^2 = I, \quad (47)$$

$$U(I + U) = I + U, \quad U_\zeta(I + U_\zeta) = I + U_\zeta, \quad (48)$$

$$U(I - U) = U - I, \quad U_\zeta(I - U_\zeta) = U_\zeta - I, \quad (49)$$

$$\{U, \Gamma_{\mu,\zeta}\} = 0, \quad \{U_\zeta, \Gamma_{\mu,\zeta}\} = 0, \quad (50)$$

$$[U, \Gamma_{\mu,\zeta} \Gamma_{\mu',\zeta'}] = 0, \quad [U_\zeta, \Gamma_{\mu,\zeta} \Gamma_{\mu',\zeta'}] = 0. \quad (51)$$

By definition of Γ , we notice that

$$\Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta} = Y_{\rho,\zeta} Z_{\rho,\zeta} = i X_{\rho,\zeta}, \quad (52)$$

then

$$\mathcal{V}_1 = (2 \sinh 2K)^{ml/2} \prod_{\rho=1}^m \prod_{\zeta=1}^l e^{iK^* \Gamma_{2\rho-1,\zeta} \Gamma_{2\rho,\zeta}}. \quad (53)$$

Similarly,

$$\Gamma_{2\rho+1,\zeta} \Gamma_{2\rho,\zeta} = i Z_{\rho,\zeta} Z_{\rho+1,\zeta}, \quad (54)$$

then we have

$$\mathcal{V}_2 = \prod_{\zeta=1}^l \left\{ e^{K Z_{m,\zeta} Z_{1,\zeta}} \prod_{\rho=1}^{m-1} e^{K Z_{\rho,\zeta} Z_{\rho+1,\zeta}} \right\} \quad (55)$$

$$= \prod_{\zeta=1}^l \left\{ e^{iK U_\zeta \Gamma_{1,\zeta} \Gamma_{2m,\zeta}} \prod_{\rho=1}^{m-1} e^{iK \Gamma_{2\rho,\zeta} \Gamma_{2\rho+1,\zeta}} \right\}. \quad (56)$$

With the identity,

$$(U_\zeta \Gamma_{1,\zeta} \Gamma_{2m,\zeta})^2 = U_\zeta \Gamma_{1,\zeta} \Gamma_{2m,\zeta} U_\zeta \Gamma_{1,\zeta} \Gamma_{2m,\zeta} = -I, \tag{57}$$

\mathcal{V}_2 can be rewritten as

$$\mathcal{V}_2 = \prod_{\zeta=1}^l \left\{ \left[\frac{1}{2}(I + U_\zeta) e^{iK\Gamma_{1,\zeta} \Gamma_{2m,\zeta}} + \frac{1}{2}(I - U_\zeta) e^{-iK\Gamma_{1,\zeta} \Gamma_{2m,\zeta}} \right] \prod_{\rho=1}^{m-1} e^{iK\Gamma_{2\rho,\zeta} \Gamma_{2\rho+1,\zeta}} \right\}. \tag{58}$$

Since U_ζ commutes with $\Gamma_{2\rho,\zeta} \Gamma_{2\rho+1,\zeta}$, the projection operators $\frac{1}{2} (I \pm U_\zeta)$ project \mathcal{V}_2 into 2^l pieces. For

$$\mathcal{V}_3 = \prod_{\rho=1}^m \left(e^{KZ_{\rho,l} Z_{\rho,1}} \prod_{\zeta=1}^{l-1} e^{KZ_{\rho,\zeta} Z_{\rho,\zeta+1}} \right), \tag{59}$$

the situation seems more complicated.

$$\begin{aligned} Z_{\rho,\zeta} Z_{\rho,\zeta+1} &= (Z_{\rho,\zeta} Z_{\rho+1,\zeta})(Z_{\rho+1,\zeta} Z_{\rho+2,\zeta}) \cdots (Z_{m,\zeta} Z_{1,\zeta+1})(Z_{1,\zeta+1} Z_{2,\zeta+1}) \\ &\quad \cdots (Z_{\rho-1,\zeta+1} Z_{\rho,\zeta+1}), \end{aligned} \tag{60}$$

$$\begin{aligned} &= (-i\Gamma_{2\rho+1,\zeta} \Gamma_{2\rho,\zeta})(-i\Gamma_{2\rho+3,\zeta} \Gamma_{2\rho+2,\zeta}) \cdots \\ &\quad (-i\Gamma_{1,\zeta+1} \Gamma_{2m,\zeta}) \cdots (-i\Gamma_{2\rho-1,\zeta+1} \Gamma_{2\rho-2,\zeta+1}), \end{aligned} \tag{61}$$

$$= i^m \Gamma_{2\rho,\zeta} \Gamma_{2\rho+1,\zeta} \Gamma_{2\rho+2,\zeta} \cdots \Gamma_{2m,\zeta} \Gamma_{1,\zeta+1} \cdots \Gamma_{2\rho-1,\zeta+1}, \tag{62}$$

$$= i^m \Gamma_{2\rho,\zeta} (\Gamma_{2\rho+1,\zeta} \cdots \Gamma_{2\rho-2,\zeta+1}) \Gamma_{2\rho-1,\zeta+1}, \tag{63}$$

$$= +i\Gamma_{2\rho,\zeta} W_{2\rho+1,\zeta} \Gamma_{2\rho-1,\zeta+1}, \tag{64}$$

$$= iW_{2\rho+1,\zeta} \Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta+1}. \tag{65}$$

$W_{2\rho+1,\zeta}$ is defined as

$$W_{2\rho+1,\zeta} = i^{m-1} \Gamma_{2\rho+1,\zeta} \Gamma_{2\rho+2,\zeta} \cdots \Gamma_{2\rho-3,\zeta+1} \Gamma_{2\rho-2,\zeta+1} \tag{66}$$

$$= I \cdots I \underbrace{\overbrace{\sigma_x^{(\rho+1,\zeta)}} \cdots \overbrace{\sigma_x^{(\rho-1,\zeta+1)}}}_{m-1 \text{ times of } \sigma_x} I \cdots I. \tag{67}$$

$W_{2\rho+1,\zeta}$ has the property that it anticommutes with $\Gamma_{\mu,\alpha}$ inside the region that the integral coordinates (μ, α) from $(2\rho + 1, \zeta)$ to $(2\rho - 2, \zeta + 1)$, whereas it commutes with $\Gamma_{\mu,\alpha}$ outside of that region.

$$Z_{\rho,l} Z_{\rho,1} = (Z_{\rho,l} Z_{\rho+1,l}) \cdots (Z_{m,l} Z_{1,1})(Z_{1,1} Z_{2,1}) \cdots (Z_{\rho-1,1} Z_{\rho,1}) \tag{68}$$

$$= -i^m U \Gamma_{2\rho,l} \Gamma_{2\rho+1,l} \cdots \Gamma_{2m,l} \Gamma_{1,1} \Gamma_{2,1} \cdots \Gamma_{2\rho-1,1} \tag{69}$$

$$= +iUW_{2\rho+1,l} \Gamma_{2\rho-1,1} \Gamma_{2\rho,l}. \tag{70}$$

$$W_{2\rho+1,l} = i^{m-1} \Gamma_{2\rho+1,l} \Gamma_{2\rho+2,l} \cdots \Gamma_{2m,l} \Gamma_{1,1} \cdots \Gamma_{2\rho-2,1} \quad (71)$$

$$= \underbrace{\sigma_x}_{(1,1)} \cdots \underbrace{\sigma_x}_{(\rho-1,1)} I \cdots I \underbrace{\sigma_x}_{(\rho+1,l)} \cdots \underbrace{\sigma_x}_{(m,l)}. \quad (72)$$

Then we have

$$\mathcal{V}_3 = \prod_{\rho=1}^m \left\{ e^{+iKUW_{2\rho+1,l} \Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} \prod_{\zeta=1}^{l-1} e^{iKW_{2\rho+1,\zeta} \Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta+1}} \right\}. \quad (73)$$

A remarkable observation of Kaufman is that decomposing \mathcal{V} of the 2D Ising model into the product of factors like $e^{\frac{\theta}{2}\Gamma}$, which is interpreted as a two-dimensional rotation with rotation angle θ in the direct product space. We follow this spirit and decompose the factors into several 2D rotations,

$$\begin{aligned} & e^{+iKUW_{2\rho+1,l} \Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} \\ &= \frac{1}{2}(I+U)e^{+iKW_{2\rho+1,l} \Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} + \frac{1}{2}(I-U)e^{-iKW_{2\rho+1,l} \Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} \end{aligned} \quad (74)$$

$$\begin{aligned} &= \frac{1}{2}(I+U) \left\{ \frac{1}{2}(I+W_{2\rho+1,l})e^{+iK\Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} + \frac{1}{2}(I-W_{2\rho+1,l})e^{-iK\Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} \right\} \\ &+ \frac{1}{2}(I-U) \left\{ \frac{1}{2}(I+W_{2\rho+1,l})e^{-iK\Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} + \frac{1}{2}(I-W_{2\rho+1,l})e^{+iK\Gamma_{2\rho-1,1} \Gamma_{2\rho,l}} \right\} \end{aligned} \quad (75)$$

$$\begin{aligned} & e^{iKW_{2\rho+1,\zeta} \Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta+1}} \\ &= \frac{1}{2}(I+W_{2\rho+1,\zeta})e^{iK\Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta+1}} + \frac{1}{2}(I-W_{2\rho+1,\zeta})e^{-iK\Gamma_{2\rho,\zeta} \Gamma_{2\rho-1,\zeta+1}}. \end{aligned} \quad (76)$$

In the 2D Ising model the \mathcal{V} are decomposed into 2 pieces. This is not so simple in the 3D Ising model. Due to the projection operators $\frac{1}{2}(I \pm U)$, $\frac{1}{2}(I \pm U_\zeta)$, $\frac{1}{2}(I \pm W)$, \mathcal{V} has $2^l \times (2 \times 2^{ml})$ pieces. Only one piece will produce the largest eigenvalue, which dominates the value of partition function.

Since $W_{2\rho+1,\zeta}$ may commute or anticommute with $\Gamma_{\mu,\alpha}$, we have to check the commutation relations between the projection operators and the product of the factors like $e^{\frac{1}{2}\theta\Gamma}$, since the dogma states that two matrices are simultaneously diagonalized if and only if these two matrices commute. \mathcal{V} comprises the product of projection operators and a lot of $e^{\frac{1}{2}\theta\Gamma}$. So if the commutation relations are not valid, the whole scheme may break down. Commuting $\frac{1}{2}(I \pm U)$ with the product of all factors like $e^{\frac{1}{2}\theta\Gamma}$ does not give any trouble. Any single projection operator $\frac{1}{2}(I \pm U_\zeta)$ or $\frac{1}{2}(I \pm W)$ may do not commute with some $e^{\frac{1}{2}\theta\Gamma}$. However, fortunately, the product of all the projections in any one piece of \mathcal{V} , e.g.

$$P = \frac{1}{2}(I+U) \left(\prod_{\zeta'=1}^l \frac{1}{2}(I+U_{\zeta'}) \right) \left(\prod_{\rho=1}^m \prod_{\zeta=1}^l \frac{1}{2}(I+W_{2\rho-1,\zeta}) \right), \quad (77)$$

do commute with any $e^{\frac{1}{2}\theta\Gamma}$, because $e^{\frac{1}{2}\theta\Gamma}$ passes through P will change the sign of $\frac{1}{2}\theta\Gamma$ an even number times and it does not change sign eventually.

How to choose the proper piece and obtain the largest eigenvalue? We have no answer. A possible rule may be followed that all eigenvalue equations should reduce to one equation. We will show this point in the next section. This is a beautiful feature in the 2D Ising model. Let us consider one possible piece of \mathcal{V} ,

$$\tilde{\mathcal{V}} = (2 \sinh 2K)^{ml/2} \tilde{\mathcal{V}}', \quad (78)$$

$$\begin{aligned} \tilde{\mathcal{V}}' = & \left\{ \prod_{\rho=1}^m e^{+iK\Gamma_{2\rho-1,1}\Gamma_{2\rho,l}} \prod_{\zeta=1}^{l-1} e^{iK\Gamma_{2\rho,\zeta}\Gamma_{2\rho-1,\zeta+1}} \right\} \\ & \left\{ \prod_{\zeta'=1}^l e^{iK\Gamma_{1,\zeta'}\Gamma_{2m,\zeta'}} \prod_{\rho'=1}^{m-1} e^{iK\Gamma_{2\rho,\zeta}\Gamma_{2\rho+1,\zeta}} \right\} \\ & \left\{ \prod_{\zeta''=1}^l \prod_{\rho''=1}^m e^{ik^*\Gamma_{2\rho''-1,\zeta''}\Gamma_{2\rho'',\zeta''}} \right\}. \end{aligned} \quad (79)$$

In essence, $\tilde{\mathcal{V}}$ includes the repetition l times of the same rotations as in the 2D Ising model, appearing in the second and third brackets of (79), and the new rotations in the first bracket of (79), relating to the third dimensional coupling beyond the 2D Ising model.

IV. Eigenvalue equations

The rotation operator in the spinor representation,

$$S_{\lambda\sigma}(\theta) = e^{\frac{1}{2}\theta\Gamma_\lambda\Gamma_\sigma} \quad (\lambda \neq \sigma), \quad (80)$$

has a one-to-one correspondence to the 2D rotational matrix $\omega(\lambda\sigma | \theta)$ of the Γ matrix.

$$S_{\lambda\sigma}^{-1}(\theta)\Gamma_\alpha S_{\lambda\sigma}(\theta) = \sum_{\kappa} \omega(\lambda\sigma | \theta)_{\alpha\kappa} \Gamma_\kappa, \quad (81)$$

$$S_{\lambda\sigma}^{-1}(\theta)\Gamma_\lambda S_{\lambda\sigma}(\theta) = \Gamma_\lambda \cos \theta + \Gamma_\sigma \sin \theta, \quad (\lambda \neq \sigma), \quad (82)$$

$$S_{\lambda\sigma}^{-1}(\theta)\Gamma_\sigma S_{\lambda\sigma}(\theta) = -\Gamma_\lambda \sin \theta + \Gamma_\sigma \cos \theta, \quad (\sigma \neq \lambda), \quad (83)$$

$$S_{\lambda\sigma}^{-1}(\theta)\Gamma_\alpha S_{\lambda\sigma}(\theta) = \Gamma_\alpha, \quad (\alpha \neq \lambda, \alpha \neq \sigma). \quad (84)$$

$S_{\lambda\sigma}(\theta)$ is a 2D rotations in the direct product space. The rotations, $e^{\pm\frac{\theta}{2}\Gamma}$, have different rotational angles, $+\theta$ and $-\theta$. We mean they have different directions of rotations. The eigenvalues of the rotational matrix ω are 1 with $(2ml-2)$ -fold degeneracies and $e^{\pm i\theta}$ two nondegenerate eigenvalues, whereas the eigenvalues of $S_{\lambda\sigma}$ in the spinor representation are $e^{\pm i\frac{\theta}{2}}$ each with 2^{ml-1} -fold degeneracies.

The correspondence with $\tilde{\mathcal{V}}$ is

$$\tilde{\omega} = (2 \sinh 2K)^{ml/2} \tilde{\omega}', \quad (85)$$

$$\begin{aligned} \tilde{\omega}' = & \left\{ \prod_{\rho=1}^m \omega(2\rho - 1, 1; 2\rho, l \mid +2iK) \prod_{\zeta=1}^{l-1} \omega(2\rho, \zeta; 2\rho - 1, \zeta + 1 \mid 2iK) \right\} \\ & \left\{ \prod_{\zeta'=1}^l \omega(1, \zeta'; 2m, \zeta' \mid 2iK) \prod_{\rho'=1}^{m-1} \omega(2\rho, \zeta; 2\rho + 1, \zeta \mid 2iK) \right\} \\ & \left\{ \prod_{\zeta''=1}^l \prod_{\rho''=1}^m \omega(2\rho'' - 1, \zeta''; 2\rho'', \zeta'' \mid 2iK^*) \right\} \end{aligned} \quad (86)$$

$$= \omega_3 \omega_2 \omega_1. \quad (87)$$

$$\omega_1^{\frac{1}{2}} \omega_2 \omega_1^{\frac{1}{2}} = \begin{pmatrix} & & & & & \\ & & & & & \\ & & \ddots & & & \\ & & & \ddots & & \\ & & & & \ddots & \\ & & & & & \ddots \end{pmatrix}_{2ml \times 2ml}, \quad (88)$$

$$= \begin{pmatrix} A & B & 0 & \cdots & 0 & -B^\dagger \\ B^\dagger & A & B & 0 & \cdots & 0 \\ 0 & B^\dagger & A & B & 0 & \cdots \\ & & & \ddots & & \\ 0 & \cdots & 0 & B^\dagger & A & B \\ -B & 0 & \cdots & 0 & B^\dagger & A \end{pmatrix}_{2m \times 2m}, \quad (89)$$

$$A = \begin{pmatrix} c^*c & is^*c \\ -is^*c & c^*c \end{pmatrix}, \quad B = \begin{pmatrix} -\frac{1}{2} & -is(\frac{-1+c^*}{2}) \\ is(\frac{1+c^*}{2}) & -\frac{1}{2} \end{pmatrix}, \quad (90)$$

$$B^\dagger = \begin{pmatrix} -\frac{1}{2} & -is(\frac{1+c^*}{2}) \\ is(\frac{-1+c^*}{2}) & -\frac{1}{2} \end{pmatrix}, \quad (91)$$

$$s \equiv \sinh 2K, \quad c \equiv \cosh 2K, \quad s^* \equiv \sinh 2K^*, \quad c^* \equiv \sinh 2K^*. \quad (92)$$

The matrix ω_3 is just the same matrix considered in the 2D Ising model. $\omega_1^{1/2}\omega_2\omega_1^{1/2}$ is in symmetric form such that its eigenvalue equations are much more easier to handle.

$$\omega_3 \equiv \prod_{\rho=1}^m \omega(2\rho - 1, 1; 2\rho, l \mid 2iK) \prod_{\zeta=1}^{l-1} \omega(2\rho, \zeta; 2\rho - 1, \zeta + 1 \mid 2iK) \tag{93}$$

$$= \begin{pmatrix} \mathcal{A} & \mathcal{B} & 0 & \cdots & 0 & -\mathcal{B}^\dagger \\ \mathcal{B}^\dagger & \mathcal{A} & \mathcal{B} & 0 & \cdots & 0 \\ 0 & \mathcal{B}^\dagger & \mathcal{A} & \mathcal{B} & 0 & \cdots \\ & & & \ddots & & \\ 0 & \cdots & 0 & \mathcal{B}^\dagger & \mathcal{A} & \mathcal{B} \\ -\mathcal{B} & 0 & \cdots & 0 & \mathcal{B}^\dagger & \mathcal{A} \end{pmatrix}_{2ml \times 2ml}, \tag{94}$$

$$\mathcal{A} = \begin{pmatrix} c & & & & \\ & c & & & \\ & & \ddots & & \\ & & & c & \end{pmatrix}_{2m \times 2m}, \mathcal{B}^\dagger = \begin{pmatrix} 0 & -is & 0 & \cdots & & \\ 0 & 0 & 0 & \cdots & & \\ 0 & 0 & 0 & -is & 0 & \cdots \\ \vdots & \vdots & \vdots & 0 & 0 & \cdots \\ & & & \vdots & & \ddots \\ & & & & 0 & -is \\ & & & & 0 & 0 \end{pmatrix}_{2m \times 2m}, \tag{95}$$

$$\mathcal{B} = \begin{pmatrix} 0 & 0 & \cdots & \cdots & & \\ is & 0 & 0 & \cdots & & \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & is & 0 & 0 & \cdots \\ & & & \ddots & & \\ & & & & 0 & 0 \\ & & & & is & 0 \end{pmatrix}_{2m \times 2m}. \tag{96}$$

Now we proceed to solve the eigenvalue equation

$$\tilde{\omega}\Psi = \lambda\Psi, \tag{97}$$

where $\tilde{\omega} = (2 \sinh 2K)^{ml/2}\omega_3[\omega_1^{1/2}\omega_2\omega_1^{1/2}]$,

$$\Psi = \begin{pmatrix} z \psi_0 \\ z^2 \psi_0 \\ z^3 \psi_0 \\ \vdots \\ z^l \psi_0 \end{pmatrix}, \psi_0 = \begin{pmatrix} y u \\ y^2 u \\ y^3 u \\ \vdots \\ y^m u \end{pmatrix}, u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}. \tag{98}$$

By imposing the constraint,

$$z^l = -1, \quad \text{or } z = e^{i\frac{\pi t_2}{l}} \quad (t_2 = 1, 3, 5 \dots), \quad (99)$$

one reduces eigenvalue equation (97) to

$$(\mathcal{A} + z\mathcal{B} + z^{-1}\mathcal{B}^\dagger) \psi_0 = \lambda \psi_0. \quad (100)$$

Further, imposing the constraint,

$$y^m = -1, \quad \text{or } y = e^{i\frac{\pi t_1}{m}} \quad (t_1 = 1, 3, 5 \dots), \quad (101)$$

(100) is reduced to

$$\mathcal{D}(A + yB + y^{-1}B^\dagger) u = \lambda u, \quad (102)$$

where

$$\mathcal{D} = \begin{pmatrix} c & -iz^{-1}s \\ izs & c \end{pmatrix}, \quad (103)$$

$$\begin{aligned} & A + yB + y^{-1}B^\dagger \\ &= \begin{pmatrix} c^*c - \cos \frac{\pi t_1}{m} & is^*c - i\left(\frac{-1+c^*}{2}\right)se^{i\frac{\pi t_1}{m}} - i\left(\frac{1+c^*}{2}\right)se^{-i\frac{\pi t_1}{m}} \\ -is^*c + i\left(\frac{1+c^*}{2}\right)se^{i\frac{\pi t_1}{m}} + i\left(\frac{-1+c^*}{2}\right)se^{-i\frac{\pi t_1}{m}} & c^*c - \cos \frac{\pi t_1}{m} \end{pmatrix}. \end{aligned} \quad (104)$$

The eigenvalue equation (102) is further reduced to

$$\lambda^2 - 2 \cosh \gamma \lambda + 1 = 0. \quad (105)$$

$\lambda = \exp(\pm\gamma)$ is the solution of λ . γ is determined by

$$\cosh \gamma = \frac{c^3}{s} - c(\cos \theta_1 + \cos \theta_2) + sc \cos \theta_1 \cos \theta_2 + s^2 \sin \theta_1 \sin \theta_2, \quad (106)$$

where two continuous variables, θ_1, θ_2 , are obtained by taking the thermodynamic limit, $m, l \rightarrow \infty$, $\frac{\pi t_1}{m} \rightarrow \theta_1, \frac{\pi t_2}{l} \rightarrow \theta_2$.

The partition function of \mathcal{V} is

$$\mathcal{Z} \sim \lambda^N. \quad (107)$$

The free energy per site under the thermodynamic limit is

$$f = -\frac{1}{\beta} \lim_{N \rightarrow \infty} N^{-1} \ln \mathcal{Z} \quad (108)$$

$$= -\frac{1}{\beta} \ln (2 \sinh 2K)^{1/2} - \frac{1}{8\pi^2\beta} \int_0^{2\pi} \int_0^{2\pi} \gamma(\theta_1, \theta_2) d\theta_1 d\theta_2, \quad (109)$$

where $\beta \equiv \frac{1}{T}$. For convenience, $J \equiv 1$, the internal energy per site is

$$u = \frac{\partial}{\partial \beta} (\beta f) \quad (110)$$

$$= -\coth 2K - \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{\partial \gamma}{\partial K} d\theta_1 d\theta_2. \quad (111)$$

V. High temperature limit

Let us expand u in terms of x at high temperature limit, x small, and compare the series of u obtained from the computer graphic method [2].

$$x \equiv \tanh K, \quad c = \cosh 2K = \frac{1+x^2}{1-x^2}, \quad s = \sinh 2K = \frac{2x}{1-x^2}, \quad (112)$$

$$\begin{aligned} \cosh \gamma &= \frac{(1+x^2)^3}{(1-x^2)^2 2x} - \frac{1+x^2}{1-x^2} (\cos \theta_1 + \cos \theta_2) \\ &+ \frac{2x(1+x^2)}{(1-x^2)^2} \cos \theta_1 \cos \theta_2 + \frac{4x^2}{(1-x^2)^2} \sin \theta_1 \cos \theta_2, \end{aligned} \quad (113)$$

$$\begin{aligned} \frac{\partial \gamma}{\partial K} &= 2(\sinh \gamma)^{-1} \left\{ -\frac{(1+x^2)^2(1-10x^2+x^4)}{(1-x^2)^2 4x^2} - \frac{2x}{1-x^2} (\cos \theta_1 + \cos \theta_2) \right. \\ &\left. + \frac{1+6x^2+x^4}{(1-x^2)^2} \cos \theta_1 \cos \theta_2 + \frac{4x(1+x^2)}{(1-x^2)^2} \sin \theta_1 \sin \theta_2 \right\}. \end{aligned} \quad (114)$$

With the help of computer program Maple V Release 5.1, we get our result

$$u = -3x - 8x^3 - 28x^5 - 132x^7 - 832x^9 + O(x^{11}). \quad (115)$$

Comparing the result obtained by the computer graphic method, the series expansion of u for a simple cubic lattice can be transformed from the partition function,

$$\mathcal{Z}^{\frac{1}{N}} = 2 \cosh^3 K (1 + 3x^4 + 22x^6 + 187.5x^8 + 1980x^{10} + O(x^{12})), \quad (116)$$

so

$$u = -\frac{\partial}{\partial K} \ln \mathcal{Z}^{\frac{1}{N}} \quad (117)$$

$$= -3x - 12x^3 - 120x^5 - 1332x^7 - 17676x^9 + O(x^{11}). \quad (118)$$

(115) and (118) have very similar structures. The coefficient of x^{-1} does not exist in our result (115) though it exists naively in $\coth 2K$ of (111). The first nonvanishing term $-3x$ of (115) and the vanishing of all coefficients of even powers of x are the same as (118). All terms, up to $O(x^9)$, with minus signs in (115) are also the same as (118). The reason why (115) and (118) do not have the same first three or four coefficients may come from the fact that we cannot decipher precisely the largest eigenvalue of \mathcal{V} . On the other hand, if we choose different directions for the 2D rotations, the eigenvalue equations may not be reduced to only one equation. This is a dilemma.

The correct relation of $\cosh \gamma$ implies the correct thermodynamic quantities of the 3D Ising model. To guess the correct relation as (106) may be a promising way for finding the right resolution of the 3D Ising model. For example, trying to repair (106), if we multiply the matrices \mathcal{A} , \mathcal{B} and \mathcal{B}^\dagger , or ω_3 , with a correcting factor $\Phi(x)$, then we have

$$\cosh \gamma = \frac{c^3}{s} - c \cos \theta_1 + \Phi(-c \cos \theta_2 + sc \cos \theta_1 \cos \theta_2 + s^2 \sin \theta_1 \sin \theta_2). \quad (119)$$

With the help of Maple V, setting

$$\Phi(x) = 1 - x^2 - \frac{27}{2}x^4 - \frac{249}{2}x^6 - \frac{12325}{8}x^8 - O(x^{10}), \quad (120)$$

then the series expansion of u has the same result as (118). $\Phi(x)$ may be explained as, something like, a weighting function for different directions of 2D rotations.

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References

- [1] L. Onsager Phys. Rev. **65**, (1944) 117.
- [2] C. Domb and M. S. Green, *Phase Transitions and Critical phenomena*, (Academic Press, New York). **Vol.3**, (1974).
- [3] B. Kaufman, Phys. Rev. **76**, (1944) 1232.
- [4] J. Zinn-Justin, J. Physique **42**, (1981) 783.
- [5] A. J. Liu and M. E. Fisher, Physica **A156**, (1989) 35.
- [6] A. J. Guttmann and I. G. Enting, J. Phy. **A27**, (1994) 8007.
- [7] G. F. Newell and E. W. Montroll, Rev. Mod. Phys. **25**, (1953) 353.
- [8] G. S. Rushbrooke, and J. Eve, J. Math. Phys. **3**, (1962) 185.
- [9] C. Itzykson, Nucl. Phys. **210**, (1982) 477. Itoi, Phys. Lett. **73**, (1994) 3335. M. Asano, C. Itoi and S. Kojima, Nucl. Phys. **B448**, (1995) 533. Shi He, Xu Yi-Chan and Hao Bai-Lin Acta Physica Sinica **27**, (1978) 47; **29**, (1980) 1564; **30**, (1981) 1225. M. E. Fisher, J. Phys. **A28**, (1995) 6323. R. Guida and Zinn-Justin, Nucl. Phys. **B489**, (1997) 626. M. Caselle and M. Hasenbusch, J. Phys. **A30**, (1997) 4963.