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Ising model with real spin

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Abstract. The derivation is discussed of a novel generalisation of the Ising model which allows us to formally include an arbitrary (positive) value for the spin. This extends the domain in which such questions as the spin independence of critical indices can be considered. This is relevant to universality. The immediate extension of the formalism to cover the case of mixed-spin Ising systems is made. Certain consequences of the new model are also explored.

1. Introduction

The standard spin S (where S is one of the usual integral or odd-half integral values) Ising model has, in the usual notation, the partition function

$$Z_N = \text{tr}_1 \dots \text{tr}_N \exp\left(K \sum_{\langle ij \rangle} S_i^z S_j^z + L \sum_{i=1}^N S_i^z\right) \quad (1.1)$$

where $K = \beta J/S^2$, $L = \beta mH/S$ and $\text{Tr} = \text{tr}_1 \dots \text{tr}_i \dots \text{tr}_N$ stands for the total trace. The partial trace tr_i in (1.1) is defined by the condition that

$$\text{tr}_i \mathcal{A}(S_i^z) = (2S+1)^{-1} \sum_{S_i^z \in \mathcal{S}} \mathcal{A}(S_i^z) \quad (1.2)$$

in which the observable \mathcal{A} is any suitable function of S_i^z and \mathcal{S} is the set

$$\mathcal{S} = \{-S, -S+1, \dots, S-1, S\}. \quad (1.3)$$

The factor $(2S+1)^{-1}$ is introduced in (1.2) so that $\text{tr}_i 1 = 1$, which is a convenient normalising condition. The connection with thermodynamics is provided via the Helmholtz free energy F_N :

$$-\beta F_N = \ln Z_N. \quad (1.4)$$

Equations (1.1)-(1.4) allow various properties of the Ising model to be calculated as explicit functions of S . As a first example of this, we note that the leading coefficients in certain exact high-temperature series expansions (in powers of K , of course) have been obtained explicitly as functions of S . Table 1 makes this clear by quoting some results from Domb and Sykes (1957) and Yousif and Bowers (1984) for the reduced zero-field susceptibility coefficients of the FCC and BCC lattices (the results of the latter are, in fact, for a mixed-spin Ising model). As a second example of explicit results

Table 1. Reduced zero-field susceptibility coefficients of the single-spin FCC and the mixed-spin (of magnitudes $\frac{1}{2}$ and S) BCC lattices. Here $x = S(S+1)$.

FCC
$a_0 = 1$
$a_1 = 2x$
$a_2 = (x/30)(114x^2 + 114x - 3)$
$a_3 = (x/300)(2124x^4 + 4248x^3 + 1988x^2 - 136x + 1)$
$a_4 = (x/453\ 600)(5909\ 832x^6 + 17\ 729\ 496x^5 + 17\ 092\ 548x^4 + 4635\ 936x^3 - 616\ 050x^2 + 20\ 898x - 135)$
BCC
$b_0 = (1/11)(4x + 3)$
$b_1 = (16x/11)$
$b_2 = (2x/165)(148x + 99)$
$b_3 = (2x/165)(516x - 22)$
$b_4 = (x/6930)(52\ 148x^2 + 31\ 159x - 1305)$
$b_5 = (x/1155)(29\ 018x^2 - 2775x + 92)$
$b_6 = (x/415\ 800)(12\ 482\ 576x^3 + 6589\ 456x^2 - 645\ 199x + 19\ 971)$
$b_7 = (x/207\ 900)(20\ 370\ 104x^3 - 3075\ 616x^2 + 202\ 329x - 5871)$

involving S , we turn to the mean-field approximation. Here the complete thermodynamics may be shown to follow (Smart 1966) from the partition function

$$Z_N = Z^N \quad Z = (2S+1)^{-1} \frac{\sinh[(S+\frac{1}{2})H_e]}{\sinh(\frac{1}{2}H_e)} \quad (1.5)$$

where H_e is an effective field. Similar results apply in other approximation schemes. As a third example of our theme, we refer to the Kac-Hubbard-Stratonovich (KHS) transformation (Berlin and Kac 1952, Stratonovich 1957, Hubbard 1959) used by Hubbard (1972). This allows (1.1) to be re-expanded in the zero-field form:

$$Z_N = \frac{1}{[(\pi/2)^N \det(K)]^{1/2}} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \exp\left(-\frac{1}{4} \sum_{ij} (K^{-1})_{ij} x_i x_j\right) \prod_{i=1}^N \Omega_S(x_i) dx_i. \quad (1.6)$$

Here $L=0$ and K is now a matrix, the couplings K_{ij} between spins i and j generalising the previous couplings K . The explicit spin dependence is given by the formula

$$\Omega_S(x_i) = (2S+1)^{-1} \frac{\sinh[(S+\frac{1}{2})x_i]}{\sinh(\frac{1}{2}x_i)}. \quad (1.7)$$

The importance of (1.6) and (1.7) is that for any spin $S = \frac{1}{2}, 1, \frac{3}{2}, \dots$, they cast the Ising model in a form suitable for the application of Wilson's (1971) field theoretical techniques (see Hubbard 1972).

The first and third examples (and, to a lesser extent, the second) indicate methods by which studies have been made of the variation with spin of critical point parameters of the Ising model. Such studies have provided strong evidence in favour of that aspect of the universality referred to as spin independence of critical exponents. An intriguing point follows from the fact that the above results involve explicit algebraic functions of S . This means that, in an *ad hoc* manner at least, the study of spin independence need not be restricted to $S = \frac{1}{2}, 1, \frac{3}{2}, \dots$; any real value of S may be considered (for simplicity we leave aside the possibility of complex values here). To give an example,

if we put $S = -3.1, \sqrt{2}, \pi$ (say) respectively in the series for susceptibility $\chi_0(K)$ of BCC lattice as given by table 1, and then form Padé approximants to $(d/dK) \ln \chi_0(K)$, we find the estimates of table 2 for the critical exponent γ ($\chi_0(K)$ of FCC yields very short Padé tables and are therefore not included). These suggest a value of γ near 1.25 just as for the usual 'quantum' spin values (for estimates using such values see Yousif and Bowers (1984)). Another example follows if we put the same 'unphysical' values in (1.6) and (1.7). The argument of Hubbard based on applying Wilson's ideas to (1.6) and (1.7) suggests that the fixed point is unchanged in going even to these values of the spin. This supports the idea that the spin independence of critical indices may be extended to real S .

Table 2. Estimates for γ provided by forming $[N, D]$ PA to the series $(d/dK) \ln \chi_0(K)$, on the mixed-spin (of magnitudes $\frac{1}{2}$ and S) BCC lattice. S takes the values $-3.1, \sqrt{2}, \pi$.

D	N = 1	N = 2	N = 3	N = 4	N = 5
<hr/>					
$(S = -3.1)$					
2	1.5100	1.0071	1.3254	—	—
3	1.1263	1.2251	1.2611	1.4434	
4	1.2843	1.2695	1.2243		
5	1.2684	1.2842			
6	—				
<hr/>					
$(S = \sqrt{2})$					
2	1.3901	1.0425	1.3154	—	—
3	1.1134	1.2184	1.2502	1.4377	
4	1.3282	1.2545	1.2175		
5	1.2305	1.3245			
6	—				
<hr/>					
$(S = \pi)$					
2	1.5895	1.0403	1.2892	—	—
3	1.1686	1.2350	1.2781	1.3755	
4	1.2547	1.3069	1.2342		
5	1.2892	1.2542			
6	—				
<hr/>					

The above is, as previously observed, *ad hoc*: it uses formalism (1.1)–(1.3) which is only valid when $S = \frac{1}{2}, 1, \frac{3}{2}, \dots$, and then quite arbitrarily treats resulting formulae as if they apply when $S = \pi$ or any other real number. The purpose of this paper is to legitimise this. We restrict our attention to the case where S takes positive values. The idea is to generalise (1.2) and (1.3) in such a way that the resulting model applies for any positive S and gives the same results, at least in our examples, for explicit spin dependence as the previous *ad hoc* procedure. In this way we define an Ising model for any positive-spin S and so extend the domain in which such questions as universality can be considered.

2. Definition of the model

Moments of powers of the spin components S_i^r are simply $\text{tr}_i (S_i^r)^r, r = 0, 1, 2, \dots$, in

the standard Ising model. These are given (on using equations (2.7)) by

$$\text{tr}_i (S_i^z)^r = \begin{cases} (2S+1)^{-1} \frac{2}{2n+1} B_{2n+1}(S+1) & r = 2n \\ 0 & r = 2n+1 \end{cases} \tag{2.1}$$

where $B_r(x)$ denotes the Bernoulli polynomial of degree r .

As is known from the theory of probability distributions, a knowledge of the full set of such moments is completely equivalent to the distribution function of spin components. With respect to discussion of § 1, it is therefore sufficient to generalise equations (1.2) and (1.3) such that (2.1) is formally valid for any $S \in \mathbb{R}^+$. This will then determine the spin distribution function uniquely, defining the generalised model via (1.1). We shall start by defining the new trace tr'_i and subsequently examine whether the requirements mentioned at the end of § 1 for a successful candidate are met. We write, for all $S \geq 0$,

$$(2S+1) \text{tr}'_i \mathcal{A}(S_i^z) = \sum_{S_i^z \in \mathcal{S}'} \mathcal{A}(S_i^z) + \int_{-\infty}^{+\infty} W_{S-[S]}(u) \mathcal{A}(u) du \tag{2.2}$$

where $[S]$ is the greatest integer $\leq S$, and the distribution function $W_{S-[S]}(u)$ is given in terms of the quantity $0 \leq S - [S] < 1$ by

$$W_{S-[S]}(u) = \frac{i \sin 2\pi(S-[S])}{\cos 2\pi u - \cos 2\pi(S-[S])}. \tag{2.3}$$

Here \mathcal{S}' is the set

$$\mathcal{S}' = \{-S, -S+1, \dots, -S+[S], S-[S], \dots, S-1, S\}. \tag{2.4}$$

The generalised moments $\text{tr}'_i(S_i^z)^r$ are thus defined from

$$(2S+1) \text{tr}'_i (S_i^z)^r = \sum_{S_i^z \in \mathcal{S}'} (S_i^z)^r + \int_{-\infty}^{+\infty} W_{S-[S]}(u) u^r du. \tag{2.5}$$

We must now prove that (2.5) indeed yields the same explicit spin dependence as in (2.1) for arbitrary positive S . First, consider the situation for non-integer spins where $0 < S - [S] < 1$. We have (Erdelyi *et al* 1953); for $r = 2n = 0, 2, 4, \dots$:

$$\begin{aligned} & \int_{-\infty}^{+\infty} W_{S-[S]}(u) u^{2n} du \\ &= \int_{-\infty}^{+\infty} (-1)^{n+1} \frac{t^{2n} \sin 2\pi(S-[S])}{\cosh 2\pi t - \cos 2\pi(S-[S])} dt \\ &= \frac{2}{2n+1} B_{2n+1}(S-[S]) \end{aligned} \tag{2.6}$$

which holds for $0 < S - [S] < 1$. The summation in (2.5) may be calculated via relations (Erdelyi *et al* 1953)

$$\int_x^{x+1} B_r(t) dt = x^r \quad \int_x^y B_r(t) dt = \frac{B_{r+1}(y) - B_{r+1}(x)}{r+1} \tag{2.7}$$

where $r = 0, 1, 2, \dots$. Whence for $0 < S - [S] < 1$, i.e. for non-integers,

$$\sum_{S_i^z \in \mathcal{S}'} (S_i^z)^{2n} = \frac{2}{2n+1} [B_{2n+1}(S+1) - B_{2n+1}(S-[S])]. \tag{2.8}$$

Thus (2.8), together with (2.6), yield via (2.5)

$$\text{tr}'_i (S_i^z)^{2n} = (2S + 1)^{-1} \frac{2}{2n + 1} B_{2n+1}(S + 1) \tag{2.9}$$

which holds for every non-integer spin and checks with (2.1) if, in it, S is literally taken to belong to non-integer \mathbb{R}^+ . When $r = 2n + 1$ is odd, the integral and summation in (2.5) are easily seen to vanish, implying zero moment for odd powers of S_i^z , consistent with (2.1). We remark the interesting case of 'physical' spins $S = \frac{1}{2}, \frac{3}{2}, \dots$ (where $S - [S] = \frac{1}{2}$, a particular case of $0 < S - [S] < 1$) for which the integral in (2.2) vanishes and \mathcal{S}' coincides with \mathcal{S} , so that $\text{tr}'_i \equiv \text{tr}_i$ and thus (1.2) and (1.3) are recovered for $s = \frac{1}{2}, \frac{3}{2}, \dots$.

Next we consider the case of integer spins where $S - [S] = 0$. It is seen that the value $S - [S] = 0$ is counted twice in \mathcal{S}' as given by (2.4). This will obviously affect the summation in (2.5) only when $r = 0$. Also the weight function $W_0(u)$ is now everywhere zero except at the origin $u = 0$. To work out the integral part of the moments in (2.5) we expand informally in a small neighbourhood of the origin to get

$$\begin{aligned} & \int_{-i\infty}^{i\infty} W_0(u) u^r du \\ &= \lim_{s-[S] \rightarrow 0} \int_{-\epsilon}^{\epsilon} -\frac{1}{\pi} \frac{S - [S]}{t^2 + (S - [S])^2} (it)^r dt \\ &= \begin{cases} -1 & r = 0 \\ 0 & r = 1, 2, 3, \dots \end{cases} \end{aligned} \tag{2.10}$$

This is because $(S - [S]) / [t^2 + (S - [S])^2] \pi$ is a delta sequence (see, for example, Gel'fand and Shilov 1964). Thus the problem with $\text{tr}'_i 1$ in (2.5), i.e. when $r = 0$, is automatically taken care of by the delta function behaviour of $W_0(u)$ to yield $\text{tr}'_i 1 = 1$, as before. Equations (2.5) and (2.10) then imply

$$\text{tr}'_i (S_i^z)^r = \begin{cases} (2S + 1)^{-1} \frac{2}{2n + 1} B_{2n+1}(S + 1) & r = 2n \\ 0 & r = 2n + 1 \end{cases} \tag{2.11}$$

for any positive integer S , which again checks with (2.1).

In this manner, we have defined a new model with the partition function

$$Z_N = \text{tr}'_1 \dots \text{tr}'_N \exp \left(K \sum_{\langle ij \rangle} S_i^z S_j^z + L \sum_{i=1}^N S_i^z \right) \tag{2.12}$$

where tr'_i are given by (2.2)–(2.4). As we set out to achieve, it is a generalisation of the standard Ising model which reduces to it (in that its moments are identical to those of the standard model) when $S = \frac{1}{2}, 1, \frac{3}{2}, \dots$, and remain consistent for any other positive-spin value. Everything derived from this partition function is now formally valid for any $S \in \mathbb{R}^+$.

The extension of the above formalism to include mixed-spin Ising systems is immediate. Let our loose-packed lattice consist of two (non-equivalent) sublattices A and B containing spins S_A and S_B . Then the partition function is

$$Z_N = \text{Tr} \exp \left(K \sum_{\langle ij \rangle} S_{i,A}^z S_{j,B}^z + L_A \sum_{i \in A} S_{i,A}^z + L_B \sum_{j \in B} S_{j,B}^z \right)$$

where $K = \beta J / S_A S_B$, $L_A = \beta m_A H_A / S_A$ and $L_B = \beta m_B H_B / S_B$. Here the total trace is

$$\text{Tr} = (\text{tr}_{1,A} \dots \text{tr}_{N_A,A}) (\text{tr}_{1,B} \dots \text{tr}_{N_B,B})$$

where N_A and N_B represent the number of sites on A and B sublattices respectively and

$$\text{tr}_{i,A} \mathcal{A}(S_{i,A}^z) = (2S_A + 1)^{-1} \sum_{S_{i,A}^z \in \mathcal{S}_A} \mathcal{A}(S_{i,A}^z)$$

$$\text{tr}_{i,B} \mathcal{A}(S_{j,B}^z) = (2S_B + 1)^{-1} \sum_{S_{j,B}^z \in \mathcal{S}_B} \mathcal{A}(S_{j,B}^z)$$

in which

$$\mathcal{S}_A = \{-S_A, -S_A + 1, \dots, S_A - 1, S_A\}$$

$$\mathcal{S}_B = \{-S_B, -S_B + 1, \dots, S_B - 1, S_B\}.$$

Equation (2.1) clearly holds:

$$\text{tr}_{i,A} (S_{i,A}^z)^r = \begin{cases} (2S_A + 1)^{-1} \frac{2}{2n+1} B_{2n+1}(S_A + 1) & r = 2n \\ 0 & r = 2n + 1 \end{cases} \quad (2.13a)$$

and

$$\text{tr}_{i,B} (S_{j,B}^z)^r = \begin{cases} (2S_B + 1)^{-1} \frac{2}{2n+1} B_{2n+1}(S_B + 1) & r = 2n \\ 0 & r = 2n + 1. \end{cases} \quad (2.13b)$$

We can thus proceed in exactly the same manner as before by writing down (2.2) for $\text{tr}'_{i,A} \mathcal{A}(S_{i,A}^z)$ and $\text{tr}'_{i,B} \mathcal{A}(S_{j,B}^z)$ with (2.3) and (2.4) defined in terms of S_A and S_B , respectively. Clearly the mathematics is identical to the single-spin case and we end up with the result that equations (2.13a, b) become formally valid for any $S_A, S_B \in \mathbb{R}^+$. So the partition function with Tr replaced by Tr' defines the required generalisation for mixed-spin Ising models.

3. Some consequences

Considering the example of high-temperature expansions, MFT and KHS transformations (as used by Hubbard), we show that our generalised model does indeed yield the same results for explicit spin dependence as discussed in § 1. (The extension of the following analysis to the mixed-spin Ising model is trivial).

(i) High-temperature expansions. Writing the partition function (1.1) in the form

$$Z_N = \text{Tr} \prod_{\langle ij \rangle} \exp(K S_i^z S_j^z) \prod_{i=1}^N \exp(L S_i^z) \quad (3.1)$$

enables one to apply the method of Brout (1959, 1960) for obtaining high-temperature series expansions in the following manner. Expand the above exponentials in powers of K and L . When the first product term is multiplied out, the coefficient of K^l gives a contribution from every possible multiply-bonded graph of l lines; every such graph is associated with an appropriate product of the $S_i^z, S_j^z, \dots, S_k^z$, there being $S_i^z S_j^z$ for each bond. These must now be multiplied by the expansion of the second product term, whose typical coefficient is again an appropriate product of the S_i^z . Finally, take the trace to get factors like $\text{tr}_i (S_i^z)^r, r = 0, 1, 2, \dots$, which must be calculated at vertex i .

These then determine the coefficients of K' in the final (exact up to a given order) expansion. In our generalised model we clearly end up with factors $\text{tr}'_i \langle S_i^z \rangle^r$ which, as proved in the last section, yield the same explicit spin dependence. As a consequence the high-temperature series expansion obtained from the new model are identical to those of the standard Ising system, with the advantage that they are formally valid for all $S \in \mathbb{R}^+$. The smoothness of estimates of table 2 now looks plausible in view of an extended form for the spin independence of critical exponents.

(ii) MFT. The standard spin- S Ising Hamiltonian

$$\mathcal{H} = \frac{J}{S^2} \sum_{\langle ij \rangle} S_i^z S_j^z - \frac{mH}{S} \sum_{i=1}^N S_i^z$$

can be written as a sum of the site-spin Hamiltonian \mathcal{H}_i in the following manner:

$$\mathcal{H} = \sum_{i=1}^N \mathcal{H}_i \tag{3.2a}$$

where

$$\mathcal{H}_i = \left(-\frac{mH}{S} - \frac{J}{S^2} \sum_{j=1}^q S_j^z \right) S_i^z \tag{3.2b}$$

q being the coordination number of the lattice. The basic assumption of MFT is that the spin-spin interactions are approximately equivalent to the effect of an applied magnetic field proportional to their mean value $\langle S_j^z \rangle$. We thus let

$$\sum_{j=1}^q S_j^z = q \langle S^z \rangle$$

with $\langle S_j^z \rangle = \langle S^z \rangle, \forall j$. Hence (3.2b) yields

$$Z_i = \text{tr}_i \exp(H_e S_i^z) \quad \forall i \tag{3.3}$$

for the partition function of the site-spin i , where the effective field H_e is given by

$$H_e = L + Kq \langle S^z \rangle.$$

The total partition function is obviously $Z_N = Z_i^N$.

For our generalised model (3.3) becomes

$$Z_i = \text{tr}'_i \exp(H_e S_i^z) \quad Z_N = Z_i^N \tag{3.4}$$

or

$$(2S+1)Z_i = \sum_{S_i^z \in \mathcal{S}'} \exp(H_e S_i^z) + \int_{-\infty}^{+\infty} W_{S-[S]}(u) \exp(H_e u) du. \tag{3.5}$$

Here the integral contribution is equal to (for $0 < S - [S] < 1$)

$$I = \int_{-\infty}^{\infty} -\frac{\sin 2\pi(S-[S]) \exp(-iH_e t)}{\cosh 2\pi t - \cos 2\pi(S-[S])} dt$$

which is just the inverse Fourier transform of

$$-(2\pi)^{1/2} \frac{\sin 2\pi(S-[S])}{\cosh 2\pi t - \cos 2\pi(S-[S])}$$

where

$$F(t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} f(x) \exp(itx) dx$$

$$f(x) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} F(t) \exp(-itx) dt$$

define the Fourier transform $F(t)$ of $f(x)$ and its inverse, respectively. Thus I is found from tables (see, for instance, Gradshteyn and Ryzhik (1980)) to be

$$I = \frac{\sinh[(S - [S] - \frac{1}{2})H_e]}{\sinh(\frac{1}{2}H_e)} \tag{3.6}$$

for $0 < S - [S] < 1$. Now equation (2.4) implies for non-integer S

$$\sum_{S_i^z \in \mathcal{S}'} \exp(H_e S_i^z) = \frac{\sinh[(S + \frac{1}{2})H_e] - \sinh[(S - [S] - \frac{1}{2})H_e]}{\sinh(\frac{1}{2}H_e)}$$

This, together with (3.6), yields the same form as (1.5) on using (3.5). For integers ($S - [S] = 0$) the integral contribution becomes -1 , because of the delta function behaviour of $W_0(u)$ and this again takes care of the fact that $S - [S] = 0$ is included twice in \mathcal{S}' , so that once again we obtain

$$\text{tr}'_i \exp(H_e S_i^z) = (2S + 1)^{-1} \frac{\sinh[(S + \frac{1}{2})H_e]}{\sinh(\frac{1}{2}H_e)}$$

for integer spins. Thus the new model gives the equivalent of (1.5), valid formally for any positive spin.

(iii) KHS transformation. In zero field, equation (1.1) reduces to

$$Z_N = \text{Tr} \exp \sum_{ij} S_i^z K_{ij} S_j^z \tag{3.7}$$

where the couplings have been generalised as described in § 1. The KHS transformation is, for any symmetric positive-definite matrix (this is necessary for the convergence of the multiple integral; there exist other transformations, however, which hold true for any symmetric matrix (see Baker 1962) so that Hubbard's arguments will not be affected in principle),

$$\exp \sum_{ij} S_i^z K_{ij} S_j^z$$

$$= \frac{1}{[(\pi/2)^N \det(K)]^{1/2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp\left(-\frac{1}{4} \sum_{ij} (K^{-1})_{ij} x_i x_j + \sum_{i=1}^N x_i S_i^z\right) d^N x_i. \tag{3.8}$$

Taking the trace as instructed by (3.7) yields equation (1.6) with $\Omega_S(x_i) = \text{tr}'_i \exp(x_i S_i^z)$. This in turn gives (1.7) after simple manipulations. These partial traces involved in Ω_S are similar to those which come in the MFT (see (ii) above), justifying the resemblance between (1.5) and (1.7). In the generalised zero-field Ising model everything remains as before, except that

$$\Omega_S(x_i) = \text{tr}'_i \exp(x_i S_i^z).$$

From arguments given in (ii), this equation (whose right-hand side is identical to (3.4) with H_c replaced by x_i) also yields

$$\Omega_S(x_i) = (2S + 1)^{-1} \frac{\sinh[(S + \frac{1}{2})x_i]}{\sinh(\frac{1}{2}x_i)}$$

for any $S \in \mathbb{R}^+$ and is consistent with (1.7). The reasoning of Hubbard (see § 1) thus becomes formally valid for any positive real spin, supporting the idea that the spin independence of critical indices may be extended to positive real S .

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