Linked-cluster series analysis of the Blume-Capel model

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Linked-cluster series have been obtained for the Blume-Capel model in an fcc lattice to the eighth order. We show that the linked-cluster series aided by the standard extrapolation techniques provide an effective method in the study of models which display first-order phase transitions as well as second-order phase transitions. The full phase diagram and the tricritical phenomena have been studied. Results are compared with those of the Monte Carlo simulation and the high-temperature and low-temperature series analysis.

I. INTRODUCTION

The Blume-Capel model[1] which displays a tricritical point in its phase diagram has attracted a lot of attention from research workers. As first pointed out by Griffiths,[2] in a full three-dimensional thermodynamic space three critical lines intersect at the tricritical point. The tricritical phenomena have been shown to be different from the ordinary critical phenomena. In a renormalization-group calculation, Riedel and Wegner[3] showed that the tricritical behavior of a three-dimensional Gaussian model is described by the classical (mean-field) exponents with logarithmic corrections. Tricritical behavior in the metamagnetic transitions of DAG (dysprosium aluminum garnet) (Ref. 4) and $FeCl_2$ (Ref. 5), phase separations of the ^{3}He-^{4}He mixture,[6] and the structural phase transition[7] of NH_4Cl have been extensively studied experimentally.

To calculate the detailed behavior near the tricritical point, the Blume-Capel model is one of very few models which are amenable to such studies. The series-expansion method[8] has been one of the most powerful methods in the study of phase transitions and critical phenomena. It not only can provide accurate critical exponents as the renormalization-group theory does, but also gives the accurate phase diagram for the system. The method has been applied to study the Blume-Capel model with much success.[9,10]

Difficulties, however, have arisen in the determination of the first-order branch of the phase boundary. While the series-expansion method has provided the most accurate estimates of the critical temperature utilizing the strong divergent behavior of certain thermodynamic quantities at the critical point,[8] the same method cannot be applied when the phase transition is of first order. Normally it is then necessary to calculate the free energies of the two phases and to locate the transition point where the free energies are equal. In the series method, Saul, Wortis, and Stauffer[10] (hereafter referred to as SWS) have used the low-temperature and the high-temperature series to estimate the free energies of the two phases, respectively. The intersection of the free energies then determines the transition point. This method gives quite accurate results for the first-order phase boundary when the discontinuity of the order parameter is large but the accuracy is lost as the tricritical point is approached. As SWS pointed out, the line of equal free energy has failed to merge, at the tricritical point and thereafter, with the second-order phase boundary which can be found to a very high accuracy by considering the divergence of the susceptibility function. SWS (Ref. 10), however, have given the most careful and detailed analysis within the limits of the method. Indeed, it is this fine work which gave us the impetus for attempting a different approach.

In this paper we show that the first-order phase boundary can be found accurately, and the tricritical behavior can be explored fully using the linked-cluster series aided by the standard extrapolation techniques. This restores the full availability of the series method in the study of phase transition and critical phenomena. The linked-cluster series-expansion method has been used to generate high-temperature series[11] and to compute the thermodynamic quantities in the "high-density approximation."[12] Extensive reviews have been given by Wortis[11] and Callen.[12] Our use of it in conjunction with the extrapolation techniques[13] enables us to obtain accurate results both in the ordered and the disordered phases. This method has been applied to the Ising model[14] where its relations to the other series found in arbitrary field or with constant magnetization[15] have been discussed.

In the next section we briefly discuss the method applied to the Blume-Capel model. The results of the calculations are presented in Sec. III where comparisons with the Monte Carlo results[16] are also discussed. A conclusion is given in Sec. IV.

II. BLUME-CAPEL MODEL AND THE LINKED-CLUSTER SERIES EXPANSION

The Hamiltonian of the Blume-Capel model[1] is given as

$$H=-J\sum_{\langle i,j\rangle}S_i^zS_j^z+\Delta\sum_i(S_i^z)^2-h\sum_i S_i^z\,, \tag{1}$$

where $S=1$ and the ferromagnetic pair interactions are restricted to nearest-neighbor spin pairs only. The second term gives rise to the zero-field splitting raising the energy of the $S^z=\pm1$ states above the $S^z=0$ state by Δ. The last term represents the Zeeman energy.

In the mean-field approximation the phase transition

remains second order up to a tricritical point at $\Delta/zJ=\frac{2}{3}\ln 2$ ($k_BT/zJ=\frac{1}{3}$) and becomes first order thereafter, but for $\Delta/zJ>\frac{1}{2}$ no phase transition occurs. Here z is the coordination number of the lattice. Two (first-order) "wings" extend out symmetrically along the first-order phase boundary and are bounded by second-order critical lines[17] in the three-dimensional Δ-T-h phase space. Thus three critical lines meet at the tricritical point.

To analyze the model by the linked-cluster series method we first divide the Hamiltonian into two parts. The unperturbed part consists of all the single-ion potentials including an effective-field term which is extracted from the pair-interaction Hamiltonian and is characterized by an effective-field parameter. The rest of the Hamiltonian is treated as a perturbation. We write

$$H=H_0+H_1\ , \tag{2}$$

where

$$H_0=\Delta\sum_i (S_i^z)^2-(h+JzM)\sum_i S_i^z+\tfrac{1}{2}NJzM^2\ , \tag{3}$$

$$H_1=-J\sum_{\langle ij\rangle}(S_i^z-M)(S_j^z-M)\ . \tag{4}$$

In H_0 and H_1 M is a free parameter which can be chosen to minimize the free energy. It can be shown[11,14] that the parameter M so chosen is equal to the self-consistently determined magnetization or the order parameter of the system. Thus, in essence, the perturbation Hamiltonian describes correlations between spin fluctuations.

The free energy of the system per spin can be calculated by the linked-cluster series-expansion method:[11]

$$F=F_0+\Delta F\ , \tag{5}$$

$$-\beta F_0=\frac{1}{N}\ln \mathrm{Tr}\, e^{-\beta H_0}\ , \tag{6}$$

$$-\beta\Delta F=\frac{1}{N}\sum_n \frac{1}{n!}\langle(-\beta H_1)^n\rangle_c\ . \tag{7}$$

In Eq. (7) the angular brackets denote the canonical thermal average over the unperturbed Hamiltonian H_0 and c denotes the cumulant part of the average. Each term in the expansion can be represented by a graph consisting of semi-invariants linked together by the pair-interaction lines. The graphs are the same as those of the Ising model and the semi-invariants are evaluated similarly.[11,14] We shall refer the details to the review of Wortis.[11]

To proceed, *we have chosen an fcc lattice* for the calculations because of the more rapid convergence of the series. We have calculated terms up to the eighth order in the perturbations. The free energy takes the form

$$-\beta F=-\beta F_0+\sum_{n=2}^{\infty} A_n(x,y)(\beta J)^n \tag{8a}$$

with

$$-\beta F_0=\ln[1+e^{-x}(e^y+e^{-y})]-\tfrac{1}{2}\beta JzM^2\ , \tag{8b}$$

where $x=\beta\Delta$ and $y=\beta(h+12JM)$. In fact, the coefficients A_n are finite polynomials of b and c. We find

$$A_n=\frac{1}{2}\sum_{m,p}\frac{1}{n!}\alpha_{mp}^n c^m b^{2p}\ , \tag{9}$$

where

$$b=\frac{e^{-x}(e^y-e^{-y})}{1+e^{-x}(e^y+e^{-y})}\ , \tag{10}$$

$$c=\frac{e^{-x}(e^y+e^{-y})}{1+e^{-x}(e^y+e^{-y})}\ . \tag{11}$$

The coefficients α_{mp}^n are given in Table I up to $n=8$.

It should be recalled that the free energy found is a function of h and T; M is simply a free parameter. The magnetization can be found by taking derivatives of $-\beta F$ with respect to y (or βh). This gives the same equation as $\partial F/\partial M=0$; thus *M is identified as the magnetization* of the system. The series is

$$M=b+\sum_{n=2}^{\infty} B_n(x,y)(\beta J)^n\ , \tag{12}$$

where

$$B_n=\tfrac{1}{2}\sum_{m,p}\frac{1}{n!}\beta_{mp}^n c^m b^{2p+1}\ . \tag{13}$$

The coefficients β_{mp}^n are shown in Table II. The susceptibility χ is given by

$$\chi^{-1}=\chi_0^{-1}-12J\ , \tag{14}$$

where $k_BT\chi_0$ is the second-order derivative of $-\beta F$ with respect to y. The quadrupolar moment and quadrupolar susceptibility can be similarly found by taking derivatives of $-\beta F$ with respect to x,

$$q=\langle(S^z)^2\rangle=-\frac{\partial(-\beta F)}{\partial x} \tag{15}$$

and

$$k_BT\chi^Q=-\frac{\partial q}{\partial\Delta}=\frac{\partial^2(-\beta F)}{\partial x^2}\ . \tag{16}$$

All the series found reduce to the exact high-temperature series[9,10] in the disordered phase when $M=0$ ($h=0$). In the ordered phase the coefficients of the series can be evaluated for given values of x and y. The analysis of the series is presented in the next section.

III. PHASE DIAGRAMS AND TRICRITICAL PHENOMENA

A. Phase diagrams

The phase diagrams in the mean-field approximation are only qualitatively correct. In the series method the second-order phase boundary can be easily and accurately found using the susceptibility series in the disordered phase at $h=0$; the series becomes divergent at the phase transition. This has been found by Oitmaas[9] and SWS.[10] The latter authors[10] have used a longer (twelfth-order) series and have found more accurate results. Our susceptibility series reduces to the SWS high-temperature series in the disordered phase (but of shorter length). It thus provides no new information in this region.

TABLE I. Free-energy series coefficients for an fcc lattice. The coefficients α_{mp}^{n} in Eq. (9) are shown.

N	M/P	0	1	2	3	4	5	6	7	8
2	0	0	0	12						
2	1	0	−24							
2	2	12								
3	0	0	12	48	−48					
3	1	0	−72	144						
3	2	0	−180							
3	3	96								
4	0	0	0	−384	−5184	−3816				
4	1	0	480	12240	15264					
4	2	12	−8064	−19008						
4	3	792	6912							
4	4	756								
5	0	0	12	−8160	−61104	37440	78912			
5	1	0	3960	99360	−139680	−394560				
5	2	0	−26100	269280	761040					
5	3	960	−209520	−686880						
5	4	28800	237600							
5	5	8640								
6	0	0	0	−16008	593280	8729280	13524480	5172480		
6	1	0	9696	−1063440	−24197760	−57551040	−31034880			
6	2	12	292320	21036240	82607040	67443840				
6	3	5400	−5229360	−43367760	−62804160					
6	4	219420	3421440	20603160						
6	5	792720	555120							
6	6	258480								
7	0	0	12	240240	21305256	177239808	7068096	−465696000	−296421120	
7	1	0	34776	−20872656	−354575088	106968960	2519959680	2074947840		
7	2	0	3344796	174489840	−662008536	−5564280960	−5875571520			

TABLE I. (*Continued.*)

N	M/P	0	1	2	3	4	5	6	7	8
7	3	8736	−20 230 560	852 692 400	6 125 021 280	8 553 323 520				
7	4	887 040	−281 300 040	−3 083 179 680	−6 558 753 600					
7	5	17 690 400	413 683 200	2 295 669 600						
7	6	22 317 120	−197 429 400							
7	7	13 426 560								
8	0	0	0	2 643 744	111 847 680	−1 812 117 888	−32 998 017 024	−80 030 393 856	−62 869 201 920	−14 417 282 880
8	1	0	87 168	−88 611 264	4 411 532 160	106 512 344 064	367 014 606 336	388 987 764 480	115 338 263 040	
8	2	12	20 248 704	−2 603 192 256	−117 433 628 928	−604 271 549 952	−902 342 730 240	−356 532 019 200		
8	3	36 792	291 162 816	48 061 258 560	417 309 653 376	955 101 127 680	528 401 180 160			
8	4	5 423 796	−6 038 807 040	−96 710 271 840	−423 206 864 640	−362 148 433 920				
8	5	165 730 320	−1 392 068 160	34 152 814 080	66 848 302 080					
8	6	1 040 397 120	7 205 345 280	27 477 636 480						
8	7	839 129 760	−5 190 998 400							
8	8	787 653 720								

To determine the first-order phase boundary, it is necessary to find the free energies of the ordered and the disordered phases. This can be done by using the linked-cluster series for the free energy. The order parameter M in the series is equal to zero in the disordered phase while in the ordered phase it should be found self-consistently from the series for the magnetization. This can be done by considering[14,15] the divergence of the series $S/(M-S)$ where S is the series for the magnetization as shown in Eq. (12). Writing $M=y/(12\beta J)$, we can evaluate the coefficients of the series at fixed values of x and y. The series diverges at $M=S$ as intended. As discussed in Refs. 14 and 15, this series reduces to the susceptibility series as M approaches zero. Thus M vanishes at and above the critical temperature determined by the susceptibility series when the phase transition is of second order. We have determined the magnetization by the standard ratio method.[8] The Neville tables[8,18] have been constructed to aid the estimates. With the eighth-order series it appears that the best estimate is given by the average of the last two second Neville extrapolants, l_7^2 and l_8^2, where

$$l_n^m \equiv \frac{1}{m}[nl_n^{m-1} - (n-m)l_{n-1}^{m-1}] \tag{17}$$

and

$$l_n^0 = C_n/C_{n-1} \tag{18}$$

C_n are the coefficients of the series. This is substantiated to some extent by the analysis of the disordered-phase susceptibility; the phase-transition temperature so obtained differs from the values of the twelfth-order series results of SWS (Ref. 10) by only one part in a thousand. The spread in the values of the selected Neville table elements are taken to estimate the uncertainties of the results. We have also performed the Padé analysis[19] (with fixed values of x and y) on the logarithmic derivative of the series $M-S$. From these analyses we believe that for $M \geq 0.5$, T/T_c is reliable to within 1%. The accuracy tends to improve as the tricritical value of x is approached (see discussion on tricritical behavior of magnetization).

To locate the first-order phase boundary we make estimates of the differences in the free energies of the ordered and disordered phases using the Padé approximants method.[19] The phase transitions are then located where the approximants vanish. It should be noted that in the calculation of ordered-phase free energy the term $\frac{1}{2}JzM^2$ in Eq. (3) should be rewritten as $y^2/(2\beta^2 Jz)$ because the value y instead of M is fixed in the analysis. We therefore have multiplied the series for the free-energy difference by $\beta^2 Jz$. This yields a series of ninth order in βJ for the Padé analysis. Table III shows data of the phase boundary given by the [4/4], [4/5], and [5/4] Padé approximants (using the notation of Ref. 19). The uncertainties in the estimate of the phase boundary have been evaluated by considering (1) the uncertainty in the estimate of the magnetization and its effects to the phase-boundary data, and (2) the consistency of the phase-boundary data as shown in Table III.

The first-order phase boundary is traced in Fig. 1 in a dashed curve with error bars on some representative points. The tricritical point is estimated at $k_B T/12J$

TABLE II. Magnetization series coefficients for an fcc lattice. The coefficients β^n_{mp} in Eq. (13) are shown.

N	M/P	0	1	2	3	4	5	6	7	8
2	0	0	−24	−48						
2	1	24	120							
2	2	−72								
3	0	0	−96	−48	288					
3	1	24	48	−1008						
3	2	144	1296							
3	3	−648								
4	0	0	480	13 776	46 368	30 528				
4	1	24	−19 104	−130 320	−137 376					
4	2	3312	101 952	205 632						
4	3	−15 480	−110 592							
4	4	10 800								
5	0	0	3936	132 000	226 944	−694 080	−789 120			
5	1	24	−96 720	−324 864	2 799 360	4 340 160				
5	2	10 800	−126 720	−4 514 400	−9 244 800					
5	3	60 120	3 075 120	9 374 400						
5	4	−491 040	−4 173 120							
5	5	432 000								
6	0	0	9696	−999 408	−27 757 440	−127 385 280	−166 279 680	−62 069 760		
6	1	24	491 520	50 949 360	404 432 640	788 091 840	403 453 440			
6	2	35 568	−21 111 120	−401 507 280	−1 309 677 120	−984 787 200				
6	3	1 446 120	123 977 520	881 629 200	1 104 788 160					
6	4	−7 372 800	−191 224 080	−541 650 240						
6	5	4 430 160	78 526 800							
6	6	−440 640								
7	0	0	34 752	−21 833 616	−482 406 624	−1 310 949 504	2 449 278 720	7 663 299 840	4 149 895 680	
7	1	24	7 546 224	581 174 496	2 575 927 008	−12 020 601 600	−45 059 051 520	−31 124 217 600		
7	2	95 760	−157 561 488	−616 312 368	24 526 883 808	106 502 376 960	95 406 232 320			
7	3	10 211 544	−326 088 000	−22 273 616 736	−125 874 453 600	−152 842 273 920				

TABLE II. (*Continued.*)

N	M/P	0	1	2	3	4	5	6	7	8
7	4	44 442 720	7 166 985 840	72 893 913 120	134 014 124 160					
7	5	−517 149 360	−16 413 077 520	−60 013 548 000						
7	6	787 449 600	10 762 113 600							
7	7	−488 844 720								
8	0	0	87 168	−99 186 240	374 044 608 0	121 009 287 168	696 994 776 567	1 349 352 490 752	995 507 089 920	230 676 526 080
8	1	24	50 810 880	−4 092 242 112	−280 244 926 080	−2 497 134 366 720	−6 802 210 856 448	−6 650 073 803 520	−1 960 750 471 680	
8	2	284 688	438 048 576	186 272 122 176	3 043 496 744 064	12 578 164 945 920	17 081 169 477 120	6 606 183 951 360		
8	3	62 082 216	−36 023 811 264	−1 427 871 670 848	−10 282 786 738 560	−20 978 133 442 560	−11 147 599 572 480			
8	4	1 389 282 048	221 517 535 680	3 448 304 165 376	12 207 119 178 240	9 629 793 008 640				
8	5	−6 663 882 960	−333 864 538 560	−2 681 750 695 680	−3 632 518 794 240					
8	6	−3 152 610 720	42 631 505 280	126 313 447 680						
8	7	14 838 012 000	156 629 531 520							
8	8	−16 683 226 560								

TABLE III. Phase-boundary data. A series representing the free-energy difference of the ordered and disordered phases has been analyzed by the Padé-approximant method. The transition temperatures are obtained when the approximants vanish. The results from the three Padé approximants [4/4], [4/5], and [5/4] are listed (see text for the determination of magnetization in the ordered phase). An asterisk shows no satisfactory result found in the analysis.

$\Delta/(12J)$	[4/4] $kT/(12J)$	[4/5] $kT/(12J)$	[5/4] $kT/(12J)$
0.468	0.2764	0.2764	0.2764
0.469	0.2721	0.2721	0.2721
0.470	0.2670	0.2670	*
0.471	*	*	*
0.472	0.2501	0.2538	0.2565
0.4725	0.2517	0.2530	0.2518
0.473	0.2496	0.2496	0.2495
0.4735	0.2476	0.2473	0.2471
0.474	0.2456	0.2450	0.2446
0.475	0.2408	0.2400	0.2400
0.476	0.2350	0.2355	0.2355
0.477	0.2295	0.2313	0.2312
0.478	0.2251	0.2272	0.2269
0.480	0.2173	0.2186	0.2183
0.4825	0.2075	0.2079	0.2078
0.485	0.1973	0.1973	0.1973
0.491	0.1700	0.1700	0.1700

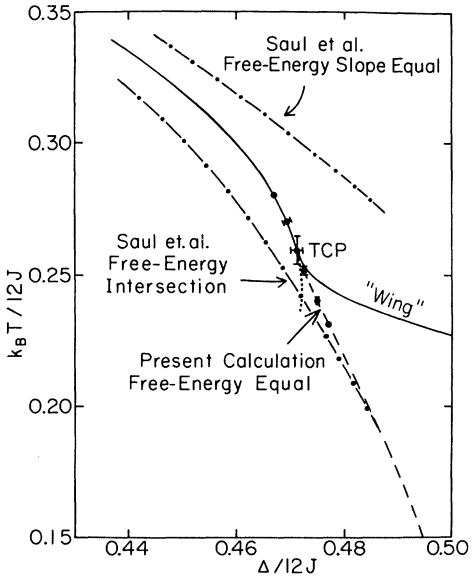

FIG. 1. Phase diagram in the Δ-T plane near the tricritical point. The first-order phase boundary found in the present calculation is drawn in dashed lines with the apparent extrapolation uncertainties shown. The free-energy intersections and free-energy slope-equal points, obtained by SWS using the high-temperature and the low-temperature series, are shown in dashed-dotted lines. In addition, the second-order phase boundary is shown in solid lines. The tricritical point is indicated by TCP. The projection of the wing boundary is drawn in solid lines with the label wing.

$=0.259\pm0.008$ and $\Delta/12J=0.471\pm0.001$ where the first-order phase boundary ends and meets the second-order phase boundary. As expected at the tricritical point and thereafter the line of equal free energy *coincides* with the second-order phase boundary determined independently by the divergence of the susceptibility. We note that the "dip" in the first-order phase boundary below the tricritical point is much less pronounced than that shown in the mean-field approximation.

An alternative and perhaps more accurate method of locating the tricritical point is to examine the behavior of the magnetization near the phase transition. This is because there is only one source of errors (i.e., from the estimate of the magnetization) that would contribute to the uncertainty in the result. It is typical that the magnetization becomes a multiple-valued function at temperatures close to the transition for a system which undergoes a first-order phase transition. Indeed, this happens as soon as Δ exceeds its tricritical value. The bulging of the magnetization curve is very evident for Δ only slightly greater than the tricritical value. We found the tricritical point at $k_BT/12J=0.258\pm0.002$ and $\Delta/12J=0.4713\pm0.001$. These values lie between the values found by SWS using the high-temperature series[10] ($k_BT=0.2615\pm0.007$, $\Delta/12J=0.4716\pm0.001$) and by Jain and Landau ($k_BT=0.256\pm0.002$, $\Delta/12J=0.471\pm0.004$) in the Monte Carlo method.[16]

In the full three-dimensional Δ-T-h space two wings which are first-order surfaces extend out symmetrically along the first-order line (in the Δ-T plane) and are bounded by second-order lines. For a fixed value of $x=\beta\Delta$ greater than the tricritical value, the magnetization becomes a single-valued function of T only when the value of βh becomes equal to or greater than its value on the wing boundary. This of course reflects the fact that the wing surfaces are of first order. To locate the wing boundary, we fix a value of x (greater than its tricritical value) and for each value of y we find values of T and βh at which the susceptibility diverges (using the Neville-ratio method). Since the susceptibility will not diverge when βh exceeds its value on the wing boundary, the wing boundary is located where T and βh attain their maximum values. To state it in another way, the method finds the minimum value of βh (at fixed x) such that the susceptibility would always remain finite. The results are collected in Table IV and drawn in Fig. 1 with a solid line labeled wing.

The quadrupole moment variable $X=1-\langle(S^z)^2\rangle$ is the "nonordering" parameter. It is of interest because it is the spin analog of the fractional concentration of ^{3}He in the ^{3}He-^{4}He mixtures.[17] We have estimated the value of X in both the ordered and the disordered phases using the Padé approximants method.[19] The phase diagram in the (T,X) space is shown in Fig. 2 where the high-temperature and low-temperature series estimates[10] and the Monte Carlo results[16] are also shown for comparison. It is clear that the low-temperature estimates[10] of SWS are in disagreement with the other calculations. Our results, however, are consistent with the conjecture of SWS.[10] While our results agree quite well with the Monte Carlo values in general, they depart from each other near the tricritical point. The discrepancies could have come partly from the somewhat slow convergence of the series for X and perhaps partly from the size effects of the Monte Carlo simulation.

TABLE IV. Wing critical end points. Employing the susceptibility and magnetization series in a finite field the boundaries of the wings in the $\Delta-h-T$ space are found. See text for the details.

$\beta\Delta$	$T/(12J)$	$\Delta/(12J)$	$\pm h/(12J)$	$\pm M$
1.85	0.255	0.472	5.1×10^{-5}	0.18
1.88	0.2516	0.473	3.47×10^{-4}	0.24
1.9	0.250	0.474	6.8×10^{-4}	0.27
2.0	0.241	0.481	3.8×10^{-3}	0.33
2.1	0.233	0.490	9.2×10^{-3}	0.37
2.2	0.227	0.500	1.66×10^{-2}	0.40
2.4	0.219	0.526	3.7×10^{-2}	0.43
2.8	0.211	0.590	9.5×10^{-2}	0.47
3.2	0.207	0.662	1.65×10^{-2}	0.49
4.5	0.204	0.920	4.2×10^{-2}	0.50

B. Tricritical phenomena

The tricritical behavior has been investigated extensively by SWS (Ref. 10) and Jain and Landau.[16] The former authors have also examined the crossover phenomena from the critical region to the tricritical region using the high-temperature series. As mentioned, our series reduce to the high-temperature series in the disordered phase but can be used to explore the ordered phase as well. We shall concentrate on the latter aspect of the series in its application to examine the tricritical phenomena, especially those not yet obtained in the conventional high-temperature and low-temperature series treatments.

We first show the tricritical behavior of the order parameter M. Taking a tricritical path $\beta\Delta=1.826$ we calculate M using the magnetization series by the ratio method

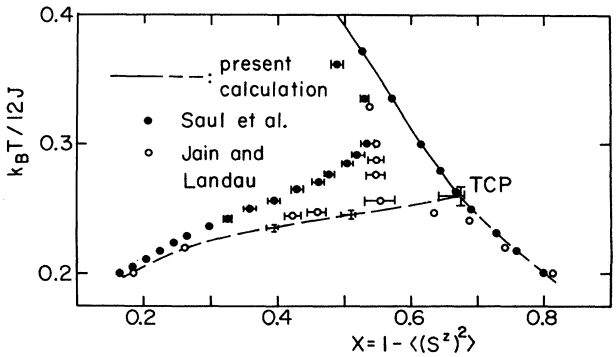

FIG. 2. Phase diagram in the X-T plane near the tricritical point. The first-order and second-order phase boundaries are drawn in dashed and solid lines with some error bars shown. The closed circles represent results of SWS calculation using the high-temperature series and the low-temperature series. The open circles show data of Monte Carlo simulation. The results of present calculations agree quite well with the Monte Carlo simulation but they depart from each other in the vicinity of the tricritical point.

as discussed above. The results are shown in Fig. 3 in circles. The uncertainties are believed to be smaller than the size of the circles shown unless they are indicated by error bars. The prediction of the renormalization-group analysis,[3] $M=A\,|\,t\ln t\,|^{1/4}$ ($t=1-T/T_t$, T_t as the tricritical temperature), is drawn in a solid line, while the classical behavior, $M\propto t^{1/4}$, is shown in a dashed line. The logarithmic correction[3] to the classical behavior has manifested itself evidently in this calculation. We find $A_\beta^t=1.19\pm0.02$. A similar conclusion has also been reached in the Monte Carlo simulation[16] but our series method allows the temperature to approach more closely to the tricritical point without loss of accuracy. The mean-field results are also shown for comparison.

At the tricritical temperature, the field dependence of M is given by a power law,

$$\beta h=A_\delta^t M^{\delta_t}\ . \tag{19}$$

Following Gaunt and Baker[15] we have estimated the values of δ_M^* defined as $\ln(\beta h)/\ln(M)$ at the tricritical temperature. The extrapolation of δ_M^* to $\beta h=0$ for $0.6<M<0.9$ finds $\delta_t=5.2\pm0.4$, $A_\delta^t=0.42\pm0.02$ in agreement with results obtained by the low-temperature series[10] and the Monte Carlo simulation.[16]

The discontinuity in the order parameter across the first-order phase boundary as the tricritical point is approached should behave as[3,20]

$$\Delta M=A_\beta^u t^{\beta_u}\ . \tag{20}$$

The low-temperature series[10] gave $\beta_u=0.2$ which is at variance with the predicted values 0.5. Our series results are shown in Fig. 4 where the log-log plot of ΔM vs t is made. The slope of the plot gives the value of β_u and it is seen that the slope starts with the value ~0.25 away from the tricritical point but becomes consistent with the value 0.5 as the tricritical point is approached. This is in good agreement with the results of Monte Carlo simulation.[16] The value of A_β^u which we found is 1.9 ± 0.2. For comparison the Monte Carlo method[16] yields $A_\beta^u=2.2\pm0.2$.

The discontinuity of the quadrupole moments on X across the first-order phase-transition boundary behaves similarly as the tricritical point is approached:

$$\Delta X=A_\omega^u t^{\omega_u}\ . \tag{21}$$

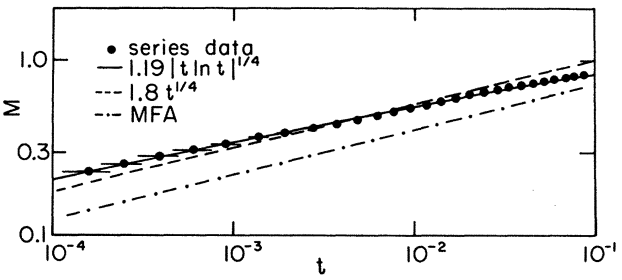

FIG. 3. Tricritical behavior of the ordering parameter M in temperature along a tricritical path $\beta\Delta=1.826$. To show the logarithmic correction to the classical behavior, a solid line $\sim|\,t\ln t\,|^{1/4}$ and a dashed line $\sim t^{1/4}$ are drawn. The mean-field results are also included (in dashed-dotted line) for comparison.

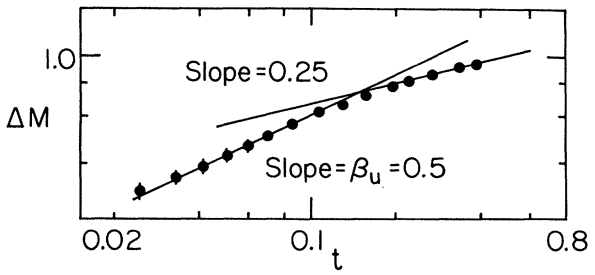

FIG. 4. Log-log plot of ΔM vs t. The discontinuity of the ordering parameter M across the first-order phase boundary near the tricritical point is plotted against the reduced temperature $1-T/T_t$ where T_t is the tricritical temperature. The slope which gives the value of β_u is seen changing from ~0.25 to 0.5 as T_t is approached.

As discussed earlier X has been estimated by the Padé-approximants[19] method. We show the log-log plot of ΔX vs t in Fig. 5. It is evident that ω_u is consistent with the value 1.0 as predicted.[3] This is in agreement with the Monte Carlo[16] finding. A_ω^u is found as 3.6 ± 0.3 which agrees with the Monte Carlo value 3.9 ± 0.3 within the uncertainties.

Finally, the shape of the wing critical line as it approaches the tricritical point is expected, according to the scaling theory,[21] as

$$k_B(T_t-T_c)/12J=A(h_c/12J)^\rho\ . \tag{22}$$

The log-log plot of (T_t-T_c) vs h_c is shown in Fig. 6. In the figure a wide range (10^{-5}—10^{-1}) of h_c is included. ρ is equal to $\frac{2}{5}$ to a very high accuracy. We find $\rho=0.40\pm0.02$. The Monte Carlo simulation[16] has given similar results but with less accuracy. The value of a is found as 0.16 ± 0.02.

IV. CONCLUSIONS

We have shown that the linked-cluster series-expansion method is a very valuable tool in the theoretical study of a

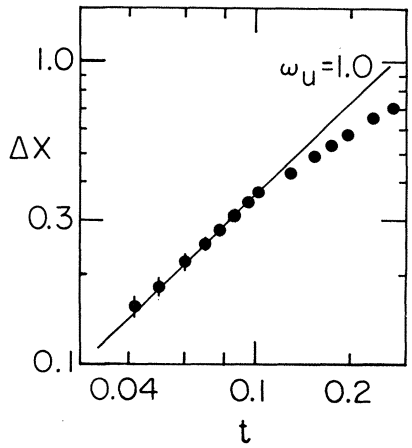

FIG. 5. Log-log plot of ΔX vs t. The discontinuity of the nonordering parameter $X=1-\langle(S^z)^2\rangle$ is plotted against the reduced temperature $t=1-T/T_t$. The slope ω_u [Eq. (21)] is consistent with the value 1.0 as predicted.

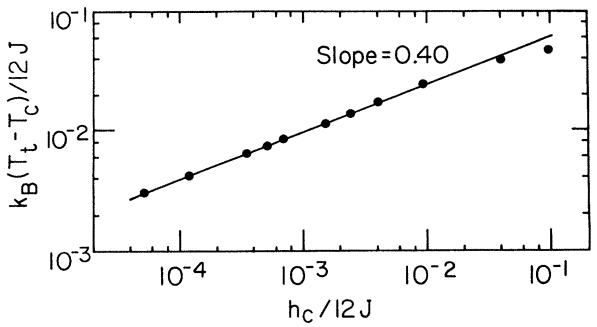

FIG. 6. Log-log plot of $(T_t - T_c)$ vs h_c. The shape of the wing boundary given by Eq. (22) is confirmed in this plot with the exponent $\rho = \frac{2}{5}$ to a very high accuracy over a wide range of h_c.

model which displays complicated phase-transition behavior. Successive applications of the method to the study of the Blume-Capel model have been reported in this paper. The use of the method to study the Blume-Emery-Griffiths model will be reported elsewhere.

The linked-cluster series-expansion method treats the single-ion potentials exactly. It is the most effective technique to generate the high-temperature series for systems with single-ion anisotropy of arbitrary strength which are essential for high-precision analysis of real (physical) magnetic systems. Its application in the ordered phase is one of very few methods which allow the physical quantities in the ordered phase to be estimated with high accuracy.

The linked-cluster series-expansion method can be applied to quantum spin systems with single-ion anisotropy. While the computation is complicated by the noncommutivity of the operators and the integrals of the ordered products, the introduction of standard basis operators has made the calculations feasible.[22,23] Much effort is needed to develop the method for higher-order calculations and for more complicated physical systems.

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