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Article

Spinor Approach for Three-Dimensional Ising Model

Degang Zhang [1,2]

1 College of Physics and Electronic Engineering, Sichuan Normal University, Chengdu 610101, China; dgzhang@sicnu.edu.cn
2 Institute of Solid State Physics, Sichuan Normal University, Chengdu 610101, China

Abstract: The three-dimensional Ising model on the m×n×l cubic lattice with the screw boundary condition along the **X** direction and the periodic boundary conditions along both **Y** and **Z** directions is exactly solved by using the 2^{mn}-dimensional representation of the rotation group in $2mn$-dimensions, similar to the Kaufman's spinor approach in two dimensions. The exact partition function is obtained from two sets of 2^{mn-1} eigenvalues of the 2^{mn}-dimensional transfer matrix **V** corresponding to the even and odd eigenvectors, respectively. Such the eigenvalues are determined by the angles of the 2mn-dimensional rotation associated with **V**.

Keywords: 3D Ising model; spinor approach; partition function

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The Ising model has been widely studied for understanding the order-disorder phase transitions in many physical or chemical systems since its establishment by Ising's research director, Wilhelm Lenz, in 1920 [1]. It is known that one-dimensional (1D) Ising model does not possesses a phase transition to a ferromagnetic ordered state at any temperature [2]. However, this result seems not to be generalized to higher dimensions [3]. In Ref. [4], Kramers and Wannier located the transition point in 2D Ising model by using the dual transformation and determined the critical temperature. In 1944, Onsager successfully solved the 2D Ising model by the operator algebra and obtained the exact partition function in the thermodynamic limit [5]. Later, Kaufman gave the complete eigenvalues of the 2D Ising model by spinor analysis [6]. Since then, a great deal of effort has been devoted to exploring the exact solution of 3D Ising model. Recently, we have exactly solved the 3D Ising model with the screw boundary condition along the **X** direction and the periodic boundary conditions along both **Y** and **Z** directions by employing the Onsager's approach [7]. The critical temperature and some thermodynamic quantities have been calculated in the thermodynamic limit. We note that under this kind of boundary conditions, the Hamiltonian along the **Y** direction is fully equivalent to an operator (physical quantity) along the the **X** direction. Therefore, the 3D classical Ising model can reduce to the 1D quantum Ising system through the transfer matrix method and operator renormalization. Eventually the 3D Ising model can be exactly diagonalized.

In this work, by employing the spinor approach, we compute the exact partition function for the 3D Ising model in terms of the complete eigenvalues of the 2^{mn}-dimensional transfer matrix V. From Ref. [7], we have the following expression for the partition function of the 3D Ising model on a m×n×l cubic lattice imposed by the screw boundary condition along the **X** direction and the periodic boundary conditions along both **Y** and **Z** directions

$$Z = [2\sinh(2H)]^{mnl/2}\mathrm{tr}(V_1V_2V_3)^l, \tag{1}$$

where

$$\begin{aligned} V_1 &= \exp(H_1 \textstyle\sum_{r=1}^{mn} \sigma_r^z\sigma_{r+1}^z) \equiv \exp(H_1H_x), \\ V_2 &= \exp(H_2 \textstyle\sum_{r=1}^{mn} \sigma_r^z\sigma_{r+m}^z) \equiv \exp(H_2H_y) \\ &= \exp(H_2 \textstyle\sum_{r=1}^{mn} \sigma_r^z\sigma_{r+1}^x \cdots \sigma_{r+m-1}^x\sigma_{r+m}^z), \\ V_3 &= \exp(H^* \textstyle\sum_{r=1}^{mn} \sigma_r^x) \equiv \exp(H^*H_z), \end{aligned} \tag{2}$$

where σ_r^x and $\sigma_r^z(=\pm 1)$ are the spin components on the site r and the transfer matrix $V \equiv V_1 V_2 V_3$. H and H^* are given by

$$H^* = \frac{1}{2}\ln\coth H = \tanh^{-1}(e^{-2H}). \tag{3}$$

From the expression of V_2, we can see that the Hamiltonian along the **Y** direction: $-H_2 H_y = -H_2 \sum_{r=1}^{mn} \sigma_r^z \sigma_{r+1}^x \cdots \sigma_{r+m-1}^x \sigma_{r+m}^z$, which is regarded as a operator along the **X** direction. This is the key to solving exactly the 3D Ising model [7].

Following the Kaufman's spinor analysis in two dimensions [6], we define

$$\begin{aligned} \Gamma_{2r-1} &\equiv \overbrace{\underbrace{\sigma^x \otimes \sigma^x \otimes \cdots \otimes \sigma^z}_{r} \otimes I \otimes I \cdots \otimes I}^{mn} \equiv P_r, \\ \Gamma_{2r} &\equiv \overbrace{\underbrace{\sigma^x \otimes \sigma^x \otimes \cdots \otimes \sigma^y}_{r} \otimes I \otimes I \cdots \otimes I}^{mn} \equiv Q_r, \end{aligned} \tag{4}$$

where $1 \le r \le mn$, I and $\sigma^{x,y,z}$ are the 2×2 unit matrix and Pauli matrices, respectively. Obviously, Γ_k are the 2^{mn}-dimensional matrices, and satisfy a set of canonical anti-commutation relations

$$\Gamma_l \Gamma_k + \Gamma_k \Gamma_l = 2\delta_{lk}, \tag{5}$$

which form the Clifford algebra. From Eq. (4), we have

$$\begin{aligned}
&\sigma_r^x = iP_r Q_r = I \otimes I \otimes \cdots \otimes \sigma^x \otimes I \otimes I \cdots \otimes I, \\
&\sigma_r^z = \sigma_1^x \sigma_2^x \cdots \sigma_{r-1}^x P_r = I \otimes I \otimes \cdots \otimes \sigma^z \otimes I \otimes I \cdots \otimes I, \\
&\sigma_{r+1}^z \sigma_r^z = -iP_{r+1} Q_r \quad \text{for} \quad 1 \le r \le mn-1, \\
&\sigma_1^z \sigma_{mn}^z = iP_1 Q_{mn} \sigma_1^x \sigma_2^x \cdots \sigma_{mn}^x \equiv iP_1 Q_{mn} U, \\
&\sigma_{r+m}^z \sigma_{r+m-1}^x \cdots \sigma_{r+1}^x \sigma_r^z = -iP_{r+m} Q_r \\
&\qquad\qquad\qquad\qquad \text{for} \quad 1 \le r \le m(n-1), \\
&\sigma_{r+mn}^z \sigma_{r+mn-1}^x \cdots \sigma_{r+m(n-1)+1}^x \sigma_{r+m(n-1)}^z \\
&\quad = iP_r Q_{r+m(n-1)} U \qquad \text{for} \quad 1 \le r \le m.
\end{aligned} \tag{6}$$

Note that $\sigma_{r+mn}^{x,y,z} \equiv \sigma_r^{x,y,z}$. Therefore,

$$\begin{aligned}
V_1 &= \textstyle\prod_{r=1}^{mn-1} \exp(-iH_1 P_{r+1} Q_r) \exp(iH_1 P_1 Q_{mn} U), \\
V_2 &= \textstyle\prod_{r=1}^{m(n-1)} \exp(-iH_2 P_{r+m} Q_r) \\
&\quad \times \textstyle\prod_{k=1}^{m} \exp(iH_2 P_k Q_{k+m(n-1)} U), \\
V_3 &= \textstyle\prod_{r=1}^{mn} \exp(iH^* P_r Q_r).
\end{aligned} \tag{7}$$

Because $U^2 = 1$ and $[U, V] = 0$, the eigenvalues of the transfer matrix V are classified by the $U = 1$ or -1 sector. We note that V_3 is the representative of a rotation with the angles $\frac{1}{2}\theta_r = iH^*, 1 \le r \le mn$. Similarly, V_1 and V_2 are also the representatives of plane rotations depending on U. For simplicity, we first diagonalize V^2 because V_3^2 has the rotation angles θ_r. As soon as the eigenvalues of V^2 are obtained, we immediately know those of V, i.e. the square roots of the eigenvalues of V^2.

We note that V_1^2, V_2^2 and V_3^2 are described by the following $mn \times mn$ matrices:

$$\begin{bmatrix}
b & c & & & & -Uc^+ \\
c^+ & b & c & & & \\
& c^+ & b & c & & \\
& & \ddots & \ddots & \ddots & \\
& & & c^+ & b & c \\
-Uc & & & & c^+ & b
\end{bmatrix}, \tag{8}$$

$$\begin{bmatrix} d & & \overbrace{e}^{m+1} & & \overbrace{-Ue^{+}}^{m(n-1)+1} & \\ & \ddots & & \ddots & & \ddots \\ e^{+} & & d & & e & \\ & \ddots & & \ddots & & \ddots \\ -Ue & e^{+} & & d & & \\ & \ddots & & \ddots & \ddots & \\ & \underbrace{-Ue}_{m} & & \underbrace{e^{+}}_{m(n-1)} & & d \end{bmatrix}, \tag{9}$$

$$\begin{bmatrix} a & & & \\ & a & & \\ & & \ddots & \\ & & & a \end{bmatrix}, \tag{10}$$

where $a = \cosh(2H^*)I - \sinh(2H^*)\sigma^y$, $b = \cosh(2H_1)I$, $c = i\sinh(2H_1)\sigma^-$, $d = \cosh(2H_2)I$, $e = i\sinh(2H_2)\sigma^-$, and $\sigma^\pm = (\sigma^x \pm i\sigma^y)/2$.

Obviously, $V^2 = V_1^2 V_2^2 V_3^2$ is a k-circulant matrix

$$\begin{bmatrix} a_0 & a_1 & a_2 & \cdots & a_{mn-1} \\ ka_{mn-1} & a_0 & a_1 & \cdots & a_{mn-2} \\ ka_{mn-2} & ka_{mn-1} & a_0 & \cdots & a_{mn-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ ka_1 & ka_2 & ka_3 & \cdots & a_0 \end{bmatrix} \tag{11}$$

with $k = -U$. The eigenvalues and eigenvectors of k-circulant matrix have been widely investigated in the literatures. If $k = 1$ or -1, the k-circulant matrix is called as the circulant or skew circulant matrix, respectively.

(I) $U = -1$, i.e. $k = 1$.

The eigenvectors of V^2 have the form

$$\frac{1}{\sqrt{mn}} \begin{bmatrix} \epsilon^{2r}\Psi_{2r} \\ \epsilon^{4r}\Psi_{2r} \\ \vdots \\ \epsilon^{2rmn}\Psi_{2r} \end{bmatrix}, \quad \epsilon = e^{\frac{i\pi}{mn}}, \quad 1 \le r \le mn. \tag{12}$$

Here, Ψ_{2r} is an eigenvector of the 2-dimensional matrix

$$\begin{aligned} \alpha_{2r} &= a_0 + a_1\epsilon^{2r} + a_2\epsilon^{4r} + \cdots + a_{mn-1}\epsilon^{2r(mn-1)} \\ &= \{cd\epsilon^{2r} + c^+e\epsilon^{2r(m-1)} + be\epsilon^{2rm} + be^+\epsilon^{2rm(n-1)} \\ &\quad + ce^+\epsilon^{2r[m(n-1)+1]} + c^+d\epsilon^{2r(mn-1)} + bd\}a \\ &= \begin{bmatrix} \mathcal{D}_{2r} - i\mathcal{C}_{2r} & -\mathcal{B}_{2r} + i\mathcal{A}_{2r} \\ -\mathcal{B}_{2r} - i\mathcal{A}_{2r} & \mathcal{D}_{2r} + i\mathcal{C}_{2r} \end{bmatrix}, \end{aligned} \tag{13}$$

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where

$$\begin{aligned}
\mathcal{A}_{2r} &= \cosh(2H_1)\cosh(2H_2)\sinh(2H^*) \\
&\quad - \sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\cos\tfrac{2r\pi}{mn} \\
&\quad - \cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\tfrac{2r\pi}{n} \\
&\quad + \sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{2(m-1)r\pi}{mn}, \\
\mathcal{B}_{2r} &= \sinh(2H_1)\cosh(2H_2)\cosh(2H^*)\sin\tfrac{2r\pi}{mn} \\
&\quad + \cosh(2H_1)\sinh(2H_2)\cosh(2H^*)\sin\tfrac{2r\pi}{n} \\
&\quad + \sinh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{2(m-1)r\pi}{mn}, \\
\mathcal{C}_{2r} &= \sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\sin\tfrac{2r\pi}{mn} \\
&\quad + \cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\sin\tfrac{2r\pi}{n} \\
&\quad + \sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\sin\tfrac{2(m-1)r\pi}{mn}, \\
\mathcal{D}_{2r} &= \cosh(2H_1)\cosh(2H_2)\cosh(2H^*) \\
&\quad - \sinh(2H_1)\cosh(2H_2)\sinh(2H^*)\cos\tfrac{2r\pi}{mn} \\
&\quad - \cosh(2H_1)\sinh(2H_2)\sinh(2H^*)\cos\tfrac{2r\pi}{n} \\
&\quad + \sinh(2H_1)\sinh(2H_2)\cosh(2H^*)\cos\tfrac{2(m-1)r\pi}{mn},
\end{aligned} \tag{14}$$

which completely coincide with Eq. (19) in Ref. [7]. Because the determinant of α_{2r} is 1, i.e. $\mathcal{D}_r^2 + \mathcal{C}_r^2 - \mathcal{A}_r^2 - \mathcal{B}_r^2 \equiv 1$, its eigenvalues can be written as $\exp(\mu_{2r}\xi_{2r})$, $\mu_{2r} = \pm 1$, which can be seen as the sign of the rotation angle ξ_{2r}, and ξ_{2r} is determined by [7]

$$\begin{aligned}
\tfrac{1}{2}\mathrm{tr}\alpha_{2r} = \tfrac{1}{2}(e^{\xi_{2r}} + e^{-\xi_{2r}}) = \cosh\xi_{2r} &= \mathcal{D}_{2r}, \\
\sinh\xi_{2r}\cos\eta_{2r} &= \mathcal{A}_{2r}, \\
\cosh(2a_{2r})\sinh\xi_{2r}\sin\eta_{2r} &= \mathcal{B}_{2r}, \\
\sinh(2a_{2r})\sinh\xi_{2r}\sin\eta_{2r} &= \mathcal{C}_{2r}.
\end{aligned} \tag{15}$$

Here, it must be emphasized that when $H_2 = 0$ or $H_1 = 0$, Eqs. (15) and (14) with $a_{2r} = H^*$ become Eq. (89) in Ref. [5] or Eqs. (51) and (52) in Ref. [6]. Let $2a_{2r} = i\delta_{2r}$, we get the normalized eigenvectors of α_{2r}

$$\Psi_{2r}^{\mu_{2r}} = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{1 + \mu_{2r}\sin\delta_{2r}\sin\eta_{2r}}e^{-i\theta_{2r}} \\ -\mu_{2r}\sqrt{1 - \mu_{2r}\sin\delta_{2r}\sin\eta_{2r}}e^{i\theta_{2r}} \end{bmatrix}, \tag{16}$$

where $\theta_{2r} = \frac{1}{2}\arctan(\cot\eta_{2r}/\cos\delta_{2r})$. Therefore, the 2^{mn-1} exact eigenvalues of V^2 are

$$(\lambda^-)^2 = e^{\mu_2\xi_2 + \mu_4\xi_4 + \cdots + \mu_{2mn}\xi_{2mn}} = e^{\sum_{r=1}^{mn}\mu_{2r}\xi_{2r}}, \tag{17}$$

where only an even number of $\mu_2, \mu_4, \cdots, \mu_{2mn}$ can be allowed to equal -1 [6]. In other words, only those eigenvalues remain in which an even number of the rotation angles ξ_{2r} appear with a minus sign.

If $\mu_2 = \mu_4 = \cdots = \mu_{2mn} = 1$, we have the maximal eigenvalue

$$(\lambda_{\max}^-)^2 = e^{\sum_{r=1}^{mn}\xi_{2r}}. \tag{18}$$

(II) $U = 1$, i.e. $k = -1$.

The eigenvectors of V^2 have the form

$$\frac{1}{\sqrt{mn}}\begin{bmatrix} \epsilon^{2r-1}\Psi_{2r-1} \\ \epsilon^{2(2r-1)}\Psi_{2r-1} \\ \vdots \\ \epsilon^{mn(2r-1)}\Psi_{2r-1} \end{bmatrix}. \tag{19}$$

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Here, Ψ_{2r-1} is an eigenvector of the 2-dimensional matrix

$$\begin{aligned}\alpha_{2r-1} &= a_0 + a_1\epsilon^{2r-1} + a_2\epsilon^{2(2r-1)} \\ &\quad + \cdots + a_{mn-1}\epsilon^{(2r-1)(mn-1)} \\ &= \{cd\epsilon^{2r-1} + c^+e\epsilon^{(2r-1)(m-1)} + be\epsilon^{(2r-1)m} \\ &\quad - be^+\epsilon^{(2r-1)m(n-1)} - ce^+\epsilon^{(2r-1)[m(n-1)+1]} \\ &\quad - c^+d\epsilon^{(2r-1)(mn-1)} + bd\}a \\ &= \begin{bmatrix} \mathcal{D}_{2r-1} - i\mathcal{C}_{2r-1} & -\mathcal{B}_{2r-1} + i\mathcal{A}_{2r-1} \\ -\mathcal{B}_{2r-1} - i\mathcal{A}_{2r-1} & \mathcal{D}_{2r-1} + i\mathcal{C}_{2r-1} \end{bmatrix}.\end{aligned} \tag{20}$$

We note that α_{2r-1} are completely consistent with α_{2r} if $2r-1$ are replaced by $2r$. Therefore, we have another set of 2^{mn-1} eigenvalues of V^2

$$(\lambda^+)^2 = e^{\mu_1\xi_1 + \mu_3\xi_3 + \cdots + \mu_{2mn-1}\xi_{2mn-1}} = e^{\sum_{r=1}^{mn}\mu_{2r-1}\xi_{2r-1}} \tag{21}$$

with the allowed sign combinations. The maximal eigenvalue reads

$$(\lambda^+_{\max})^2 = e^{\sum_{r=1}^{mn}\xi_{2r-1}}. \tag{22}$$

We have obtained the complete eigenvalues $(\lambda^-)^2$ and $(\lambda^+)^2$ of V^2. Therefore, the exact partition function of the 3D Ising model with the transfer matrix V is

$$\begin{aligned} Z &= [2\sinh(2H)]^{mnl/2}\sum_{i=1}^{2^{mn}}\lambda_i^l \\ &= [2\sinh(2H)]^{mnl/2}[\sum(\lambda^-)^l + \sum(\lambda^+)^l] \\ &= \tfrac{1}{2}[2\sinh(2H)]^{mnl/2}\{\prod_{r=1}^{mn}(2\cosh\tfrac{l}{2}\xi_{2r}) \\ &\quad + \prod_{r=1}^{mn}(2\sinh\tfrac{l}{2}\xi_{2r}) + \prod_{r=1}^{mn}(2\cosh\tfrac{l}{2}\xi_{2r-1}) \\ &\quad + \prod_{r=1}^{mn}(2\sinh\tfrac{l}{2}\xi_{2r-1})\}, \end{aligned} \tag{23}$$

which is similar to that of the 2D Ising model [6]. Here the summations are performed over the allowed configurations of $\mu_2, \mu_4, \cdots, \mu_{2mn}$ in λ^- and $\mu_1, \mu_3, \cdots, \mu_{2mn-1}$ in λ^+.

From Eqs. (14) and (15), we can see that all the ξ_{2r} and ξ_{2r-1}, except $\xi_{2mn} \equiv \xi_0$, are positive. However, ξ_0 has different behavior in comparison with the other ξ_r. Because

$$\cosh\xi_0 = \mathcal{D}_0 = \cosh[2(H^* - H_1 - H_2)], \tag{24}$$

ξ_0 changes sign at the critical point $H^* = H_1 + H_2$ [7], i.e.

$$\sin(2H)\sin(2H_1 + 2H_2) = 1, \tag{25}$$

which fixes the critical temperature T_c. Therefore, when mn is large enough, except in the vicinity of the critical point, we can take $\xi_{2r} = \xi_{2r+1}(1 \le r \le mn-1)$, and

$$\xi_0 = \begin{cases} \xi_1 & \text{for } T < T_c \\ -\xi_1 & \text{for } T > T_c. \end{cases} \tag{26}$$

As a result, we have

$$\frac{\lambda^-_{\max}}{\lambda^+_{\max}} = \begin{cases} 1 & \text{for } T < T_c \\ e^{2(H_1+H_2-H^*)} & \text{for } T > T_c, \end{cases} \tag{27}$$

$$\begin{aligned} [2\sinh(2H)]^{-mnl/2}Z &\cong \prod_{r=1}^{mn}(2\cosh\tfrac{l}{2}\xi_{2r-1}) \\ &\sim (\lambda^+_{\max})^l \quad \text{for } T > T_c, \end{aligned} \tag{28}$$

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and

$$\begin{aligned}[2\sinh(2H)]^{-mnl/2}Z &\cong \prod_{r=1}^{mn}(2\cosh\tfrac{l}{2}\xi_{2r-1}) \\ &\quad + \prod_{r=1}^{mn}(2\sinh\tfrac{l}{2}\xi_{2r-1}) \\ &= \prod_{r=1}^{mn}(2\cosh\tfrac{l}{2}\xi_{2r-1}) \\ &\quad \cdot[1+\prod_{r=1}^{mn}\tanh[\tfrac{l}{2}\xi_{2r-1})] \\ &\sim 2(\lambda_{\max}^{+})^{l} \quad \text{for } T < T_c. \end{aligned} \tag{29}$$

We can see from the equation above that the maximal eigenvalue of the 3D Ising model has two degeneracy for $T < T_c$ in the thermodynamic limit, i.e. $\lambda_{\max}^{+} = \lambda_{\max}^{-}$.

In summary, we have exactly solved the 3D Ising model with the suitable boundary conditions by the spinor approach. Two sets of exact eigenvalues and eigenvectors are derived. The exact expression for the partition function is also presented. We note that this exact solution is completely consistent with that by the operator algebra [7]. When the interaction energy in the third dimension vanishes, i.e. $H_1 = 0$ or $H_2 = 0$, the Onsager's exact solution of 2D Ising model is recovered immediately. Therefore, the correctness of the exact solution of the 3D Ising model is guaranteed.

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