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On the critical polynomial of the simple cubic Ising model

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Abstract. In 1985 Rosengren conjectured that the critical point of the symmetric, simple cubic (SC) Ising model is given by $v_c \equiv \tanh(J/k_BT_c) = v_R \equiv (\sqrt{5}-2)\cos(\pi/8)$. This guess is examined in the context of attempting to construct the *full critical polynomial* $P_3(v_x, v_y, v_z)$, with a root $v_c(J_x, J_y, J_z)$, for the anisotropic SC Ising model with couplings J_x, J_y and J_z. It transpires that v_R is a surd which satisfies $R(v_R^2) = 0$, where $R(x)$ is a quartic polynomial with integral coefficients; but $R(v^2)$ is a poor candidate for $P_3(v, v, v)$ since it does not display various 'nice' properties embodied in the critical polynomial $P_2(v_x, v_y)$ for the square, 2D Ising lattices. Methods for constructing nice polynomials $Q_k(v_x, v_y, v_z)$ that provide excellent approximations for v_c *and* for v_R are demonstrated. However, scaling arguments, etc, for the dimensional crossover induced when, say, $J_z \to 0$ cast doubt on the *existence* and nature of the sought-for critical polynomial P_3.

1. Introduction and summary

In 1944 Onsager [1] presented his exact solution of the two-dimensional Ising model with nearest-neighbour interactions on a square lattice (in zero magnetic field): if spins $s_i, s_j, \ldots = \pm 1$ occupy each lattice site, then nearest-neighbour bonds parallel to the x and y axes each contribute a term $J_x s_i s_j$ and $J_y s_k s_l$, to the total Hamiltonian. In subsequent years many authors [2–6] attempted to solve or, at least, guess exact answers for the corresponding three-dimensional Ising model on a simple cubic lattice with the additional couplings $J_z s_m s_n$ for bonds parallel to the z axis. Difficulties were soon appreciated: see, e.g., [7]. Thus Onsager showed that the crucial contribution to the free energy per spin for the square lattice ($J_z \equiv 0$) could be written [1, 8]

$$f = \frac{1}{2}\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\ln[C_xC_y - S_x\cos\theta - S_y\sin\phi] \tag{1}$$

where, with $\lambda = x, y, z$, one has

$$C_\lambda = \cosh 2K_\lambda \qquad S_\lambda = \sinh 2K_\lambda \qquad K_\lambda = J_\lambda/k_BT. \tag{2}$$

A natural generalization is to add a term $S_z \sin\psi$ in the argument of the logarithm in (1), etc, and to perform a further integration [2]; however, it was found that this fails at a rather low order of expansion in powers of the K_λ.

Less ambitiously one may seek an equation for the critical point of the three-dimensional model. The only singularities as a function of T of the double integral in (1) arise from the vanishing of the argument of the logarithm; that is possible only when $\theta = \phi = 0$. In terms of the natural, high-temperature counting variables [8]

$$u = \tanh K_x \qquad v = \tanh K_y \qquad \text{and} \qquad w = \tanh K_z \tag{3}$$

the logarithmic argument then reduces to a simple rational function decomposable into quadratic factors. (Of course we set $w = 0$ for the two-dimensional situation.) One of the factors is simply

$$P_2(u, v) = 1 - u - v - uv. \tag{4}$$

(Some others simply entail replacing u by $-u$ and v by $-v$.)

It now follows that for *ferromagnetic* couplings, $J_\lambda \geqslant 0$ (to which, for the square and SC lattices, we may restrict attention with no loss of generality) the *vanishing* of the polynomial $P_2(u, v)$ specifies the *critical point* of the square lattice Ising model for general J_x/J_y. Thus, in the one-dimensional case with, say, $K_x = u = 0$, we find $v_c = \tanh K_c = 1$ implying $K_c = \infty$ or $k_B T_c/J = 0$ ($J_y = J$) which, of course, is the correct answer first found by Ising [8]. For the symmetric square lattice with $u = v$ we recapture Onsager's famous result

$$v_c = \sqrt{2} - 1 = 0.414\,21\ldots \qquad \text{or} \qquad K_c = \tfrac{1}{2}\ln(1 + \sqrt{2}) \tag{5}$$

corresponding to $k_B T_c/J = 2.269\,18\ldots$ [1, 8].

We remark that the *critical polynomial* (4) also arises naturally from the self-duality of the planar Ising model at criticality [8]. Furthermore, if $\kappa_x(T)$ is the inverse of the true range of correlation for decays parallel to the x axis *above* T_c, one has [8–10]

$$\exp(-\kappa_x a) = u\frac{1 + v}{1 - v} = \exp(\Sigma_x a/k_B T) \tag{6}$$

where a is the lattice spacing while, on the right-hand side, $\Sigma_x(T)$ denotes the interfacial tension of a domain wall parallel to the x axis *below* T_c. The criticality conditions $\kappa_x(T \to T_c^+) \to 0$, $\Sigma_x(T \to T_c) \to 0$ lead directly back to the critical-point equation $P_2(u, v) = 0$. As noted originally by Temperley [11, 12], powers of the factor $u(1 + v)/(1 - v)$ have a natural interpretation as generating functions of *directed lattice walks* that move up or down the y axis but advance only parallel to the positive x axis. It follows on physical grounds from (6) that for any ratio of J_x/J_y, the polynomial $P_2(u, v)$ *decreases monotonically* from $P_2(0, 0) = 1$ and vanishes, for the *first* time, at the critical point (u_c, v_c). (Of course, this can also be easily verified numerically.)

The natural question now is: 'Can one find the polynomial, $P_3(u, v, w)$, whose vanishing specifies the critical points of the anisotropic, *three*-dimensional, SC Ising model?' Note, first, that the premise of the question may well be false! Indeed, as discussed in section 4, the critical points of the truly three-dimensional models (with u, v and w all non-zero) may not be the root of *any* polynomial. Nevertheless, it is tempting to hunt for a *critical polynomial* even if one is prepared to find that it must be of infinite order!

One such search was, in fact, reported in 1985 by Rosengren [13] who based his study on the construction of walk generating functions [11, 12] as inspired by the Kac–Ward approach to solving the planar Ising model [7, 14]. Rosengren showed that a certain 'natural extension' to $d = 3$ dimensions was false but, at the same time, he advanced the conjecture that the critical value $v_c = \tanh K_c$ for the symmetric simple cubic model ($u = v = w$) was equal to

$$v_R \equiv (\sqrt{5} - 2)\cos(\pi/8) = 0.218\,098\,372_7. \tag{7}$$

It is not unfair to say that the basis for this guess remains somewhat obscure: Rosengren did sketch an argument suggesting that a relevant class of weighted lattice walks with no backsteps would yield the factor $\sqrt{5} - 2$ [13]; but the second factor in (7) was then selected to match various critical point estimates based on series and Monte Carlo studies published in 1981–84 [15–18]: these estimates varied from $v_c \simeq 0.218\,085$ up to $v_c \geqslant 0.218\,110$ which nicely bracket v_R!

In the last decade further estimates of v_c (for the symmetric model have become available [19–23], many being more precise (and, one hopes, more accurate). With further computational developments still in view, Rosengren's conjecture has attracted renewed attention [24]. Accordingly, it seems appropriate to bring it under some theoretical scrutiny: that is the object of this paper.

Explicitly, it transpires that v_R can be expressed wholly in terms of quadratic surds since

$$\cos(\pi/8) = \tfrac{1}{2}\sqrt{(2+2\sqrt{2})}. \tag{8}$$

Thence one finds that v_R is a root of a polynomial

$$R(v^2) = 1 - r_2 v^2 - r_4 v^4 - r_6 v^6 - r_8 v^8 \tag{9}$$

which has integral coefficients r_k. However, $R(v^2)$ is a poor candidate for the desired critical polynomial, $P_3(v, v, v)$, in the symmetric case ($u = v = w$) since it has a second root, v_R' which is *smaller* than $v_R \simeq v_c$; thus $R(v^2)$ varies *non*-monotonically when v rises from 0 to v_R-. In other words it does *not* mimic the natural properties of the $d = 2$ polynomial, $P_2(u, v)$, discussed above. Furthermore, since $R(v^2)$ lacks any linear term, it is hard to envisage how it might derive from some three-variable polynomial, say $\tilde{R}(u, v, w)$, which would yield the appropriate $d = 2$ factors, $P_2(v, w)$, $P_2(w, u)$ and $P_2(u, v)$, when, respectively, u, v or w vanished.

On the other hand, in section 3, it is shown that one can systematically construct putative critical polynomials, $Q_k(u, v, w)$, of appropriate symmetry, which (a) have integral coefficients, (b) reduce to $P_2(v, w)$, etc, when u, v or w vanishes, that (c) decrease monotonically as u, v and w increase to the locus of zeros and (d) yield (approximate) values for v_c (when $u = v = w$) which match the numerical estimates with essentially the same precision as does v_R.

Explicitly, the sixth-order polynomial

$$\begin{aligned} Q_6(u, v, w) = {} & 1 - u - v - w - uv - vw - wu - 18uvw - 2uvw(u+v+w) \\ & - uvw(u^2+v^2+w^2+uv+vw+wu) - \tfrac{1}{2}uvw[uvw - (u+v)w^2 \\ & - (v+w)u^2 - (w+u)v^2] \end{aligned} \tag{10}$$

clearly satisfies the criteria (a), (b) and (c); furthermore, the smallest root of

$$Q_6(v, v, v) = 1 - 3v - 3v^2 - 18v^3 - 6v^4 - 6v^5 + \tfrac{5}{2}v^6 \tag{11}$$

is found to be

$$v_F = 0.218\,098\,074_4. \tag{12}$$

But this differs from v_R by only about 1.7×10^{-9}, which is about 1000 times smaller than the best precision currently claimed for v_c estimates!

The remarkably close correspondence of v_R and v_F is partly accidental: indeed, if the coefficient $\frac{5}{2}$ of v^6 in (11) is replaced by one of the closest integers, 2 or 3, the deviations from v_R increase in magnitude to

$$\Delta v \simeq -7.485 \times 10^{-6} \qquad \text{or} \qquad +7.490 \times 10^{-6} \tag{13}$$

respectively. These are comparable to the deviations of recent estimates from v_R: see table 1. Nevertheless, the good approximation of v_R by v_F clearly illustrates the dangers of being overly impressed even by extremely close numerical coincidences if they are not backed by respectable theory. Of course, one must not now claim that v_F is likely to be the true value of v_c; nevertheless, v_F could reasonably be regarded as a *better guess* for the exact value than v_R! However, the method of construction illustrated below (see table 1) demonstrates that the various current estimates of v_c, and others likely to be forthcoming in the next decade, can probably all be matched within their numerical precision by the roots of 'nice' polynomials like (10), although perhaps of higher order if one wants such simple coefficients.

Table 1. Comparison of simple-cubic-lattice critical point estimates and conjectural values. The last column lists the values of $\Delta v \equiv v_c^{\mathrm{est}} - v_R$ multiplied by 10^6, where $v_c = \tanh(J/k_B T_c)$ and Rosengren's surd v_R is given in equations (7) and (8); the polynomials $Q_k(u, v, w; \{p_i\})$ are specified in the text.

Source of estimate/conjecture	$10^6 \Delta v$
Guttmann [19, 23]	-5.373
Liu and Fisher [20]	-27.37 ± 10.00
Ferrenberg and Landau [21] (FL)	0.827 ± 2.6
Baillie *et al* [23] (BP)	-6.328 ± 3.8
$Q_k(v, v, v; \{p_i\})$	
$k = 3$: $p_0 = 137/7 \simeq 19.571428$	-4.926
$724/37 \simeq 19.567567$	0.715
$3 \cdot 7 \cdot 41/44 \simeq 19.568181$	-0.183
$1585/3^4 \simeq 19.567901$	0.227
$2446/5^3 \simeq 19.568000$	0.083
$k = 4$: $p_1 = 12/5 \simeq 2.400000$	-3.255
$p_0 = 18$, $67/28 \simeq 2.392857$	3.502
$103/43 \simeq 2.395349$	1.144
$139/58 \simeq 2.396551$	0.007_3
$151/63 \simeq 2.396826$	-0.252
$149/62 \simeq 2.403059$	-6.306
$k = 5$: $p_0 = 18$, $p_1 = 2$, $p_2 = 1$	-37.40
$p_2 = 10/11$	0.016

Finally, however, the caveat concerning the *existence* of the critical polynomial $P_3(u, v, w)$ must be kept strongly in mind. In particular, section 4 considers the *dimensional crossover* in critical behaviour that must occur when, say, $w \to 0$. General scaling arguments, explicitly verified for spherical models (for all $d > 2$), indicate that $v_c(u, w)$ varies *non-analytically* with w (at $w = 0$); that is inconsistent with the existence of simple critical polynomials of the sort illustrated above (and in section 3) since these allow a Taylor expansion of $v_c(u, w)$ in powers of w. Nevertheless, for the Ising model, a degenerate crossover scaling function (diverging at infinite argument) could still allow a critical polynomial. Moreover, because the susceptibility exponent γ of the two-dimensional Ising model is a rational number, one can even construct model critical polynomials with roots depending non-analytically on $w(\to 0)$; but these cannot have all the nice properties listed above.

2. Rosengren's surd

It is well known that trigonometric functions of angles which are rational fractions of π can be expressed as the roots of algebraic equations. In the present case one merely needs to (i) write

$$t \equiv \cos(\pi/8) = \tfrac{1}{2}(\epsilon + \epsilon^{-1}) \qquad \text{with} \qquad \epsilon = \mathrm{e}^{\mathrm{i}\pi/8} \tag{14}$$

(ii) note that $\epsilon^{\pm 8} = -1$, and (iii) calculate successively the squares of t, $(4t^2 - 2)$ and $[(4t^2-2)^2 - 2]$. The last square yields the quadratic equation

$$8t^4 - 8t^2 + 1 = 0 \tag{15}$$

for t^2 from which (8) follows immediately.

The definition (7) then gives

$$4v_{\mathrm{R}}^2 = (9 - 4\sqrt{5})(2 + \sqrt{2}) = 18 + 9\sqrt{2} - 8\sqrt{5} - 4\sqrt{10}. \tag{16}$$

Clearly, all higher powers $(4v_{\mathrm{R}}^2)^k$ can equally be expressed as linear combinations of 1, $\sqrt{2}$, $\sqrt{5}$ and $\sqrt{10}$ with integer coefficients. Between the four equations for $k = 1, 2, 3$ and 4, one may thus eliminate the three surds. This leads to a quartic equation satisfied by v_{R}^2 of the form (9) with the integral coefficients

$$r_2 = 144 \qquad r_4 = -2640 \qquad r_6 = 1152 \qquad r_8 = -64. \tag{17}$$

Because each root containing $\sqrt{2}$ and $\sqrt{5}$ must be paired with like roots with $-\sqrt{2}$ and $-\sqrt{5}$ it is clear that no rational algebraic equation of lower degree can have v_{R} as a root.

What proves significant about the coefficients (17) is the large value of r_2 (relative to $1/v_{\mathrm{c}}^2 \simeq 4.6$) and the subsequent negative sign of r_4 (and of r_8). By evaluating the corresponding polynomial, $R(v^2)$, for increasing v one finds that it drops rapidly from $R(0) = 1$ and first vanishes at $v = v'_{\mathrm{R}} \simeq 0.09034$; this value is, of course, less than $\frac{1}{2}v_{\mathrm{c}}$. Then $R(v^2)$ drops to a minimum, $R_{\mathrm{m}} \simeq -0.9876$, at $v \simeq 0.1666$ before rising and vanishing again at $v = v_{\mathrm{R}}$. For larger $v \leqslant 1$ (which is all that is physically relevant) $R(v^2)$ rises increasingly steeply to $R(1) = 1409$. As explained in the introduction, the absence of a term linear in v and this non-monotonic behaviour is quite unlike what is seen in the exact critical polynomials for two-dimensional Ising models which, in addition, remain of magnitude around unity for all $0 \leqslant u, v, w \leqslant 1$. It seems unlikely, therefore, that Rosengren's polynomial can resemble the true critical polynomial (should one exist).

Let us, nonetheless, compare Rosengren's surd with some more recent estimates of v_{c} for the simple cubic Ising lattice. Table 1 lists the deviations from v_{F} of v_{c} estimates adopted in studies by Guttmann [19, 23], Liu and Fisher [20], Ferrenberg and Landau [21] and Baillie and coworkers [23]. The Liu and Fisher series-based value for v_{c} lies significantly below the other estimates. It should be borne in mind, however, that workers using Monte Carlo methods [18, 21, 22] typically quote only 'one-sigma' uncertainties so that one must not be surprised to find the correct value lying at a distance two or three times further from the quoted central estimate. In all the approximate methods, systematic errors are difficult to assess with confidence. However, one sees from table 1 that the Ferrenberg–Landau (FL) estimate is rather close to v_{F}: but, as will now be shown, it is also close to the roots of other polynomials which seem much better candidates for $P_3(u, v, w)$.

3. Plausible critical polynomials

Consider polynomials of the form

$$Q_k(u, v, w; \{p_i\}) = 1 - u - v - w - uv - vw - wu - uvwS_{k-3}(u, v, w; \{p_i\}) \tag{18}$$

for $k \geqslant 2$, where S_l is a symmetric polynomial of degree l (with $S_{-1} \equiv 0$) having rational coefficients p_i. Clearly $Q_k(u, v, w; \{p_i\})$ reduces directly to the appropriate $d = 2$ critical polynomial, $P_2(u, v)$, etc, for all k whenever u, v or w vanish. One may now attempt to choose the p_i so that the closest root to the origin of $Q_k(v, v, v)$ represents an acceptable approximation to v_c; then $Q_k(u, v, w)$ should be a reasonable candidate for $P_3(u, v, w)$. More concretely one might try to select $S_l(\{p_i\})$ so that the closest root is a good approximation to Rosengren's surd, v_R. The form of (18) and the value of v_R virtually ensure the desired monotonic decrease with u, v, and w.

The first non-trivial cases to examine are the cubic approximations for P_3 with $k = 3$ and $S_0 \equiv p_0$. If one could choose p_0 equal to

$$p_{0R} = v_R^{-3} Q_2(v_R, v_R, v_R) \simeq 19.568\,057_4 \tag{19}$$

the root of $Q_3(v, v, v)$ would be *precisely* v_R. Unfortunately p_{0R} is not rational; but merely by multiplying the fractional part of p_{0R} by successive integers and inspecting the products, one can find rational fractions p_0, with relatively small denominators say, q_0, that provide acceptable approximations to p_{0R}. The polynomial $q_0 Q_3(u, v, w; p_0)$ then has integer coefficients and a root approximating v_R.

This process is illustrated in the second section of table 1. Note: (i) the lowest denominator, $q_0 = 7$, yields a value close to the Baillie *et al* (BP) estimate for v_c; (ii) the denominator $q_0 = 37$ leads to a value that is *closer* to the central FL estimate than is v_R! Finally, (iii) the denominator $q_0 = 125$ yields a root differing from v_R by less than 1×10^{-7}.

Of course there is no need to stop at $k = 3$. In light of the sixfold symmetry of the simple cubic lattice and the value of p_{0R}, it is natural for $k = 4$ to try

$$S_1 = p_0 + p_1(u + v + w) \tag{20}$$

with $p_0 = 18$. In analogy to (19) one then finds $p_{1R} \simeq 2.396\,559_9$ and obtains the family of quartic polynomials shown in the third part of table 1: (i) the denominator $q_1 = 5$ yields a root close to the mean of the BP and LF estimates; (iii) $q_1 = 43$ yields a root closer to the LF central value than is v_R; (iii) the root for denominator $q_1 = 58$ differs from v_R by only about 0.7×10^{-8}. On the other hand (iv) the central BP estimate is matched to within 2.5×10^{-8} by $q_1 = 62$: see the last entry in the third part of the table.

If one dislikes large denominators one may examine quintics. To that end keep $p_0 = 18$, adopt $p_1 = 2$ and consider

$$S_2 = p_0 + p_1(u + v + w) + p_2(u^2 + v^2 + w^2 + uv + vu + wv). \tag{21}$$

Then (i) the integral value $p_2 = 1$ generates a root within the range of the Liu–Fisher estimate: see the last section of table 1. Further, (ii) the simple fraction $p_2 = 10/11$ reproduces v_R to within $\Delta v = 2 \times 10^{-8}$.

In sixth order one can take $p_2 = 1$ and write

$$S_3(u, v, w) = S_2(u, v, w) + p_3 C_3(u, v, w) \tag{22}$$

where C_3 is a homogeneous polynomial of degree three. As illustrated already in (10) above, the simple assignment $p_3 = \frac{1}{2}$ and a judicious choice for C_3 with coefficients ± 1, leads to a root differing from v_R by less than 2×10^{-9}. Other, perhaps less appealing choices for $C_3(u, v, w)$ that yield the same result (since $C_3(1, 1, 1) = -5$) are

$$-5uvw, \qquad -(2uvw + u^2 + v^2 + w^2)$$

and

$$4uvw - (u + v + w)(u^2 + v^2 + w^2). \tag{23}$$

If one insists on an integral value for p_3 one could instead take $p_3 = 1$ and try, for example,

$$C_{3a} = uvw - u^3 - v^3 - w^3 \qquad \text{or} \qquad C_{3b} = -(u^3 + v^3 + w^3) \tag{24}$$

but, as shown in (13) above, this entails relatively large deviations of the nearest roots from v_R. On the other hand, at the same order, the integral assignment

$$p_0 = 15 \qquad p_1 = 6 \qquad p_2 = 2 \qquad \text{and} \qquad p_3 = 1 \tag{25}$$

with $C_3(1, 1, 1) = 7$, which can be realized by

$$C_{3c} = uvw + (u + v)w^2 + (v + w)u^2 + (w + u)v^2 \tag{26}$$

yields a root with $\Delta v = -1.603 \times 10^{-6}$: this falls within the FL range (see table 1).

As a final example, the seventh-order polynomial $Q_7(v, v, v)$ constructed with

$$\begin{aligned} S_4 = 18 &+ 2(u + v + w) + uv + vu + wu + 2(u + v)w^2 + 2(v + w)u^2 + 2(w + u)v^2 \\ &+ 2(u + v + w)(uvw + u^3 + v^3 + w^3) \end{aligned} \tag{27}$$

leads to $v_c \simeq 0.218\,098\,687$ which exceeds v_R by only 0.315×10^{-6} and thus once more lies closer to the FL estimate than does v_R (see table 1).

4. Why there may be no critical polynomial

Can one can decide theoretically if the hypothesis that a critical polynomial exists for the simple cubic Ising model with general (u, v, w) is acceptable? To approach this question, suppose J_z and, hence, w is small (while $u, v > 0$). If $p_3(u, v, w)$ exists in the natural form (18) it can be written

$$P_3(u, v, w) = 1 - u - v - uv - wZ(u, v, w) \tag{28}$$

where $Z(u, v, w)$ is a polynomial with leading behaviour $1 + u + v + p_0 uv[1 + O(u, v, w)]$. For convenience let us regard u as a fixed parameter; then it follows from (28) that the critical value $v_c(u, w)$ can be expanded as a Taylor series in powers of w. This seems very reasonable; but is it?

When $J_z = w = 0$, the susceptibility per spin of the $d = 3$ SC lattice must diverge as

$$\chi(u, v, 0) \approx C_+(u)/\tau^{\gamma_2} \tag{29}$$

when the deviation from criticality, defined conveniently as

$$\tau(u, v, w) \equiv v_c(u, w) - v \tag{30}$$

approaches 0 from above: the exponent $\gamma_2 = \frac{7}{4}$ is the well known susceptibility exponent for the $d = 2$ Ising model; $C_+(u)$ is the critical amplitude. (See e.g., [20].) On the other hand, for J_z, $w > 0$ the divergence of $\chi(u, v, w)$ when $\tau \to 0+$ will be controlled by the $d = 3$ exponent $\gamma_3 \simeq 1.238_5$ [20]. If J_z, $w < 0$ the model will represent a metamagnet, ordering, beneath criticality, with ferromagnetic (x, y) lattice layers stacked *anti*ferromagnetically; in this case $\chi(u, v, w)$ will no longer diverge: however, it will exhibit a $\tau^{1-\alpha}$ singularity with $\alpha \simeq 0.10_5$, when $\tau \to 0+$ where $\tau(u, v, -w) = \tau(u, v, w)$ (by the symmetry of the SC Ising model in zero magnetic field under $J_z \to -J_z$).

Said in other words, the model (for fixed u) displays a *bicritical* point in the (v, w) plane at $[v = v_c(u, 0), w = 0]$ at which two distinct critical lines meet [25, 26]. Scaling and renormalization group principles then assert that

$$\chi(u, v, w) \approx C_+(u)\tau_0^{-\gamma_2} X(w/\tau_0^{\phi}) \tag{31}$$

when w and $\tau_0(v) \equiv \tau(u, v, 0)$ become small. Here ϕ is the appropriate *crossover exponent* while the *crossover scaling function* has a normalized expansion

$$X(x) = 1 + X_1 x + \cdots \tag{32}$$

[25–27]. For this *dimensional crossover* the exponent ϕ is known to be $\phi = \gamma_2 = \frac{7}{4}$ [27]; this can be seen quite generally for such a layered Ising lattice by computing $(\partial\chi/\partial w)$ at $w = 0$ and noting that it is proportional to $[\chi(w = 0)]^2 \sim 1/\tau_0^{2\gamma_2}$.

The $d = 3$ divergence for $w > 0$ is normally embodied in the scaling function which varies as

$$X(x) \approx X_c/(x_c - x)^{\gamma_3} \tag{33}$$

when $x \to x_c-$ with $0 < x_c < \infty$ [25, 26]. It follows from this that $(\tau_{0c})^\phi \equiv \tau_0^\phi[v_c(u, w)] \approx w/x_c$ so that the critical locus for small w must vary in *singular* fashion as

$$v_c(u, w) = v_c(u, 0) - (w/x_c)^{4/7} + \cdots. \tag{34}$$

For bicritical points as observed in anisotropic antiferromagnets in a uniform external field, the analogous non-analytic dependence of the critical locus with exponent $1/\phi$ has been verified experimentally [26, 28, 29]. Evidently, the appearance of the power $w^{4/7}$ in (34) is quite inconsistent with the Taylor series expansion for $v_c(u, w)$ implied by the existence of a critical polynomial $P_3(u, v, w)$ as in (28).

It would appear, therefore, that the considerations of the previous section are quite empty! But this is overly pessimistic on at least two scores: first, even if no full critical polynomial $P_3(u, v, w)$ exists, it is possible that there *is* a critical polynomial, say $P_3^{\text{sym}}(v)$, with a root v_c in the *symmetric* case, $u = v = w$; second, the crossover scaling function may embody the γ_3 divergence only in the limit $x_c = \infty$. In that case $\tau_0(v)$ in the scaling form (31) must be replaced by the *nonlinear scaling field*

$$\tilde{\tau}(u, v, w) = \tilde{P}_3(u, v, w) \geqslant 0 \tag{35}$$

where, even if $\tilde{P}_3$ is not a polynomial, it serves the same role as a critical polynomial, being analytic in u, v and w through and above the critical locus $v = v_c$ but vanishing when v approaches v_c. Then, since $\phi = \gamma_2$, the correct $d = 3$ behaviour for $w > 0$ is ensured by

$$X \approx X_\infty x^{(\gamma_3-\gamma_2)/\gamma_2} \qquad \text{as} \qquad x \to +\infty. \tag{36}$$

(It might be remarked parenthetically that even when $x_c < \infty$ and (33) applies, the scaling form (31) holds over a broader range if τ_0 *and* w are replaced by appropriate nonlinear scaling variables $\tilde{\tau}$ and $\tilde{w}$.)

Can one choose between the expected scaling option (31), forbidding a natural critical polynomial like (28), and the special scaling form (36) which allows one? One possibility is that careful numerical studies for small w might be able to detect the presence of a $w^{4/7}$ power provided the critical parameter x_c, is not too large. Beyond that the spherical model [30] should provide some guidance.

Accordingly, consider the spherical model on a d-dimensional hypercubic lattice with couplings

$$J_\lambda = \eta_\lambda J_0 \qquad \text{with} \qquad \eta_0 = 1, \qquad \eta_d = \zeta \tag{37}$$

where $\lambda = 0, 1, \ldots, d$. The critical point is given by [30]

$$\frac{J_0}{k_B T_c} \equiv K_c^d(\{\eta_\lambda\}) = \prod_{\lambda=1}^{d} \int_{-\pi}^{\pi} \frac{d\theta_\lambda}{2\pi} [\Gamma(\theta_1, \ldots, \theta_{d'}) + \zeta\Delta(\theta_d)]^{-1} \tag{38}$$

where $d' \equiv d-1$ while

$$\Gamma = 2\sum_{\lambda=1}^{d-1} \eta_\lambda(1-\cos\theta_\lambda), \qquad \Delta(\theta) = 2(1-\cos\theta). \tag{39}$$

When $\zeta \to 0$ (so J_d vanishes) the lattice decomposes into uncoupled d'-dimensional layers with a critical point given by $K_c^d(\eta_1, \ldots, \eta_{d'})$, where we suppose none of the η_λ vanish for $\lambda \leqslant d'$. Since one has $\Gamma \approx \sum_\lambda^{d'} \eta_\lambda \theta_\lambda^2$ for small θ_λ the integral defining $K_c^{d'}$ converges provided $d' > 2$, which we also suppose.

Now we may write a *formal* Taylor series for $K_c^d(\zeta)$ by expanding $(\Gamma + \zeta\Delta)^{-1}$ in powers of ζ in (38). This yields

$$K_c^d(\zeta) = K_c^{d'} + \sum_{s=1}^{\infty} G_s \zeta^s \tag{40}$$

where the coefficients have the form

$$G_s(\eta_1, \ldots, \eta_{d'}) = (2\pi)^{-d} \int_{-\pi}^{\pi} \Delta^s(\theta)\, \mathrm{d}\theta \prod_{\lambda=1}^{d'} \int \mathrm{d}\theta_\lambda / \Gamma^{s+1}(\theta_1, \ldots, \theta_{d'}). \tag{41}$$

The first integral factor here converges for all s; however, the d'-fold multiple integral diverges at small θ_λ whenever $s \geqslant \frac{1}{2}d - 1$. It follows that for any d, however large, $K_c^d(\zeta)$ does *not* have a Taylor series expansion in powers of ζ. Thus, the spherical model for $d > 2$ cannot have a natural critical polynomial like (28).

For those who prefer a more explicit demonstration, the appendix examines the case $2 < d \leqslant 4$, for which the layer critical behaviour is nonclassical with susceptibility exponent $\gamma_{d'} = 2/(4-d')$ (and a logarithmic factor appearing when $d' = 4$). It is shown that

$$K_c^d(\zeta) = K_c^d(0) - H(\eta_1, \ldots, \eta_{d'})\zeta^{1/\phi} + \cdots \tag{42}$$

where $\phi = \gamma_{d'}$ while the coefficient H is a product of explicit (non-vanishing) integrals: a factor $\ln\zeta$ appears when $d' = 4$. This result is evidently in full accord with the general scaling analysis presented above. This behaviour of the spherical model, which is, of course, just that of the general n-component vector-spin model in the limit $n \to \infty$, thus suggests that the Ising model ($n = 1$) obeys (34) and so does *not* have a natural critical polynomial like (28) in variables analytic in the J_λ.

Nevertheless, one can *still* salvage the possibility of a critical polynomial if, first, one notes that $1/\phi = 4/7$ is *rational* and, second, one relaxes the 'naturalness' assumption embodied in (28)! Specifically, consider the symmetric polynomial of degree 22:

$$\begin{aligned} Q_{22}(u, v, w) = {} & u^4v^4(1-u-v-uv)^7 + v^4w^4(1-v-w-vw)^7 \\ & + w^4u^4(1-w-u-wu)^7 - bu^4v^4w^4 \end{aligned} \tag{43}$$

which vanishes as u, v, $w \to 0$. Note that setting $w = 0$ yields a polynomial in u and v with four many-fold repeated roots, namely, $u = 0$, $v = 0$, and the desired roots of the $d = 2$ critical polynomial $P_2(u, v)$. For simplicity let us take $u = v$ so that $P_2(u, v) = (v - v_0)(v_1 - v)$, with $v_0 = \sqrt{2} - 1 = v_c(w = 0)$ and $v_1 = -(1 + \sqrt{2})$, and attempt to expand about $v_c = v_0$ in powers of w. Equating Q_{22} to zero, rearranging and taking the real seventh root yields

$$1 - 2v - v^2 = (w/v)^{4/7}[bv^4 - 2(1-v-w-vw)^7] \tag{44}$$

whence one directly obtains the expansion

$$v_c(w) = v_0 - c(w/v_0)^{4/7}[1 + \mathrm{O}(w^{4/7})] \tag{45}$$

with, for sufficiently large b, the positive coefficient

$$c = \tfrac{1}{4}\sqrt{2}[bv_0^4 - 2(1-v_0)^7]^{1/7}. \tag{46}$$

Hence, at the cost of sacrificing the nice monotonicity properties of the putative critical polynomial, we have been able to achieve consistency with the singular scaling-law expansion (34).

In conclusion, then, we have been able to propose a goodly number of candidates for the critical polynomial of the simple cubic Ising model supposing that it exists! These 'nice' polynomials reduce appropriately to the exact two-dimensional forms and they approximate the symmetric simple cubic critical point rather well; in addition they have an attractive monotonicity property. It seems likely, however, that such nice polynomials are ruled out by the singularity structure required by the scaling theory of dimensional crossover. If a simple-cubic critical polynomial exists at all, therefore, it probably cannot have all the natural and pleasing features found in the two-dimensional Ising model.

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Appendix. Dimensional crossover in the spherical model

This appendix elucidates the variation of the critical point of a d-dimensional hypercubic spherical model with coupling parameters (37) in the limit that $\zeta = J_d/J_0 \to 0$ for $2 < d' \equiv d-1 \leqslant 4$ [30]. Following the explicit formula (38) consider the derivative

$$\mathrm{D}(\zeta) \equiv \frac{\mathrm{d}K_c^d}{\mathrm{d}\zeta} = -\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta}{2\pi}\Delta(\theta)\prod_{\lambda=1}^{d-1}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_\lambda}{2\pi}[\Gamma + \zeta\Delta(\theta)]^{-2} \tag{A1}$$

and recall that Γ varies as $\sum_{\lambda=1}^{d-1}\eta_\lambda\theta_\lambda^2$ with $\eta_\lambda > 0$. It follows easily that $\mathrm{D}(\zeta) \to \infty$ as $\zeta \to 0+$. Since the divergence arises from small θ_λ we set

$$\sqrt{\eta_\lambda}\theta_\lambda = 2\pi\sqrt{\zeta\Delta(\theta)}\psi_\lambda \qquad (\eta_\lambda > 0) \tag{A2}$$

which, when $\zeta \to 0$, yields

$$\mathrm{D}(\zeta) \approx -\zeta^{(d-5)/2}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta}{2\pi}\Delta^{(d-3)/2}(\theta)\prod_{\lambda=1}^{d-1}\int\frac{\mathrm{d}\psi_\lambda}{\sqrt{\eta_\lambda}}(1+4\pi^2\psi_\lambda^2)^{-2} \tag{A3}$$

where $\psi^2 = \sum_{\lambda=1}^{d-1}\psi_\lambda^2$ while the limits on the ψ_λ integrals are $\pm\sqrt{\eta_\lambda/4\zeta\Delta(\theta)}$.

For $d-1 < 4$ the overall ψ integral converges at ∞ and so one may take $\zeta \to 0$ in the integration limits which then become independent of θ. Since $\Delta(\theta)$ is positive and varies as θ^2, while $d > 3$, the θ integral always converges and cannot vanish. If C_d is the area of a unit sphere in d dimensions we thus obtain

$$\mathrm{D}(\zeta) \approx -C_d I\left(\prod_{\lambda=1}^{d-1}\eta_\lambda^{-1/2}\right)\zeta^{(d-5)/2} \tag{A4}$$

as $\zeta \to 0$, where the coefficient is

$$I = \int_{-\pi}^{\pi}\frac{\mathrm{d}\theta}{2\pi}\Delta^{(d-3)/2}(\theta)\int_0^\infty\frac{\psi^{d-2}\,\mathrm{d}\psi}{(1+4\pi^2\psi^2)^2}. \tag{A5}$$

The observation that $\frac{1}{2}(d-5) = 1/\gamma_{d'} - 1$ and integration with respect to ζ leads to the result (42) with an explicit, non-zero expression for the coefficient H.

In the case $d - 1 = 4$ the ψ integral in (A5) diverges logarithmically at ∞. Then the integration limits in (A5) can no longer be set to ∞; rather, they lead to an upper cutoff in (A5) varying as $\zeta^{-1/2}$ which then leads to a factor $|\ln\zeta|$ in the result (A4) and, correspondingly, in (42).

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