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Susceptibility Expansion for Classical Scalar Models*

J. P. Van Dyke and William J. Camp
Sandia Laboratories, Albuquerque, New Mexico 87115
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We present high-temperature series through tenth order for the susceptibility of *all* classical scalar models with bilinear nearest-neighbor interactions in the absence of symmetry-breaking fields. As an example of the use of these results we examine the tricritical behavior of triple-well Landau-Wilson models which interpolate between the Blume-Capel and Riedel-Wegner models. The general series are given for the fcc, bcc, and simple cubic lattices.

We have derived new tenth-order, high-temperature series for the susceptibility tensor χ of a broad class of classical lattice models, and present *in closed form* the series coefficients for the subclass of models with scalar order parameter on the three cubic lattices. We believe that these results represent a breakthrough of fundamental importance. All previous treatments[1] have involved numerically deriving the series for a single model at a time; and many specialized techniques which have been used to obtain series of useful length apply only to limited classes of models (e.g., models for which all articulated diagrams and/or diagrams with multiple bonds are absent from the linked-cluster expansion[1]). We know of no prior method which produces series of comparable length for as broad a class of models as is encompassed by our method. In addition to its generality, our method has the advantage that the linked-cluster expansion is obtained *formally* (through tenth order) for *all* models at once. Thus we obtain *analytical* expressions for the series coefficients for all models of a given class. The fact that we obtain the series coefficients analytically rather than numerically makes it particularly easy to study the dependence of critical-point properties on parameters entering the Hamiltonian, to map out universality classes, to investigate crossover behavior near unstable fixed points, and to make direct contact with the renormalization-group approach to critical phenomena.[2]

The models to which our results are applicable include *all* classical models with Hamiltonians of the form

$$-\frac{\mathcal{H}}{kT}=\sum_{\vec{r}}W[S(\vec{r})]+\frac{1}{2}\frac{J}{kT}\sum_{\vec{r}}\sum_{\vec{\delta}}S(\vec{r})\cdot S(\vec{r}+\vec{\delta}). \quad (1)$$

Here, $S(\vec{r})$ is a scalar, m-component vector, or $n\times n$ tensor variable with discrete or continuous (but even) domain, J is the exchange energy, the sums over $\vec{r}$ and $\vec{\delta}$ extend over all nearest-neighbor pairs of lattice sites, W is an even function of the components of S, and $S(\vec{r})\cdot S(\vec{r}+\vec{\delta})$ is the (most generally, weighted) inner product of $S(\vec{r})$ and $S(\vec{r}+\vec{\delta})$. There are several familiar cases to which these results apply, including (i) scalar models—the spin-S Ising models,[3] the Blume-Capel model,[4] and the one-component Landau-Wilson continuous-spin models[2]; and (ii) vector models—the anisotropic Heisenberg and planar Heisenberg models[5] and the m-component Landau-Wilson models.[2] As an example of the usefulness and generality of these results, we analyze below the loci of tricritical points of a particular class of scalar Landau-Wilson models which interpolate between the Blume-Capel[4] and Riedel-Wegner models.[6] Less familar applications of these results also include lattice models for liquid crystals with tensor order parameters,[7] and classical phonon models for displacive and order-disorder structural phase transitions.[8]

The series for χ were obtained by first solving for the outer-product correlation function, $G(\vec{R}) = \langle S(\vec{r}) * S(\vec{r}+\vec{R})\rangle$, and then using the fluctuation theorem to obtain the reduced susceptibility tensor $\chi = \sum_{\vec{r}} G(\vec{R})$. To obtain the series for $G(\vec{R})$, we employed the excluded-volume linked-cluster expansion[9] in a generalized Stanley-Kaplan recursive form.[10] The uniqueness of our treatment lies in the fact that we do not reperform the expansion for each new model and lattice, but rather incorporate the particular lattice and class of models (which are specified by sets of lattice constants and graph weights, respectively[9]) with the previously calculated (through tenth order) formal structure of the linked-cluster expansion. Since the lattice constants need only be evaluated once for a given lattice, we ultimately only need to specify the set of graph weights appropriate to a given class of models.

For models with a scalar order parameter, a further significant simplification obtains. Namely, the weight associated with any graph is obtained as a finite sum of finite products of "bare-vertex weights." This enables us—for each lattice—to obtain the series coefficients analytically as polynomials of these bare-vertex weights. The primary purpose of this publication is to present the results for scalar models in a form which can be used by the reader for any model within the class and for any of the cubic lattices.[11] Full details will be published elsewhere.

In Table I we present the susceptibility series for all scalar models of the form in Eq. (1). To explain the use of these results we first define the bare-vertex weights, I_{2l}, by

$$I_{2l} = \mathrm{Tr}(S^{2l} e^{W[S]})/\mathrm{Tr}(e^{W[S]}). \tag{2}$$

Thus I_{2l} is the average of the $2l$th power of S with respect to the potential well $W[S]$. Here the trace operation indicates the sum (or integral) over the domain of definition of S. We can now discuss Table I. The results are tabulated in each order for all three lattices at once. That is, the order $1, 2, \ldots, 10$ is specified, followed by a table of data describing the coefficient of that order for the three lattices. The numbers $(m_2, m_4, m_6, m_8, m_{10}, m_{12})$ in parentheses at the start of each line represent a product of vertex weights:

$$(m_2, m_4, m_6, m_8, m_{10}, m_{12}) \to \prod_{l=1}^{6} (I_{2l})^{m_{2l}}. \tag{3}$$

(Through eighth order, only $m_2, \ldots, m_{10}$ are listed since $m_{12} \equiv 0$.) The three numbers following $(m_2, \ldots, m_{12})$ in a given line are the factors multiplying that particular product in Nth order for the simple cubic (sc), bcc, and fcc lattices, respectively. If we denote such a factor as $F_L{}^N(m_2, \ldots, m_{12})$, where N is the order and L (= sc, bcc, and fcc) is the lattice, we write the coefficient $\chi_N(L)$ of $(J/kT)^N$ on lattice L as[12]

$$(N!)\chi_N(L) = \sum_{\{m_2, \ldots, m_{12}\}} F_L{}^N(m_2, \ldots, m_{12}) \prod_{l=1}^{6} (I_{2l})^{m_{2l}}. \tag{4}$$

For example we can write $\chi_3(\mathrm{sc})$ as

$$\chi_3(\mathrm{sc}) = \tfrac{1}{6}[180(I_2)^2 I_4 + 702(I_2)^4 + 6(I_4)^2]. \tag{5}$$

The zeroth-order coefficient $\chi_0(L)$ equals I_2 for all lattices, L.

As an example of the use of these series, we examine the loci of Gaussian tricritical points for the triple-well continuous-spin model on the fcc lattice,

$$W[S] = -[AS^2(S^2-1)^2 + \Delta_n S^{2n}] \tag{6}$$

with $n = 1$, 2, and 3. For this model the vertex weights are given by

$$I_{2l} = \int_{-\infty}^{\infty} dS\, S^{2l} e^{W[S]} \Big/ \int_{-\infty}^{\infty} dS\, e^{W[S]}. \tag{7}$$

By numerically integrating Eq. (7) and using Table I we readily obtain the series coefficients for given A, n, and Δ_n. In the limit as $A \to \infty$ with Δ_n finite this model becomes the Blume-Capel $S=1$ model for tricritical phenomena[4] (independent of n). For the particular value of $\Delta_n = -\ln 2$ the model reduces to the $S=1$ Ising model. Here Δ_n plays the role of a nonordering field in the theory of tricritical phenomena.[4,6] Analysis of the series shows that for $\Delta_n < \Delta_{n,t}$ the system is Ising-like, i.e., χ diverges like $\chi_0/(K_c - K)^\gamma$ with $\gamma = 1.25$. As $\Delta_n \to \Delta_{n,t}$ the system crosses over[6] from Ising to tricritical behavior; and, exactly at the tricritical value $\Delta_{n,t}$ of the nonordering field, the susceptibility divergence is characterized by the Gaussian exponent $\gamma = 1$, i.e., $\chi \sim \chi_t/(K_t - K)$ (to within logarithmic terms[6]). For $\Delta_n > \Delta_{n,t}$ the transition is first order.[4,6] For finite A, $S^2 \neq S^4 \neq S^6$, so that the behavior of the $n=1$, 2, and 3 models can be expected to differ. In fact we shall see that only the $n=1$ model exhibits tricritical behavior at small A (the limit $A \approx 0$ corresponds to the Riedel-Wegner model[6]), the $n=2$ and $n=3$ models being Ising-like for all $\Delta_n > 0$ at small enough A.

Herein, we accept the Gaussian nature of the tricritical point, and use the crossover to $\gamma = 1$ to identify $\Delta_{n,t}$. As pointed out in Ref. 4, this provides the most accurate method of finding $\Delta_{n,t}$ and K_t $[=K_c(\Delta_{n,t})]$. In Fig. 1(a) we present the

TABLE I. Susceptibility series for scalar model, as described in text.

	sc	bcc	fcc
--- 1---			
(2,0,0,0,0)	6	8	12
--- 2---			
(1,1,0,0,0)	6	8	12
(3,0,0,0,0)	54	104	252
--- 3---			
(2,1,0,0,0)	180	336	936
(4,0,0,0,0)	702	1992	7452
(0,2,0,0,0)	6	8	12
--- 4---			
(0,1,1,0,0)	6	8	12
(1,2,0,0,0)	414	776	2412
(3,1,0,0,0)	4662	13368	61380
(5,0,0,0,0)	11772	48336	285336
(2,0,1,0,0)	90	168	396
--- 5---			
(1,1,1,0,0)	900	1680	4920
(2,2,0,0,0)	22950	62760	330300
(4,1,0,0,0)	127440	558240	4113360
(6,0,0,0,0)	248400	1464000	13461120
(0,3,0,0,0)	0	0	1920
(3,0,1,0,0)	3600	10080	54000
(0,0,2,0,0)	6	8	12
--- 6---			
(0,0,1,1,0)	6	8	12
(1,0,2,0,0)	804	1504	4992
(1,3,0,0,0)	37710	109320	814140
(3,2,0,0,0)	1013580	4321200	38494440
(2,1,1,0,0)	64440	178560	1029600
(5,1,0,0,0)	3931200	25328880	297651240
(7,0,0,0,0)	6162480	52430400	755917920
(1,1,0,1,0)	450	840	1980
(4,0,1,0,0)	128880	602640	5382360
(0,2,1,0,0)	1050	1960	12540
(3,0,0,1,0)	1800	5040	19800
--- 7---			
(1,0,1,1,0)	1680	3136	9408
(2,0,2,0,0)	85092	230832	1325352
(2,3,0,0,0)	3996720	16813440	196857360
(4,2,0,0,0)	44963100	295100400	4262970600
(3,1,1,0,0)	3767400	16070880	162524880
(6,1,0,0,0)	135898560	1274353920	23643627840
(8,0,0,0,0)	178230780	2191185360	49256038440
(0,1,2,0,0)	0	0	27888
(0,2,0,1,0)	2100	3920	12600
(1,2,1,0,0)	188160	519680	5886720
(5,0,1,0,0)	4415040	33183360	502649280
(2,1,0,1,0)	50400	141120	806400
(0,4,0,0,0)	43890	151480	897540
(4,0,0,1,0)	75600	352800	3855600
(0,0,0,2,0)	6	8	12
--- 8---			
(0,0,0,1,1)	6	8	12
(1,0,0,2,0)	1314	2456	8484
(1,1,2,0,0)	480816	1362368	18137280
(3,0,2,0,0)	5668992	23816576	264316416
(0,3,1,0,0)	293580	980560	11500440
(1,4,0,0,0)	8927100	41667920	558904920
(3,3,0,0,0)	303516360	1989657600	37158115680
(5,2,0,0,0)	2069648280	20325614400	475058213280
(2,0,1,1,0)	206136	566720	3494400
(4,1,1,0,0)	189108360	1291281600	22446012960
(7,1,0,0,0)	5174948520	70672704480	2065871772720
(9,0,0,0,0)	5853118320	103776644160	3652358441760
(1,0,1,0,1)	840	1568	3696
(2,2,1,0,0)	26412120	115673600	1691964960
(3,1,0,1,0)	3931200	17424960	189675360
(6,0,1,0,0)	174628440	1970831520	47902715280
(0,1,1,1,0)	6300	11760	90888
(0,2,0,0,1)	1050	1960	4620
(1,2,0,1,0)	342090	949480	8663340
(0,0,3,0,0)	0	0	36960
(2,1,0,0,1)	25200	70560	277200
(5,0,0,1,0)	3107160	27684720	507449880
(4,0,0,0,1)	37800	176400	1247400
--- 9---			
(1,0,0,1,1,0)	2700	5040	15336
(2,0,0,2,0,0)	230526	621576	3736044
(2,1,2,0,0,0)	70425936	299113920	6396866784
(4,0,2,0,0,0)	352651320	2341715040	44471715120
(1,3,1,0,0,0)	90039600	446019840	8154699840
(2,4,0,0,0,0)	1354041360	8918159040	199989246240
(4,3,0,0,0,0)	20411591760	206833193280	6235971507360
(6,2,0,0,0,0)	101944354680	1477552497120	54913237893360
(3,0,1,1,0,0)	19613664	82555200	921697056
(5,1,1,0,0,0)	9534445200	102238718400	2943054505440
(8,1,0,0,0,0)	216899000640	4309745408640	197749196527680
(10,0,0,0,0,0)	216250443360	5527262240640	303601312848960
(0,1,0,2,0,0)	0	0	86400
(0,5,0,0,0,0)	0	0	652821120
(0,1,1,0,1,0)	12600	23520	79632
(1,1,1,1,0,0)	1818936	5021856	71605296
(3,2,1,0,0,0)	2388022560	15969542400	379611308160
(2,2,0,1,0,0)	44180640	189332640	3119724720
(4,1,0,1,0,0)	230519520	1692290880	34358476320
(7,0,1,0,0,0)	7401119040	123195219840	4826433003840
(0,0,2,1,0,0)	0	0	215712
(1,0,3,0,0,0)	0	0	24635520
(2,0,1,0,1,0)	151200	423360	2509920
(0,2,2,0,0,0)	1775088	5916288	66265920
(1,2,0,0,1,0)	378000	1058400	6577200
(0,3,0,1,0,0)	0	0	25280640
(6,0,0,1,0,0)	115123680	1776297600	59390392320
(3,1,0,0,1,0)	2268000	10584000	123832800
(5,0,0,0,1,0)	1360800	12700800	310262400
(0,0,0,0,2,0)	6	8	12
---10---			
(0,0,0,0,1,1)	6	8	12
(1,0,0,0,2,0)	1944	3632	12888
(1,1,0,2,0,0)	1970730	5511960	87483780
(3,0,0,2,0,0)	23264820	96989040	1176654600
(0,1,3,0,0,0)	3024000	10946880	205541280
(1,2,2,0,0,0)	452571840	2294916960	54706856400
(3,1,2,0,0,0)	8032658760	54959879520	1695991515120
(5,0,2,0,0,0)	19520948160	206630827200	6827110647840
(0,2,1,1,0,0)	4698540	15155280	354475800
(1,5,0,0,0,0)	2506442400	18295401600	597611498400
(3,4,0,0,0,0)	143381107800	1455184836000	54389454512400
(2,3,1,0,0,0)	15636537000	111954124800	3328520580000
(5,3,0,0,0,0)	1345723016400	20593050811200	998371268042400
(7,2,0,0,0,0)	5316170680800	113290264483200	66806630809632000
(2,0,0,1,1,0)	507060	1386720	8912160
(4,0,1,1,0,0)	1356558840	9211839840	195028994160
(6,1,1,0,0,0)	503085945600	8182030752000	384686341905600
(9,1,0,0,0,0)	9932152608000	286074500241600	20614373055309600
(10,0,0,0,0,0)	8825075128800	325382704214400	27960309337867200
(1,0,0,1,0,1)	1350	2520	5940
(2,1,1,1,0,0)	332942400	1438819200	30999235680
(2,0,3,0,0,0)	55467720	249994080	9847661040
(4,2,1,0,0,0)	180779256000	1923859828800	73917161690400
(1,3,0,1,0,0)	156907800	771271200	20733829200
(3,0,1,0,1,0)	18779040	81849600	945967680
(5,1,0,1,0,0)	12670295400	155281341600	5446231635600
(8,0,1,0,0,0)	343399240800	8419005604800	520997701946400
(0,1,0,1,1,0)	14850	27720	241020
(0,4,1,0,0,0)	95823000	552316800	15161025600
(0,1,1,0,0,1)	6300	11760	27720
(1,1,1,0,1,0)	3031560	8410080	88567920
(3,2,0,1,0,0)	4338646200	30390519600	832911244200
(2,2,0,0,1,0)	51710400	228186000	3516420600
(0,0,2,0,1,0)	13860	25872	257544
(0,0,1,2,0,0)	0	0	624960
(2,0,1,0,0,1)	75600	211680	831600
(4,1,0,0,1,0)	185749200	1499299200	32407452000
(7,0,0,1,0,0)	5407138800	127421683200	6864442653600
(1,0,2,1,0,0)	1689660	4793040	194108040
(1,2,0,0,0,1)	189000	529200	2079000
(0,3,0,0,1,0)	693000	1940400	35947800
(3,1,0,0,0,1)	1134000	5292000	37422000
(6,0,0,0,1,0)	48308400	1191153600	49353494400
(5,0,0,0,0,1)	680400	6350400	89812800

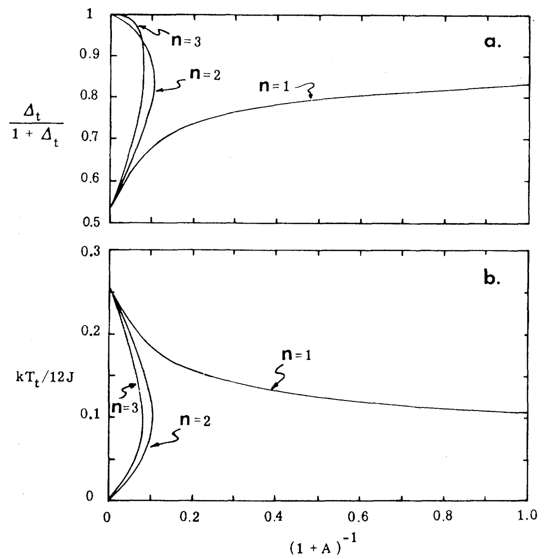

FIG. 1. (a) Loci of tricritical parameters. (b) Tricritical temperatures as a function of $(1+A)^{-1}$.

analysis of $\Delta_{n,t}$ as a function of A for *all* A. We plot $\Delta_{n,t}/(1+\Delta_{n,t})$ versus $1/(1+A)$ so as to encompass both the Riedel-Wegner ($A\to 0$) and Blume-Capel ($A\to\infty$, Δ finite) limits. All three models exhibit tricritical loci, $\Delta_{n,t}(A)$, which coincide in the $A\to\infty$, Δ-finite limit. We agree with Saul, Wortis, and Stauffer's value for $\Delta_t(\infty)$ with high precision.[4]

As $(1+A)^{-1}$ increases from zero all three $\Delta_{n,t}$ loci increase. However, only the $n=1$ locus extends all the way to the ($A=0$) Riedel-Wegner limit. For sufficiently small A neither the $n=2$ nor the $n=3$ model has a tricritical point. Instead the tricritical loci bend back to $\Delta_t=\infty$ at $A=\infty$. In Fig. 1(b) we display the loci of tricritical temperatures as a function of A. Note that the tricritical temperature decreases to zero for $n=2$ and 3 in the $A\to\infty$, $\Delta_{n,t}\to\infty$ limit. For $n=1$ the tricritical point approaches $\Delta_{1,t}\simeq 5.06$ and $kT_t/12J\simeq 0.107\pm 0.01$ as $A\to 0$.

These results may appear hard to understand, but they are eminently reasonable. In molecular-field theory the tricritical point is easily found to be located by the condition that the bare fourth-order cumulant $I_4-3I_2^{\,2}$ vanish. For sufficiently small A this can never be satisfied for our $n=2$ and $n=3$ models, whereas for any A it can always be satisfied for some $\Delta_{1,t}$ for the $n=1$ model. Indeed the results of molecular-field theory for $\Delta_{n,t}$ and $K_{n,t}$ are qualitatively identical to the series predictions. As usual molecular-field theory considerably *over*estimates T_t and *under*estimates Δ_t.

In conclusion, we have presented tenth-order susceptibility series in powers of J/kT for *all* classical scalar models in the absence of symmetry-breaking fields. As an example of the power of these results we have mapped out the tricritical behavior of a new class of models which interpolate between the Blume-Capel[4] and Riedel-Wegner[6] models. We expect that our general results will prove useful in studying new models for phase transitions.

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[12]To apply the table to the site-randomized problem, simply replace I_{2l} wherever it appears by $I_{2l}\langle p^{2l}\rangle$, where $\langle\cdots\rangle$ represents an average over the single-site random distribution.