Algebraic Derivation of the Partition Function of a Two-Dimensional Ising Model*

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(Received 2 November 1964)

In the algebraic formulation of the Ising model, the partition function is expressed as the trace of a power V^M of the transfer operator V, or equivalently, as the sum of Mth powers of the eigenvalues of V. In the derivations of Kaufman, Onsager, and more recently of Schultz, Mattis, and Lieb (SML), the transfer operator is first reduced to a more amenable form for computation and then, in principle at least, diagonalized. For the infinite lattice, only the largest eigenvalue of V is needed, and this is all Onsager and SML compute. Kaufman finds all the eigenvalues and is thus able to write down the partition function for the finite lattice. In the present work we give an alternative derivation of the SML form for V, and show how the Kaufman result can be obtained from this form without actual diagonalization. Instead of diagonalizing V, the evaluation of the trace is done directly after assigning a simple representation to V.

I. INTRODUCTION

SINCE Onsager's celebrated solution of the two-dimensional Ising model in 1944,[1] there have been numerous alternative derivations of the Onsager result, a number of derivations of correlations and spontaneous magnetization, and some generalizations to other types of two dimensional lattices. Reviews of the work prior to 1960 are given in the articles of Domb[2] and Newell and Montroll.[3]

Roughly speaking, one can divide the methods used into two categories: the combinatorial approach, which essentially counts polygons on the lattice; and the algebraic approach. The combinatorial approach began in 1952 with the work of Kac and Ward.[4] Their approach has since been refined and been given a rigorous treatment,[5] and in its present form is the most popular method.[6] The popularity is undoubtedly due to the relative simplicity of the method compared with the original formidable algebraic approach of Onsager, and even with the simplified algebraic approach of Kaufman.[7] In recent times the algebraic approach has been given little attention. Recently however, Schultz, Mattis, and Lieb[8] (called SML hereinafter) have shown how the algebraic formulation of Onsager, leads to a many-fermion problem, the solution of which requires only an elementary knowledge of spin-$\frac{1}{2}$ and the second quantization formalism for Fermions. Much of the mysticism surrounding the algebraic method is clarified by SML; their steps are simple and their language more familiar. Of particular interest is their lucid discussion of correlations and spontaneous magnetization, and their new derivation of the transfer matrix formulation, which is the heart of the algebraic approach.

In brief outline, the problem is formulated algebraically as follows. Consider a square lattice consisting of M rows and N columns with a set of NM particles of two types arranged on the vertices of the lattice. If we let only nearest-neighbor particles interact, with interaction energy $-J_2(-J_1)$ between like particles in rows (columns) and $+J_2(+J_1)$ between unlike particles in rows (columns) and assign a coordinate $\mu_{m,n}$ to the vertex at the intersection of the nth row and mth column, with values $+1$ or -1 depending on the type of particle, the Hamiltonian for the system in configuration $\{\mu_{11}, \cdots, \mu_{MN}\}$,

$$H(\mu_{11}, \cdots, \mu_{MN}) = -J_1 \sum \mu_{m,n}\mu_{m+1,n} - J_2 \sum \mu_{m,n}\mu_{m,n+1}, \qquad (1)$$

defines the rectangular two-dimensional Ising model, and the problem is to calculate the partition function Z defined by

$$Z_{MN} = \sum_{\mu_{11}=\pm1} \cdots \sum_{\mu_{MN}=\pm1} e^{-\beta H(\mu_{11}, \cdots, \mu_{MN})}, \qquad (2)$$

where $\beta = (k_B T)^{-1}$, k_B being Boltzmann's constant, and T the absolute temperature.

For boundary conditions one usually takes $\mu_{M+m,n} = \mu_{m,n}$ and $\mu_{m,N+n} = \mu_{m,n}$, so that the lattice

* Supported by U. S. Air Force Office of Scientific Research, under AF Grant No. AF-AFOSR-610-64.
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is assumed to be wrapped on a torus. In this case the sums in (1) are over n from 1 to N, and m from 1 to M. The toroidal boundary conditions will be used in the present work.

The reduction of Z_{MN} to the transfer operator form is well known, we merely quote the result. For detailed derivations, see for example the book by Huang[9] or SML.

The transfer operator V is defined by

$$V = \exp\left(K_2 \sum_{n=1}^{N} \tau_n^1\tau_{n+1}^1\right) \exp\left(-K_1^* \sum_{n=1}^{N} \tau_n^2\right), \quad (3)$$

where

$$K_i = \beta J_i, \qquad i = 1, 2, \quad (4a)$$

K_1^* is related to K_1 through

$$\tanh K_1^* = e^{-2K_1}, \quad (4b)$$

and the operators τ_n^i, $i = 1, 2$, satisfy the relations

$$[\tau_n^i, \tau_{n'}^j]_- = \tau_n^i\tau_{n'}^j - \tau_{n'}^j\tau_n^i = 0, \quad (5a)$$

$$[\tau_n^i, \tau_n^j]_+ = \tau_n^i\tau_n^j + \tau_n^j\tau_n^i = 0, \quad (5b)$$

for $i \neq j = 1, 2, n, n' = 1, 2, \ldots, N$,

and

$$(\tau_n^i)^2 = I \quad \text{for} \quad i = 1, 2, \quad n = 1, 2, \cdots, N, \quad (5c)$$

with I the unit operator and 0 the null operator.

The first term in V arises from interactions in a row and the second from interactions between nearest-neighbor rows.

In terms of V, the partition function is given by

$$Z_{MN} = (2\sinh 2K_1)^{\frac{1}{2}MN} \operatorname{Tr}(V^M). \quad (6)$$

A common feature of the Onsager, Kaufman, and SML derivations is that they all compute the eigenvalues of the transfer operator. Kaufman actually computes all the eigenvalues and is thus able to write down the partition function for the finite lattice from

$$Z_{MN} = (2\sinh 2K_1)^{\frac{1}{2}MN} \sum_{n=1}^{2^N} \lambda_n^M. \quad (7)$$

Of more interest, phase transition-wise, is the infinite lattice where it is easily shown that the free-energy per particle is given by

$$-\beta^{-1} \lim_{\substack{M,N\to\infty \\ (M/N=\text{const})}} (MN)^{-1} \ln Z_{MN}$$
$$= -(2\beta)^{-1}\ln(2\sinh 2K_1) - \beta^{-1}\lim_{N\to\infty} N^{-1}\ln\lambda_{\max} \quad (8)$$

with $\lambda_{\max}$ the largest eigenvalue of V.

For the infinite case it is therefore only necessary to find the largest eigenvalue, and this is done by Onsager and SML. Even so, one must in principle diagonalize V, and it is this part of the three calculations that is difficult, or at least complicated. In the present calculation, we do not find the eigenvalues of V. Instead we choose a representation of V in which the problem reduces to calculating traces of four-dimensional matrices of relatively simple structure. The calculation is given in the following section and the result obtained is Kaufman's expression for the finite problem. The passage to the infinite lattice can be followed in the manner suggested by Kaufman and is not included here. Our procedure, as a method for obtaining the infinite lattice result as well as the finite result, is, we feel, much less involved than the diagonalizing procedures of previous algebraic derivations. We remark also that our method can be used to evaluate the short- and long-range order (which are expressible as traces of operators). The calculations are straightforward and parallel closely those of SML so are not included here.

2. THE PARTITION FUNCTION

To express V in a more convenient form we define Fermi destruction and creation operators a_n and $a_n^\dagger (n = 1, 2, \cdots N)$, by

$$a_n + a_n^\dagger = \tau_1^2\tau_2^2 \cdots \tau_{n-1}^2\tau_n^3, \quad (9a)$$

$$a_n - a_n^\dagger = i\tau_1^2\tau_2^2 \cdots \tau_{n-1}^2\tau_n^1. \quad (9b)$$

In terms of these operators one can easily show that[10]

$$V^M = \tfrac{1}{2}(I + U)V_+^M + \tfrac{1}{2}(I - U)V_-^M, \quad (10)$$

where

$$U = \prod_{n=1}^{N} \tau_n^2 = \exp\left[i\pi \sum_{n=1}^{N} (a_n^\dagger a_n - 1)\right] \quad (11)$$

and

$$V_\pm = \prod_{n=1}^{N} \exp\left[K_2(a_{n+1}^\dagger - a_{n+1})(a_n^\dagger + a_n)\right]$$
$$\times \prod_{n=1}^{N} \exp\left[-2K_1^*(a_n^\dagger a_n - 1)\right] \quad (12)$$

with the anticyclic boundary condition

$$a_{N+l} = -a_l \quad (13a)$$

holding for V_+, and the cyclic boundary condition

$$a_{N+l} = a_l \quad (13b)$$

[9] K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963), p. 349 ff.

[10] The steps follow closely those of Kaufman.

holding for V_-, and in deriving (10) we have made use of the fact that $P_\pm = \frac{1}{2}(I \pm U)$ are projection operators (which follows from $U^2 = I$), and act on orthogonal subspaces (i.e., $P_+P_- = 0$). Equation (12) was obtained by SML by a different method.

In the remainder of this section we will focus our attention on the V_+ term in (10). The steps in the calculation of the remaining three terms in (10) are similar to those given below and are summarized briefly at the end.

To simplify V_+ further we follow SML and transform to running wave operators through

$$a_n = N^{-\frac{1}{2}} e^{i\pi/4} \sum_q e^{iqn} \eta_q, \tag{14}$$

where the anticyclic condition (13a) requires that

$$q = \pm(2j-1)\pi/N \qquad j = 1, \cdots, N/2 \tag{15a}$$

[the cyclic condition (13b) requires that

$$q = 0, \pi, \pm 2j\pi/N, \quad j = 1, 2, \cdots, N/2 - 1] \tag{15b}$$

and for convenience we have chosen N to be even. Direct substitution of (14) into (12) gives

$$V_+ = \prod_{0<q<\pi} V_q, \tag{16}$$

where in terms of operators Σ_q^1, Σ_q^2, (and Σ_q^3 for completeness)

$$\begin{aligned} \Sigma_q^1 &= \eta_q^\dagger \eta_q + \eta_{-q}^\dagger \eta_{-q} - I, \\ \Sigma_q^2 &= \eta_{-q}\eta_q + \eta_q^\dagger \eta_{-q}^\dagger, \\ \Sigma_q^3 &= i(\eta_q^\dagger \eta_{-q}^\dagger - \eta_{-q}\eta_q), \end{aligned} \tag{17}$$

$$V_q = \exp\{2K_2[\cos q\Sigma_q^1 - \sin q\Sigma_q^2]\} \times \exp\{-2K_1^*\Sigma_q^1\}. \tag{18}$$

We will make use of the commutation relations for the Σ_q^i operators

$$\begin{aligned} &[\Sigma_q^i, \Sigma_{q'}^j]_- = -2i\delta_{qq'}\Sigma_q^k, \ (ijk) \quad \text{cyclic (123)} \\ &\text{and} \qquad [\Sigma_q^i, \Sigma_q^j]_+ = 0 \quad \text{for} \quad i \neq j. \end{aligned} \tag{19}$$

These follow directly from (17) and the Fermi anticommutation relations for the η_q -operators. We remark in passing that the sequence of equations (16)–(18)–(19) was obtained originally by Onsager using a slightly more involved method.

In all previous algebraic derivations, $V_\pm$ were diagonalized (simultaneously because of their commutability). Let us show that for the purpose of computing the trace, the most convenient representation is not the diagonal one but one based on the occupation number representation of the η_q-Fermi operators. Thus, since the eigenvalues of $\eta_{\pm q}^\dagger \eta_{\pm q}$ are 0 and 1 (with equal degeneracy), the eigenvalues of Σ_q^1 are 1, -1, 0, 0 (equal degeneracy). A representation of the Σ-operators in which Σ_q^1 is diagonal is therefore [from (19)]

$$\Sigma_q^i = I_4 \otimes \cdots \otimes I_4 \otimes \sigma^i r^+ \otimes I_4 \otimes \cdots \otimes I_4, \qquad i = 1, 2, 3, \tag{20}$$

where

$$\sigma^i = \begin{bmatrix} \tau^i & 0_2 \\ 0_2 & \tau^i \end{bmatrix}, \qquad r^+ = \begin{bmatrix} I_2 & 0_2 \\ 0_2 & 0_2 \end{bmatrix}. \tag{21}$$

τ^i are the conventional Pauli matrices

$$\tau^1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \tau^2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \tau^3 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}. \tag{22}$$

I_4 and I_2 are the four- and two- dimensional unit matrices, respectively, 0_2 is the two-dimensional null matrix, and in the direct product (denoted by $\otimes$), there are $N/2$ terms, with the $\sigma^i r^+$ occuring in the jth ($q = 2j - 1$) place.

Using the property

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD) \tag{23}$$

of direct product, we then have

$$V_+ = \bigotimes_{j=1}^{N/2} V_{2j-1} = \bigotimes_{p+} V_{p+}, \tag{24}$$

where

$$V_{p+} = \exp\{2K_2[\cos(p+)\sigma_+^1 - \sin(p+)\sigma_+^2]\} \times \exp\{-2K_1^*\sigma_+^1\} \tag{25}$$

and

$$\sigma_+^i = \sigma^i r^+. \tag{26}$$

If we then use the property

$$\mathrm{Tr}\,(A \otimes B) = \mathrm{Tr}\,(A)\,\mathrm{Tr}\,(B), \tag{27}$$

we have

$$\mathrm{Tr}\,(V_+^M) = \prod_{j=1}^{N/2} \mathrm{Tr}\,(V_{2j-1}^M). \tag{28}$$

The problem has now been reduced to the evaluation of traces of four-dimensional matrices with relatively simple structure. Let us consider V_p (p will henceforth be used for $p+$). Since the σ^i matrices satisfy the commutation relations

$$[\sigma_+^i, \sigma_+^j] = -2i\sigma_+^k \quad (ijk) \text{ cyclic (123)}. \tag{29}$$

V_p can be written in the form

$$V_p = \exp\left(\sum_{i=1}^{3} c_p^i \sigma_+^i\right). \tag{30}$$

If we then use the anticommutation relations

$$[\sigma_+^i, \sigma_+^j]_+ = 2\delta_{ij}r^+ \tag{31}$$

expansion of the exponential (30) gives

$$V_p = r^- + r^+ \cosh \gamma_p + \left(\sum_{i=1}^{3} c_p^i \sigma_+^i\right) \frac{\sinh \gamma_p}{\gamma_p}, \tag{32}$$

where

$$r^- = I_4 - r^+ \tag{33}$$

and γ_p is defined by

$$\gamma_p^2 = \sum_{i=1}^{3} (c_p^i)^2. \tag{34}$$

If we also expand the exponentials in (18) in a similar manner, we obtain

$$\begin{aligned} V_p = r^- &+ r^+[\cosh 2K_2 \cosh 2K_1^* - \sinh 2K_2 \sinh 2K_1^* \cos p] \\ &+ \sigma_+^1[\sinh 2K_2 \cosh 2K_1^* \cos p - \sinh 2K_1^* \cosh 2K_2] \\ &+ \sigma_+^2[-\sinh 2K_2 \cosh 2K_1^* \sin p] \\ &+ \sigma_+^3[\sinh 2K_1^* \sinh 2K_2 \sin p]. \end{aligned} \tag{35}$$

This expression must be identical with (32), so equating coefficients of r^+ gives the connection

$$\cosh \gamma_p = \cosh 2K_2 \cosh 2K_1^* - \sinh 2K_2 \sinh 2K_1^* \cos p \tag{36}$$

between the c_p^i parameters in (30) and K_2, K_1^*, and p. It turns out that (36) is the only relation needed to evaluate the trace (28). The steps needed are as follows. From (30) we have

$$\begin{aligned} (V_p)^M &= \exp\left(\sum_{i=1}^{3} (Mc_p^i)\sigma_+^i\right) \\ &= r^- + r^+ \cosh (M\gamma_p) + \left(\sum_{i=1}^{3} c_p^i \sigma_+^i\right) \frac{\sinh (M\gamma_p)}{\gamma_p} \end{aligned} \tag{37}$$

and recalling expressions (21) and (33) for r^+ and r^-, and noting that $\mathrm{Tr}\,(\sigma_+^i) = 0$, we have

$$\mathrm{Tr}\,(V_p^M) = 2[1 + \cosh (M\gamma_p)] = 4 \cosh^2 (\tfrac{1}{2}M\gamma_p). \tag{38}$$

To evaluate $\mathrm{Tr}\,(UV_+^M)$ in (10) we use the representation (20) to get

$$U_+ = \bigotimes_{p+} (-e^{i\pi\sigma_+'}) = \bigotimes_{p+} (r^+ - r^-) \tag{39}$$

and then from (23) and (27)

$$\mathrm{Tr}\,(UV_+^M) = \prod_{p+} \mathrm{Tr}\,[(r^+ - r^-)V_{p+}^M] \tag{40}$$

where, using $r^+r^- = 0_4 = r^-\sigma_+^i$, $(r^+)^2 = r^+$, and (37),

$$\begin{aligned} \mathrm{Tr}\,[(r^+ - r^-)V_{p+}^M] &= 2[-1 + \cosh (M\gamma_p)] \\ &= 4 \sinh^2 (\tfrac{1}{2}M\gamma_p). \end{aligned} \tag{41}$$

To evaluate the corresponding minus quantities $\mathrm{Tr}\,(V_-^M)$ and $\mathrm{Tr}\,(UV_-^M)$ in (10), one uses the representation (20) with $\sigma^i r^-$ in place of $\sigma^i r^+$ [to preserve the orthogonality of the two terms in (10)]. The above calculation then goes through with essentially just a minus sign in place of a plus [although some special care must be taken with the $q = 0$ and $q = \pi$ terms (15b) arising from the cyclic boundary conditions (13b).]

If we now define γ_k to be the positive solution of Eq. (36), that is, the positive solution of ($p = k\pi/N$)

$$\cosh \gamma_k = \cosh 2K_2 \cosh 2K_1^* - \sinh 2K_2 \times \sinh 2K_1^* \cos\left(\frac{k\pi}{N}\right) \qquad k = 0, 1, \cdots \tag{42}$$

and note that $\gamma_{2N-k} = \gamma_k$ for $k = 0, 1, \cdots, N$, we have finally, after combining (10), (28), (38), (40), and (41) and the corresponding minus results, the Kaufman expression for the partition function of the finite lattice,

$$\begin{aligned} Z_{MN} &= (2 \sinh 2K_1)^{\frac{1}{2}MN}\, \mathrm{Tr}\,(V^M) \\ &= \tfrac{1}{2}(2 \sinh 2K_1)^{\frac{1}{2}MN} \\ &\quad \times \left\{\prod_{j=1}^{N} 2 \cosh\left(\frac{M\gamma_{2j-1}}{2}\right) + \prod_{j=1}^{N} 2 \sinh\left(\frac{M\gamma_{2j-1}}{2}\right) \right. \\ &\quad \left. + \prod_{j=1}^{N} 2 \cosh\left(\frac{M\gamma_{2j}}{2}\right) + \prod_{j=1}^{N} 2 \sinh\left(\frac{M\gamma_{2j}}{2}\right)\right\}. \end{aligned} \tag{43}$$

The partition function for the infinite lattice can be obtained straightforwardly from (43) in the manner suggested by Kaufman. The reader is referred to Kaufman's article for details.

ACKNOWLEDGMENT

The author is grateful to Professor H. Suhl for the hospitality extended to him at the University of California, San Diego.