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Analytical Properties of the Anisotropic Cubic Ising Model

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We combine an exact functional relation, the inversion relation, with conventional high-temperature expansions to explore the analytic properties of the anisotropic Ising model on both the square and simple cubic lattice. In particular, we investigate the nature of the singularities that occur in partially resummed expansions of the partition function and of the susceptibility.

KEY WORDS: Lattice statistics; critical phenomena; Ising model; lattice anisotropy; high-temperature expansion; inversion relation; analytical properties.

1. INTRODUCTION

One of the promising recent developments in the continuing quest for exact results in statistical mechanics is the so-called "inversion relation." This is a functional equation satisfied by the eigenvalues of the transfer matrix, which leads to a corresponding functional equation for the partition function and for the correlation functions. The reader is referred to reviews[1,2] for an introduction to these ideas. Similar ideas occur in S-matrix theory, for $(1+1)$-dimensional S-matrix models.[3]

The inversion relation has been used to obtain exact solutions for statistical mechanics models by a number of authors.[4–7] An inversion relation, and a corresponding functional relation for the partition function, also exists for a number of models that, at least at present, are not exactly

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solvable. These include the two-dimensional Ising model in a field,[1] the two-dimensional noncritical Potts model,[8] and the anisotropic cubic Ising model in zero field.[9]

In this paper we will explore some of the consequences of the inversion relation for the anisotropic Ising models on both the square lattice and the simple cubic lattice. We will show that the inversion relation, combined with conventional high-temperature series, provides some insight into the analytic structure of the partition function and susceptibility of these models.

2. THE PARTITION FUNCTION

We consider first the anisotropic Ising model on the square lattice with coupling constants K_1, K_2. It can be shown (e.g., Baxter[1]) that the partition function per site $Z(K_1, K_2)$ satisfies the inverse functional relation

$$Z(K_1, K_2)\, Z(K_1 + i\pi/2, -K_2) = 2i \sinh 2K_1 \tag{1}$$

If we introduce the standard high-temperature variables $t_i = \tanh K_i$ and define a quantity $\Lambda(t_1, t_2)$ by

$$\Lambda(t_1, t_2) = (2 \cosh K_1 \cosh K_2)^{-1}\, Z(K_1, K_2) \tag{2}$$

then it follows from (1) that

$$\ln \Lambda(t_1, t_2) + \ln \Lambda(1/t_1, -t_2) = \ln(1 - t_2^2) \tag{3}$$

The exact Onsager solution of course satisfies this relation.

The quantity $\ln \Lambda$ can also be written as a double power series

$$\ln \Lambda(t_1, t_2) = \sum_{m,n} a_{m,n} t_1^m t_2^n \tag{4}$$

The coefficients $a_{m,n}$ are obtainable by standard high-temperature expansion techniques (e.g., Domb[10]), in which $a_{m,n}$ is related to the number of embeddings of closed graphs with m, n bonds in the two lattice directions. As a consequence, only terms with m, n even occur in the expansion.

By considering the class of graphs with fixed n and m variable, we can effect a partial resummation of (4) to obtain

$$\ln \Lambda(t_1, t_2) = \sum_{n=1}^{\infty} R_n(t_1^2)\, t_2^{2n} \tag{5}$$

where $R_n(t_1^2)$ is a rational function in the variable t_1^2 and can be written as

$$R_n(t_1^2) = P_n(t_1^2)/Q_n(t_1^2) \tag{6}$$

with P_n and Q_n being polynomials of the same degree.

In Fig. 1 we illustrate the nature of this partial resummation. The exact Onsager solution shows that the only zeros of Q_n are $t_1^2 = 1$, and with this information a quick inspection of the resummed diagrams shows that

$$Q_n(t_1^2) = (1 - t_1^2)^{2n-1} \tag{7}$$

Conversely, as noted by Baxter,[1] if we assume (7), then the inversion relation (3) and the obvious symmetry relation $\Lambda(t_1, t_2) = \Lambda(t_2, t_1)$ completely determine the polynomial P_n order by order. Thus, the celebrated Onsager solution is determined completely by these two functional equations and the assumption that only $t_1^2 = 1$ singularities occur. Indeed, this is a very efficient way to obtain the high-temperature expansion for the partition function of the anisotropic square lattice Ising model.

Let us now consider the anisotropic simple cubic Ising model, with coupling constants K_1, K_2, K_3. The partition per site now satisfies the inversion relation

$$Z(K_1, K_2, K_3)\, Z(K_1 + i\pi/2, -K_2, -K_3) = 2i \sinh 2K_1 \tag{8}$$

Defining $\Lambda(t_1, t_2, t_3)$ by

$$\Lambda(t_1, t_2, t_3) = (2 \cosh K_1 \cosh K_2 \cosh K_3)^{-1}\, Z(K_1, K_2, K_3) \tag{9}$$

we obtain

$$\begin{aligned} &\ln \Lambda(t_1, t_2, t_3) + \ln \Lambda(1/t_1, -t_2, -t_3) \\ &\quad = \ln(1 - t_2^2) + \ln(1 - t_3^2) \end{aligned} \tag{10}$$

We can now use the inversion relation (10) in combination with a high-temperature expansion

$$\ln \Lambda(t_1, t_2, t_3) = \sum_{p,m,n} a_{p,m,n} t_1^{2p} t_2^{2m} t_3^{2n} \tag{11}$$

to investigate the form of the partially resummed expansion

$$\ln \Lambda(t_1, t_2, t_3) = \sum_{m,n} R_{m,n}(t_1^2)\, t_2^{2m} t_3^{2n} \tag{12}$$

and, in particular, to investigate the nature of the singularities of $R_{m,n}(t_1^2)$.

From (12) and (10) we find that the $R_{m,n}$ functions must satisfy the constraints

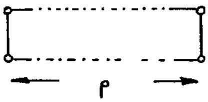
$$R_{m,0}(t_1^2) + R_{m,0}(1/t_1^2) = -1/m \tag{13a}$$

$$R_{m,n}(t_1^2) + R_{m,n}(1/t_1^2) = 0 \qquad m, n \neq 0 \tag{13b}$$

We have evaluated the coefficients a_{p+m+n} for $p+m+n \leqslant 8$, i.e., a 16-term, high-temperature expansion, and these are given in Table I. We thus have available the leading coefficients in the power series for the functions $R_{m,n}(t_1^2)$. We expect that the $R_{m,n}$ can again be written as a ratio of the two polynomials

$$R_{m,n}(t_1^2) = P_{m,n}(t_1^2)/Q_{m,n}(t_1^2) \tag{14}$$

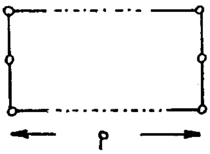
n = 1 :



$$R_1(t^2) = \sum_{p=1}^{\infty} t^{2p} = t^2/(1-t^2)$$

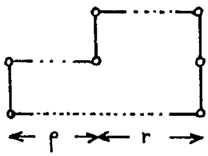
n = 2 :

(a)



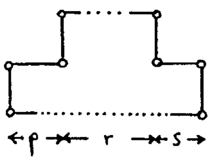
$$\sum_{p=1}^{\infty} t^{2p} = t^2/(1-t^2)$$

(b)



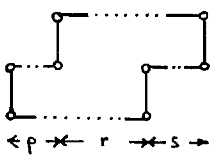
$$4\sum_{p=1}^{\infty}\sum_{r=1}^{\infty} t^{2p+2n} = 4t^4/(1-t^2)^2$$

(c)



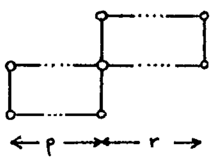
$$2\sum_{p=1}^{\infty}\sum_{r=1}^{\infty}\sum_{s=1}^{\infty} t^{2p+2r+2s} = 2t^6/(1-t^2)^3$$

(d)



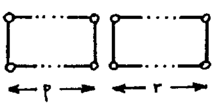
$$2\sum_{p=1}^{\infty}\sum_{r=1}^{\infty}\sum_{s=1}^{\infty} t^{2p+2r+2s} = 2t^6/(1-t^2)^3$$

(e)



$$2\sum_{p=1}\sum_{r=1} t^{2p+2r} = 2t^4/(1-t^2)^2$$

(f)



$$-\frac{1}{2}\sum_{p=1}\sum_{r=1} 3(p+r+1)t^{2p+2r}$$

$$= -\frac{3}{2}\, t^4/(1-t^2)^2 - 3t^4/(1-t^2)^3$$

$$R_2(t^2) = (a) + \dots + (f) = (t^2 - \frac{1}{2}\, t^4 + \frac{1}{2}\, t^6)/(1-t^2)^3$$

Fig. 1. Partial resummation of partition function series for the square lattice. Evaluation of the functions $R_1(t^2)$ and $R_2(t^2)$.

Table I. Coefficients $a_{p,n,m}$ Defined by Eq. (11)

Order	(p, n, m)	$a_{p,n,m}$
$O=4$	(1, 1, 0)	1
$O=6$	(2, 1, 0)	1
	(1, 1, 1)	16
$O=8$	(3, 1, 0)	1
	(2, 2, 0)	$2\frac{1}{2}$
	(2, 1, 1)	58
$O=10$	(4, 1, 0)	1
	(3, 2, 0)	5
	(3, 1, 1)	128
	(2, 2, 1)	520
$O=12$	(5, 1, 0)	1
	(4, 2, 0)	$8\frac{1}{2}$
	(4, 1, 1)	226
	(3, 3, 0)	$18\frac{1}{3}$
	(3, 2, 1)	2,262
	(2, 2, 2)	9,682
$O=14$	(6, 1, 0)	1
	(5, 2, 0)	13
	(5, 1, 1)	352
	(4, 3, 0)	51
	(4, 2, 1)	6,746
	(3, 3, 1)	17,200
	(3, 2, 2)	75,216
$O=16$	(7, 1, 0)	1
	(6, 2, 0)	$18\frac{1}{2}$
	(6, 1, 1)	506
	(5, 3, 0)	117
	(5, 2, 1)	16,014
	(4, 4, 0)	$217\frac{1}{4}$
	(4, 3, 1)	81,410
	(4, 2, 2)	359,753
	(3, 3, 2)	949,322

The rational functions $R_{m,0} = R_{0,m}$ are obtainable from the exact Onsager solution of the square lattice. The first few are

$$R_{1,0}(t_1^2) = t_1^2/(1 - t_1^2) \tag{15}$$

$$R_{2,0}(t_1^2) = t_1(2 - t_1^2 + t_1^4)/2(1 - t_1^2)^3 \tag{16}$$

$$R_{3,0}(t_1) = t_1^2(3 + 10t_1^4 - 2t_1^6 + t_1^8)/3(1 - t_1^2)^5 \tag{17}$$

The expansions of these rational functions of course agree with the high-temperature series.

The function $R_{1,1}$ is given by

$$R_{1,1}(t_1^2) = 1 + 16t_1^2 + 58t_1^4 + 128t_1^6 + 226t_1^8 + 352t_1^{10} + 506t_1^{12} + \cdots \tag{18}$$

We note that

$$(1 - t_1^2)^3 R_{1,1}(t_1^2) = 1 + 13t_1^2 + 13t_1^4 + t_1^6 + o(t_1^{14})$$

which suggests that

$$R_{1,1}(t_1^2) = (1 + 13t_1^2 + 13t_1^4 + t_1^6)/(1 - t_1)^3 \tag{19}$$

exactly. It is not difficult to obtain this result directly from a consideration of resummed diagrams. We note that, in contrast to the two-dimensional case, the function $R_{1,1}$ is not determined uniquely from the inversion and symmetry relations. The coefficient of the $t_1^2 t_2^2 t_3^2$ term in the high-temperature expansion, which is 16, is also required.

We now consider the function $R_{2,1} = R_{1,2}$, which has the expansion

$$R_{2,1}(t_1^2) = 1 + 58t_1^2 + 520t_1^4 + 2262t_1^6 + 6746t_1^8 + 16{,}014t_1^{10} + \cdots \tag{20}$$

and we seek polynomials P, Q such that $R_{2,1} = P_{2,1}/Q_{2,1}$. Consideration of the resummed diagrams suggests that $Q_{2,1}$ is divisible by $(1 - t_1^2)^5$. By inspection we find that

$$\begin{aligned}(1 - t_1^2)^5&(1 + t_1^2)\, R_{2,1}(t_1^2) \\ &= 1 + 54t_1^2 + 293t_1^4 + 472t_1^6 + 293t_1^8 + 54t_1^{10} + o(t_1^{12})\end{aligned}$$

It appears likely that this expression terminates with a term t_1^{12}, and thus that the exact expression for $R_{2,1}$ is

$$R_{2,1}(t_1^2) = \frac{1 + 54t_1^2 + 293t_1^4 + 472t_1^6 + 293t_1^8 + 54t_1^{10} + t_1^{12}}{(1 - t_1^2)^5(1 + t_1^2)} \tag{21}$$

This result reveals a new feature of the resummed high-temperature expansion for the simple cubic lattice, namely the appearance of a $t_1^2 = -1$ singularity in addition to the singularity at $t_1^2 = 1$.

It seems likely that the $t_1^2 = -1$ singularity will continue to appear in higher order, but we have insufficient terms in the high-temperature expansion to confirm this.

3. THE SUSCEPTIBILITY

An inverse functional relation can also be established for the correlation functions of the anisotropic Ising model, and hence for the susceptibility.[11] We therefore investigate the implications of the inversion relation for resummed susceptibility expansions using the same approach as in the previous section.

For the anisotropic square lattice the susceptibility satisfies the inversion relation

$$\chi(t_1, t_2) + \chi(1/t_1, -t_2) = 0 \tag{22}$$

Of course $\chi(t_1, t_2)$ is not known exactly for this model. However, the high-temperature expansion is known through 11th order.[12] This can be written in the form

$$\chi(t_1, t_2) = \sum_{m,n=0}^{\infty} c_{m,n} t_1^m t_2^n = \sum_{n=0}^{\infty} H_n(t_1)\, t_2^n \tag{23}$$

The $c_{m,n}$ coefficients for $m+n \leqslant 11$ are given in Table II.

Table II. Coefficients $c_{m,n}$ Defined by Eq. (23)

(0, 0)	1	(7, 1)	56
(1, 0)	2	(6, 2)	400
(2, 0)	2	(5, 3)	1,240
(1, 1)	8	(4, 4)	1,776
(3, 0)	2	(9, 0)	2
(2, 1)	16	(8, 1)	64
(4, 0)	2	(7, 2)	544
(3, 1)	24	(6, 3)	2,104
(2, 2)	48	(5, 4)	4,032
(5, 0)	2	(10, 0)	2
(4, 1)	32	(9, 1)	72
(3, 2)	104	(8, 2)	708
(6, 0)	2	(7, 3)	3,304
(5, 1)	40	(6, 4)	7,988
(4, 2)	180	(5, 5)	10,728
(3, 3)	296	(11, 0)	2
(7, 0)	2	(10, 1)	80
(6, 1)	48	(9, 2)	896
(5, 2)	280	(8, 3)	4,896
(4, 3)	656	(7, 4)	14,424
(8, 0)	2	(6, 5)	24,584

Consideration of the types of diagrams that contribute to a given order in t_2 suggest that the $H_n(t_1)$ are again rational functions

$$H_n(t_1) = K_n(t_1)/L_n(t_1) \tag{24}$$

with K_n and L_n being polynomials of the same degree, and with L_n having the generic form

$$L_n(t_1) \sim (1-t_1)^a(1+t_1)^b \tag{25}$$

This property of the partially resummed susceptibility expansion was noted a number of years ago by Citteur and Kasteleyn[13–15] and by Enting.[16]

The inversion relation (22) imposes a strong constraint on the functions $H_n(t_1)$ in (23), namely

$$H_n(t_1) + (-1)^n H_n(1/t_1) = 0 \tag{26}$$

which in turn means that if $L_n(t_1)$ is of the form (25), then the polynomial $K_n(t_1)$ must be either symmetric or antisymmetric.

From the results of Table II, or by a direct calculation from the resummed diagrams, we find that

$$H_0(t_1) = (1+t_1)/(1-t_1) \tag{27}$$

$$H_1(t_1) = 2(1+t_1)^2/(1-t_1)^2 \tag{28}$$

By inspection we also find that

$$(1-t_1)^3(1+t_1)\, H_2(t_1) = 2 + 12t_1 + 16t_1^2 + 12t_1^3 + 2t_1^4 + o(t_1^{10})$$

which suggests that H_2 is given exactly by

$$H_2(t_1) = 2(1 + 6t_1 + 8t_1^2 + 6t_1^3 + t_1^4)/(1-t_1)^3(1+t_1) \tag{29}$$

Similarly, by inspection, we find that

$$(1-t_1)^4\, H_3(t_1) = 2 + 16t_1 + 20t_1^2 + 16t_1^3 + t_1^4 + o(t_1^9)$$

which suggest that H_3 is given exactly by

$$H_3(t_1) = 2(1 + 8t_1 + 10t_1^2 + 8t_1^3 + t_1^4)/(1-t_1)^4 \tag{30}$$

On the basis of these results it might be expected that $H_4(t_1)$ will have a denominator of the form $(1-t_1)^5(1+t_1)^b$ with $0 \leqslant b < 5$. However, this does not appear to be the case. The closest candidate is $b = 3$, for which

$$\begin{aligned}(1-t_1)^5(1+t_1)^3\, H_4(t_1)\\ = 2 + 28t_1 + 112t_1^2 + 244t_1^3 + 296t_1^4 + 236t_1^5 + 120t_1^6 + 28t_1^7 + \cdots\end{aligned}$$

However, this is not quite symmetric, and hence does not satisfy the inversion relation. We have not found a solution for H_4 with polynomials of degree less than or equal to 13.

What makes this even more surprising is that there appears to be a fairly simple result for H_5. In particular, we find

$$(1-t_1)^6(1+t_1)^2 H_5(t_1)$$
$$= 2 + 32t_1 + 128t_1^2 + 288t_1^3 + 332t_1^4 + 288t_1^5 + 128t_1^6 + \cdots$$

which suggests that

$$H_5(t_1) = \frac{2(1+16t_1+64t_1^2+144t_1^3+166t_1^4+144t_1^5+64t_1^6+16t_1^7+t_1^8)}{(1-t_1)^6(1+t_1)^2} \tag{31}$$

exactly.

We finally consider the susceptibility of the fully anisotropic simple cubic lattice, which satisfies the inverse functional relation

$$\chi(t_1, t_2, t_3) + \chi(1/t_1, -t_2, -t_3) = 0 \tag{32}$$

The high-temperature expansion for this case can be written as

$$\chi(t_1, t_2, t_3) = \sum_{p,m,n} c_{p,m,n} t_1^p t_2^m t_3^n = \sum_{m,n} H_{m,n}(t_1)\, t_2^m t_3^n \tag{33}$$

The coefficients $c_{p,m,n}$ for $p+m+n \leqslant 11$ have been computed[1,12] and are given in Table III.

We again expect that the $H_{m,n}(t_1)$ are rational functions

$$H_{m,n}(t_1) = K_{m,n}(t_1)/L_{m,n}(t_1) \tag{34}$$

with $K_{m,n}$ and $L_{m,n}$ being polynomials. Since for $m=0$ or $n=0$ the square lattice results apply, we concentrate on the cases with $m, n \neq 0$.

By inspection we find that

$$(1-t_1)^3 H_{1,1}(t_1) = 8 + 24t_1 + 24t_1^2 + 8t_1^3 + o(t_1^{10})$$

which suggest that

$$H_{1,1}(t_1) = 8(1+3t_1+3t_1^2+t_1^3)/(1-t_1)^3 \tag{35}$$

exactly. Similarly,

$$(1-t_1)^4 H_{2,1}(t_1) = 16 + 80t_1 + 112t_1^2 + 80t_1^3 + 16t_t^4 + o(t_1^9)$$

Table III. Coefficients $c_{p,m,n}$ Defined by Eq. (33)

(0, 0, 0)	1	(9, 0, 0)	2
(1, 0, 0)	2	(8, 1, 0)	64
(2, 0, 0)	2	(7, 2, 0)	544
(1, 1, 0)	8	(7, 1, 1)	1,584
(3, 0, 0)	2	(6, 3, 0)	2,104
(2, 1, 0)	16	(6, 2, 1)	11,504
(1, 1, 1)	48	(5, 4, 0)	4,032
(4, 0, 0)	2	(5, 3, 1)	35,248
(3, 1, 0)	24	(5, 2, 2)	63,856
(2, 2, 0)	48	(4, 4, 1)	50,704
(2, 1, 1)	144	(4, 3, 2)	145,280
(5, 0, 0)	2	(3, 3, 3)	228,592
(4, 1, 0)	32	(10, 0, 0)	2
(3, 2, 0)	104	(9, 1, 0)	72
(3, 1, 1)	304	(8, 2, 0)	708
(2, 2, 1)	592	(8, 1, 1)	2,064
(6, 0, 0)	2	(7, 3, 0)	3,304
(5, 1, 0)	40	(7, 2, 1)	18,032
(4, 2, 0)	180	(6, 4, 0)	7,988
(4, 1, 1)	528	(6, 3, 1)	69,744
(3, 3, 0)	296	(6, 2, 2)	125,584
(3, 2, 1)	1,648	(5, 5, 0)	10,728
(2, 2, 2)	3,024	(5, 4, 1)	134,256
(7, 0, 0)	2	(5, 3, 2)	382,448
(6, 1, 0)	48	(4, 4, 2)	542,352
(5, 2, 0)	280	(4, 3, 3)	855,120
(5, 1, 1)	816	(11, 0, 0)	2
(4, 3, 0)	656	(10, 1, 0)	80
(4, 2, 1)	3,616	(9, 2, 0)	896
(3, 3, 1)	5,808	(9, 1, 1)	2,608
(3, 2, 2)	10,672	(8, 3, 0)	4,896
(8, 0, 0)	2	(8, 2, 1)	26,688
(7, 1, 0)	56	(7, 4, 0)	14,424
(6, 2, 0)	400	(7, 3, 1)	125,488
(6, 1, 1)	1,168	(7, 2, 2)	226,224
(5, 3, 0)	1,240	(6, 5, 0)	24,584
(5, 2, 1)	6,800	(6, 4, 1)	307,136
(4, 4, 0)	1,776	(6, 3, 2)	871,088
(4, 3, 1)	15,664	(5, 5, 1)	411,952
(4, 2, 2)	28,336	(5, 4, 2)	1,659,456
(3, 3, 2)	45,456	(5, 3, 3)	2,595,952
		(4, 4, 3)	3,685,552

which suggests that

$$H_{2,1}(t_1) = 16(1 + 5t_1 + 7t_1^2 + 5t_1^3 + t_1^4)/(1 - t_1)^4 \tag{36}$$

We also find that

$$(1 - t_1)^5 H_{3,1}(t_1) = 24 + 184t_1 + 368t_1^2 + 368t_1^3 + 184t_1^4 + 24t_1^5 + o(t_1^8)$$

which suggests that

$$H_{3,1}(t_1) = 8(3 + 23t_1^2 + 46t_1^3 + 23t_1^4 + 3t_1^5)/(1 - t_1)^5 \tag{37}$$

exactly.

This rather simple and appealing structure does not appear to persist to higher orders. In fact, we have not found a solution for $H_{2,2}$, or for any of the higher order ones.

4. CONCLUSION

The aim of this investigation has been to explore the analytical properties of resummed high-temperature expansions of the Ising model on anisotropic square and simple cubic lattices. Our approach has been to combine an analytic result, the inversion relation, with conventional high-temperature expansions. In the process we have obtainad a 16-term series for the partition function of the anisotropic cubic Ising model and an 11-term series for the susceptibility of the square lattice and of the fully anisotropic simple cubic lattice.

It is known from the exact Onsager solution that for the resummed partition function of the square lattice only $t_1^2 = 1$ singularities occur. Our analysis indicates that for the simple cubic lattice not only $t_1^2 = 1$ singularities, but also $t_1^2 = -1$ singularities occur in the partition function. This is a new result, which we feel is of some importance.

The resummed susceptibility series for the square lattice has singularities at $t_1 = 1$ and $t_1 = -1$, and for low orders of t_2 the rational functions $H_n(t_1)$ have a simple form, which has been explicitly found. However, the order of the polynomials appears to increase rapidly with increasing n, a rather surprising result. For the simple cubic lattice similar behavior is found.

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