Calculation of the zero-field susceptibility and critical temperature of Ising magnets on the basis of the principle of limit similarity

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A simple analytical approximate method for the calculation of the zero-field susceptibility and the critical temperature for the Ising model is proposed. The analysis is based on the rule of limit correspondence. Assuming that the first three terms of the high-temperature series expansion are known, accurate values for the eight types of lattices are obtained. These values (excepting the honeycomb lattice) differ from those obtained through series extrapolation by 0.8% rms, and generally compare favorably to estimates computed through the heuristic Bishop formula. In connection with an associated percolation problem, a more accurate formula for the critical bond percolation probability is proposed.

I. ASYMPTOTIC SYMMETRY, TWO-SIDED LIMIT CORRESPONDENCE AND THE MONOVARIANT INTERPOLATION

Let us consider the Ising model at an arbitrary regular lattice being D the Euclidean dimensionality and c the first coordination number. Every site $i=1,\ldots,N$ is occupied by one magnetic moment $\mu_i=\mu_0 S_i$, $S_i=\pm 1$.

The Hamiltonian is

$$H_N=-(J/2)\sum_{ij} S_i S_j-\mu_0 H\sum_i S_i \ . \tag{1}$$

The double sum is taken for the nearest neighbors i,j.

Let us introduce the variable y of the temperature T:

$$y=cJ/(k_B T)=T_M/T \ , \tag{2}$$

where

$$T_M=cJ/k_B \tag{3}$$

is the Curie temperature in the Weiss mean-field approximation;[1] the variable B of the magnetic field H,

$$B=\mu_0 H/(k_B T) \ , \tag{4}$$

the variable m of the magnetization,

$$m=\langle S_i\rangle \ , \quad -1<m<1 \ , \tag{5}$$

the variable U of the interaction energy,

$$U=\langle S_i S_j\rangle/2 \ . \tag{6}$$

In these variables the thermodynamic identity is of the form

$$d\Phi=U\,dy-B\,dm \ . \tag{7}$$

For the state functions B and U, we have the high-temperature limit corresponding to noncorrelated spins:

$$\lim_{y\to 0}[B(m,y),U(m,y)]=[B_0(m),U_0(m)] \ . \tag{8}$$

For the one-component (scalar) model (1),

$$B_0(m)=\operatorname{arctanh} m \ , \quad U_0(m)=m^2/2 \ . \tag{9}$$

Following Ref. 2, let us construct dimensionless functions—the thermic one, f, and the caloric one, g:

$$f=(\partial B/\partial B_0)_y \ , \quad g=(\partial U/\partial U_0)_y \ . \tag{10}$$

By construction, in the high-temperature limit, $f=g=$land $f>0$. Moreover, the simple analysis of the low-temperature expansion[3] also shows that $f=g=1$ in the low-temperature limit also.

Thus, the two-sided symmetric asymptotics exists:

$$\forall D,m: \ \lim_{y\to 0}(f,g)=\lim_{y\to\infty}(f,g)=1 \ . \tag{11}$$

By virtue of (11), one can call f,g the two-sided limit correspondence variables.

The mapping of the manifold of the thermodynamic states of the Ising model into the f-g plane forms a set of squares of the same size, 1×1, enumerated essentially by the Euclidean dimensionalities $D=1,2,3,\ldots$. In this connection it turns out that the f-g mappings are monovariant only for the main, exactly solvable, limiting cases and approximations. Namely, they are degenerated into the curves of the form

$$g=G(f): \ G(0)=0, \ G(1)=1, \ G''(f)<0 \ . \tag{12}$$

For example, at the Bethe-Peierls-Guggenheim quasichemical approximation[3-5] it corresponds exactly to a

one-parametric family of straight lines:

$$G(f)=(2/c)f+(c-2)/c \ . \tag{13}$$

As it is known, this approximation interpolates the exact results for a one-dimensional ($c=2$) Ising chain and the Curie-Weiss-Ising model ($c=\infty$), the last corresponding to the mean-field approximation (3) in the real situation.

In particular, the map $D=0$, $c=0$ (ideal magnet) contains one point $f=g=1$, the map $D=1$, $c=2$ contains the squares diagonal $g=f$ and the map $c=\infty$ contains the straight lines $f=0$ and $g=1$.

Generally, (12) is an approximation. By virtue of (11), one can call it a monovariant approximation of the two-sided limit correspondence, or briefly, the monovariant interpolation, $G(f)$ being the monovariant approximant.

II. STATE EQUATION, ZERO-FIELD SUSCEPTIBILITY, AND CRITICAL TEMPERATURE

Let us introduce, according to (8), instead of m, the variable B_0 and the auxiliary function W:

$$W(B_0,y)=B[m(B_0,y)] \ . \tag{14}$$

Then from (7), (9), (10), and (12) one gets for W the Hamiltonian-Jacobi-type equation:

$$\partial W/\partial y-m(B_0)G(\partial W/\partial B_0)=0 \ . \tag{15}$$

This equation has an energy-type first integral associated with a cyclic variable y. It is solved by quadratures. By use of (12), it is convenient represent it in the form

$$y=T_M/T=\int_f^1 G^{-1}(\phi)B_0'[mG(f)/G(\phi)]d\phi/B_0'(0) \ , \tag{16}$$

where, as usual, the prime denotes the derivative. Due to the boundary condition $y=0$ for $f=1$, (16) is valid only in the supercritical region $T>T_c$, $0<y<y_c=T_M/T_c$.

Let f_+ be the inverse zero-field susceptibility K_T with respect to its ideal value κ_{T0}:

$$f_+(y)=\kappa_{T0}/\kappa_T, \quad H=0, \ T>T_c \ . \tag{17}$$

Thus, for $m=0$ it follows from (16) that

$$df_+/dy+G(f_+)=0 \ . \tag{18}$$

Moreover, if $T=T_c$, then

$$y_c=T_M/T_c=\int_0^1 d\phi/G(\phi) \ . \tag{19}$$

From (18) and (19) one gets

$$y_c-y=\int_0^f d\phi/G(\phi) \ . \tag{20}$$

Thus, the calculation of the thermodynamic properties requires the construction of the monovariant approximant $G(f)$.

Some general properties of G follow from critical asymptotics of the susceptibility with amplitude F_+ and critical exponent γ:

$$f_+=F_+[(y-y_c)/y_c]^\gamma \ . \tag{21}$$

From (20), the singular part G_s of G is

$$G_s=G_c f^a \ , \quad a=1-(1/\gamma) \ , \tag{22}$$

and the amplitude is

$$F_+=(G_c y_c/\gamma)^\gamma \ . \tag{23}$$

Completely, G is constructed in the form

$$G=G_s+G_r \ , \quad G_s(1)+G_r(1)=1 \ . \tag{24}$$

In the first approximation $G_r=0$, $G=G_s$, and from (19) and (22)–(24) it follows immediately that

$$F_+=G_c=1, \quad T_c=T_M/\gamma \ . \tag{25}$$

This simple formula improves systematically the mean-field approximation, as γ grows with decrease of D. Thus, G_r is a relatively small correction for G_s. Let us take G_r, generalizing (13), of the form

$$G_r=(1-G_c)f^b \ , \tag{26}$$

where G_c and b have to be founded. Then, from (16) and (19) the susceptibility and the Curie temperature are given by

$$y=\gamma[Y(1)-Y(f)], \quad y_c=\gamma Y(1) \ , \tag{27}$$

$$Y(f)=fG_s^{-1}\sum_n(-G_r/G_s)^n/[n\gamma(b-a)+1] \ . \tag{28}$$

The series in the last formula represents the incomplete B function[6] and converges rapidly because of the small ratio G_r/G_s.

III. CALCULATION OF ZERO-FIELD SUSCEPTIBILITY AND OF THE CURIE TEMPERATURE FOR EIGHT LATTICES

In the one-component case, it follows from (9) and (16) that

$$y=\int_f^1 d\phi\, G(\phi)/[G^2(\phi)-G^2(f)] \ . \tag{29}$$

The values of the parameters G_c and b of the approximations (22), (24), and (26) are obtained by means of the four-term high-temperature expansion of the susceptibility:[1,3,7–13]

$$f_+=1-y+y^2/c+\varepsilon_3 y^3/(3c) \ , \tag{30}$$

$$\varepsilon_3=18n_3/c^2 \ . \tag{31}$$

Here n_3 is the arrangement number for closed triangular graphs on the lattice of given type: $n_3=2$, $\varepsilon_3=4$ for a hexagonal lattice,[7] $n_3=8$, $\epsilon_3=1$ for a face-centered-cubic lattice,[12] and $n_3=0$, $\varepsilon_3=0$ for other analyzed lattice types.

Together with the universal critical exponent $\gamma(D)$, the coefficients of (30) form the minimal set of individual geometric parameters which are necessary for the lattice identification. In this sense, the approximants (25) and (30) are also the minimal ones.

By combining (18), (23), (25), and (30) and equating the

coefficients of the same order in y, one obtains

$$G_c = 1/(1+a_1) ,$$
$$a_1 = 2\gamma^{-2}(1-\varepsilon_{IW})^2/[(1-\varepsilon_3)c-2] , \quad (32)$$

$$b = 2-(1+\gamma\varepsilon_3)/(1+\varepsilon_{IW}) , \quad (33)$$

$$\varepsilon_{IW} = (\gamma-1)[(c/2)-1] . \quad (34)$$

One could see that $\varepsilon_{IW}=0$ for the two basic limited universal classes corresponding to the one-dimensional Ising model ($c=2$) and the Weiss mean-field approximation ($\gamma=1$). Therefore, one can call ϵ_{IW} as the Ising-Weiss parameter. In particular, for $\gamma=1$, $\epsilon_3=0$ one obtains the linear monovariant equation (13) of the quasi-chemical approximation.

The values of y_c computed by (28) are shown in Table I. In the column labeled y_c (HT) the high-temperature extrapolation results are given (for $D=2$, the exact ones). These results are systematized in Ref. 15. The value $\gamma=1.241$ was taken from Refs. 16 and 17. The percent error relative to HT is given in the columns labeled %. The column labeled $y_c(B)$ is commented on in the next section.

The method proposed improves essentially the high-temperature series convergence. In fact, the results obtained using the input data only, or otherwise by solving the equation $f_+(y)=0$ with (30), are incorrect even qualitatively by lack of the y_c (D) dependence.

On the other hand, one can see from Table I that the second (minimal) approximation gives the results with the rms deviation (excepting the honeycomb lattice) of 0.8%. It is three times smaller than that corresponding to the best analytic approximation (41).

As for the zero-field isothermal susceptibility, the result corresponding to (26) and (27) is simplified essentially for the γ rational, in particular, for $\gamma=\frac{7}{4}$ (the exact result for $D=2$) and $\gamma=\frac{5}{4}$ (the best rational approximation of just the HT data). It turns out that in this case the exponents a and b in (25) are rational ones also. It permits ones to express (27) through the elementary functions[18]

$$y = \gamma(1+a_1)^{-1}(m+1)(2n+1)^{-1}y^{m-2n}[I(1)-I(x)] , \quad (35)$$

where

$$\ln x = (\ln f_+)/[\gamma(m+1)] , \quad (36)$$

$$\ln\xi = -(\ln a_1)/(2n+1) , \quad (36a)$$

$$I(x) = (-1)^m \ln(x+\xi) - \sum_{k=0}^{n-1} \cos[r_k(m+1)\pi]\ln(x^2+\xi^2-2x\xi\cos r_k\pi)$$
$$+2\sum_{k=0}^{n-1} \sin[r_k(m+1)\pi]\arctan[(x-\xi\cos r_k\pi)] , \quad 1<m<2n-1, \; r_k=(2k+1)/(2n+1) . \quad (37)$$

TABLE I. The Curie temperature mean-field approximation values, T_M, with respect to the calculated ones, T_c: $y_c = T_M/T_c$. In the column headings D denotes the Euclidean dimension, γ is the critical exponent of the isothermic susceptibility (Refs. 16 and 17), c is the first coordination number. The value of y_c are calculated using (28) and are compared with y_c from the high-temperature series extrapolation (HT) from references "Ref. (HT)", and with the heuristic Bishop (B) formula (41) (Refs. 5 and 19). The errors (%) are given by $[y_c - y(HT)]/y(HT)$ ($[y(B)-y(HT)]/y(HT)$).

D,γ	c	y_c	y_c (HT)	Ref. (HT)	%	y_c (B)	%
2	3	2.0365	1.9750	7	3.11	2.1063	6.65
$\frac{7}{4}$	4	1.7807	1.7629	7	1.01	1.8263	3.60
	6	1.6552	1.6486	7	0.40	1.6479	−0.04
	3	1.7039	1.7212	21	−1.00		
3	4	1.4896	1.4793	21	0.70	1.5294	3.39
1.241	6	1.3137	1.3300	11	−1.22	1.3544	1.83
	8	1.2576	1.2593	11	−0.13	1.2648	0.44
	12	1.2217	1.2250	14	−0.27	1.2162	−0.72

[m should not be confused with the magnetization in (3).] The values of m, n, and the corresponding ones of y_c from (35)–(37) are given in the Table II.

In the important case of the face-centered lattice ($c=12$, $\epsilon_3=1$), for $\gamma=\frac{5}{4}$ one obtains from (34) $\epsilon_{IW}=\frac{5}{4}$, and from (33), $b=1$. In this case (28) represents the logarithm function, and for the zero-field susceptibility one obtains

$$f_\gamma = [\exp(\kappa y_c)-\exp(\kappa y)]^\gamma/[\exp(\kappa y_c)-1]^\gamma , \quad (38)$$

where

TABLE II. The Curie temperature mean-field values with respect to the ones calculated by (35) (the last line). All symbols have the same meaning as in Table I except that m and n are defined by (35)–(37).

D,γ	$2,\frac{7}{4}$			$3,\frac{5}{4}$			
c	3	4	6	3	4	6	8
m	19	3	7	27	11	3	3
n	20	12	7	16	8	4	9
(35)	2.036	1.781	1.655	1.778	1.492	1.318	1.264

$$\kappa=2(\varepsilon_{IW}-1)/(c\gamma)\ ,\quad y_{c\gamma}=\kappa^{-1}\ln(1+\gamma\kappa)\ . \tag{39}$$

For the fcc one obtains

$$y_{\rm fcc}=30\ln\tfrac{25}{24}=1.2247\ . \tag{40}$$

According to Table I, the error is only -0.024%. Out of the fcc, the accuracy of (39) is worse than that of (27) and (28) but better than the quasichemical result [for the last in (39) $\gamma=1$, $\varepsilon_{IW}=0$].

IV. THE CURIE TEMPERATURE AND THE CRITICAL PERCOLATION PROBABILITY

The correlation between the percolation probability and the critical site percolation probability $p_{S,C}$ was established by Bishop[19] (see also Ref. 5) through the heuristic formula

$$T_M/T_c=y_{CB}=[1+(1/p_{SC})]\text{arctanh}p_{SC}\ . \tag{41}$$

The corresponding values of y are presented in the column labeled B (41) of Table I, p_{SC} have being taken from Ref. 5.

On the other hand, the evaluation through (39) shows that the equation

$$y_{CB}=y_{c\gamma}\ ,\quad p_{SC}=f_{B\gamma}(D,c) \tag{42}$$

keeps within the rms error of 1.4% (exepting 7% for the honeycomb lattice). γ being, by the scaling hypothesis, a function of D only (within the universality class considered), (14) and (42) give p_{SC} through the basic geometric lattice parameters.

As for the bond percolation, a similar correlation is known also:[20]

$$p_{bc1}=c^{-1}D/(D-1)\ . \tag{43}$$

Neither correlation of type y_c-p_{bc} was found to be sufficiently accurate. However, by a heuristic search we have arrived at

$$p_{bc2}=1/[1+(c-2)D/4]\ . \tag{44}$$

TABLE III. The critical bond percolation probabilities: $p_{b,c1}$ from (43) (Refs. 5 and 20), $p_{b,c2}$ from (44), $p_{b,ce}$ from Refs. 22 and 23.

D	2			3			
c	3	4	6	4	6	8	12
$p_{b,c1}$	0.667	0.500	0.333	0.375	0.250	0.188	0.125
$p_{b,c2}$	0.667	0.500	0.333	0.400	0.250	0.182	0.118
$p_{b,ce}$	0.653	0.500	0.347	0.388	0.247	0.178	0.119

The values obtained by (43) and (44) and the numerical (or exact) ones, p_{bce},[22,23] are given in Table III. The values obtained by (44) generally compare favorably to estimates made through formula (43).

V. CONCLUSIONS

The proposed monovariant two-sided limit correspondence method belongs to the family of approximation schemes of the type used in Refs. 24 and 25. However, we found that this method is of rather general nature and may be useful for more complicated high-spin or vector models.

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