Extended high-temperature series for the N-vector spin models on three-dimensional bipartite lattices

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High-temperature expansions for the susceptibility and the second correlation moment of the classical N-vector model [$O(N)$ symmetric Heisenberg model] on the sc and the bcc lattices are extended to order β^{19} for arbitrary N. For $N = 2, 3, 4, \ldots$ we present revised estimates of the critical parameters from the newly computed coefficients.

There has been a resurgence of interest in series expansions for the statistical mechanics of lattice models witnessed by the recent publication of several remarkably long high-temperature (HT) and low-temperature (LT) series, in particular for the N-vector model[1] with $N = 0$ (the self-avoiding walk model),[2] with $N = 1$ (the Ising model),[3] and with $N = 2$ (the XY model),[4] in 2- and 3-space dimensions. The best results, however, are still restricted to the $N = 0$ and 1 cases, where series are obtained by counting techniques which achieve maximal efficiency in low dimensions and only with discrete site variable models. Presently, on the sc lattice, the zero field susceptibility $\chi(N;\beta)$ and the second correlation moment $\mu_2(N;\beta)$ are known to $O(\beta^{24})$ and $O(\beta^{21})$ (Refs. 2 and 5), respectively, for $N = 0$, to $O(\beta^{19})$ and $O(\beta^{15})$ (Refs. 6 and 7), respectively, for $N = 1$, to $O(\beta^{17})$ (Ref. 4) for $N = 2$, and to $O(\beta^{14})$ (Refs. 8 and 9) for any other N. On the bcc lattice, χ and μ_2 have been computed to $O(\beta^{16})$ for $N = 0$,[5] to $O(\beta^{21})$ for $N = 1$,[10,11] to $O(\beta^{12})$ for $N = 2$,[12] and to $O(\beta^{11})$ for $N = 3$.[13] Apart from the interest of an increasingly precise direct determination of the critical properties of the lattice models, there is no lack of other good reasons to undertake such a laborious calculation as a long series expansion: they include more accurate tests of the validity both of the assumption of universality, on which the renormalization-group (RG) approach to critical phenomena is based, and of the approximation procedures required to produce estimates of universal quantities by field theory methods. In fact, for want of more rigorous arguments, as stressed in Ref. 14, a crucial test of the validity of Borel resummed ϵ expansions or fixed dimension g expansions[14–17] is still provided by the comparison with experimental or numerical data.

Here we present a brief analysis of a new extension from $O(\beta^{14})$ to $O(\beta^{19})$ of the high-temperature (HT) expansions in zero field for the susceptibility and the second correlation moment of the N-vector model both on the sc lattice and on the bcc lattice. More results to $O(\beta^{19})$ in $d = 2, 3, 4, \ldots$ space dimensions, and a study of the second field derivative of the susceptibility $\chi^{(4)}(N;\beta) = d^2\chi/dH^2$ will appear elsewhere. We have determined the series coefficients as explicit functions of the spin dimensionality N by using the vertex renormalized linked cluster expansion (LCE) method.[18] Our calculation substantially extends previous work in that it provides coefficient tables of considerable length irrespective of the spin dimensionality and of the lattice structure: HT series for the general N-vector model were previously available only for the (hyper)sc lattice in $d = 2, 3, 4$ dimensions up to $O(\beta^{14})$.[8,9]

Concerning the LCE technique, we have found the following works particularly useful: the review papers,[18] the $N = 1$ computations,[10,11,19–21] and the more recent work by Luescher and Weisz (LW),[8] devoted to the model, the $O(N)$ symmetric $P(\vec{\varphi}^2)$ lattice field theory, described by the partition function

$$Z = \int \Pi d\mu(\vec{\varphi}_i^2) \exp\left(\beta \sum_{\langle i,j\rangle} \vec{\varphi}_i \cdot \vec{\varphi}_j\right), \qquad (1)$$

where $\vec{\varphi}_i$ is a N-component vector. With the choice $d\mu(\vec{\varphi}_i^2) = \delta(\vec{\varphi}_i^2 - 1)d\vec{\varphi}_i$ of the single spin measure, (1) reduces to the partition function of the N-vector model, but also a broad class of other models of interest in statistical mechanics can all be represented in this form. LW have devised or simplified some algorithms required for the calculations, and have tabulated HT expansions of χ, μ_2, $\chi^{(4)}$ on the (hyper)sc lattices for the N-vector model to $O(\beta^{14})$.[8,9] Also, starting from (1), we have extended the calculation to the class of bipartite lattices, in particular to the (hyper)sc and (hyper)bcc lattices. By redesigning the algorithms in order to take full advantage of the structural properties of the bipartite lattices and by writing an entirely new optimized code, we have significantly reduced the growth of the complexity with the order of expansion. Thus, we have been able to push our calculation well beyond $O(\beta^{14})$, where LW had to give up. We can give a rough idea of the size and the complexity of the calculation by mentioning that over 2×10^6 graphs enter into the evaluation of χ and μ_2 through $O(\beta^{19})$. This should be compared with the corresponding figure: 1.1×10^4, in the LW computation. Since these figures by no means represent our computational limits, a further extension of our calculations is feasible. We are confident that our results are correct also because, in each space dimension $d = 1, 2, 3, \ldots$, by

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a single procedure, we produce numbers in agreement with all expansion coefficients already available for $N = 0,1,2,3$ and ∞ (spherical model).[22] Our codes were run on an IBM Risc 6000/530 power station with 32 Mbyte memory capacity and 1.5 Gbyte of disk storage. Typical CPU times were extremely modest, and the random access memory (RAM) is far from being saturated. For reasons of space neither a detailed discussion of the main steps of this computation can fit here nor we can display the extensive formulas giving the closed form structure of the HT series coefficients as functions of N. Therefore, as an example of our results, we shall only report here the HT series in the $N = 3$ case (classical Heisenberg model) on the sc and the bcc lattices, respectively, where we have contributed from five to eight new coefficients beyond those given in Refs. 8, 9, and 13.

The susceptibility HT series for the sc lattice is

$$\begin{aligned}\chi^{sc}(\beta) = {} & 1 + 2\beta + \frac{10}{3}\beta^2 + \frac{244}{45}\beta^3 + \frac{230}{27}\beta^4 + \frac{37612}{2835}\beta^5 + \frac{864788}{42525}\beta^6 + \frac{19773464}{637875}\beta^7 \\ & + \frac{89686514}{1913625}\beta^8 + \frac{25478812}{360855}\beta^9 + \frac{140348301868}{1326142125}\beta^{10} + \frac{477383158731608}{3016973334375}\beta^{11} \\ & + \frac{426768736125964}{1810184000625}\beta^{12} + \frac{28560817226680664}{81458280028125}\beta^{13} + \frac{775988604270248}{1491909890625}\beta^{14} \\ & + \frac{16004552656617124832}{20771861407171875}\beta^{15} + \frac{354950851980427607594}{311577921107578125}\beta^{16} \\ & + \frac{14641283528139550963126 76}{870237133653465703125}\beta^{17} + \frac{1068764655864454858376417828}{430767381158465523046875}\beta^{18} \\ & + \frac{259814093690188797550933157144}{71076617891146811302734375}\beta^{19} + \dots .\end{aligned}$$

The second correlation moment HT series for the sc lattice is

$$\begin{aligned}\mu_2^{sc}(\beta) = {} & 2\beta + 8\beta^2 + \frac{964}{45}\beta^3 + \frac{2192}{45}\beta^4 + \frac{57116}{567}\beta^5 + \frac{8340368}{42525}\beta^6 + \frac{33324872}{91125}\beta^7 + \frac{1263947744}{1913625}\beta^8 \\ & + \frac{73478278372}{63149625}\beta^9 + \frac{13325285538064}{6630710625}\beta^{10} + \frac{3434294378983784}{1005657778125}\beta^{11} + \frac{51819882101501984}{9050920003125}\beta^{12} \\ & + \frac{773005999283909656}{81458280028125}\beta^{13} + \frac{19031243835736702816}{1221874200421875}\beta^{14} + \frac{225650609227937809568}{8902226317359375}\beta^{15} \\ & + \frac{267912260258927725784384}{6543136343259140625}\beta^{16} + \frac{171544906778131647970688684}{2610711400960397109375}\beta^{17} \\ & + \frac{45158335170568649028207863344}{430767381158465523046875}\beta^{18} + \frac{19874973349328684680550746792}{119456500657389598828125}\beta^{19} + \dots .\end{aligned}$$

The susceptibility HT series for the bcc lattice is

$$\begin{aligned}\chi^{bcc}(\beta) = {} & 1 + \frac{8}{3}\beta + \frac{56}{9}\beta^2 + \frac{1936}{135}\beta^3 + \frac{12904}{405}\beta^4 + \frac{119600}{1701}\beta^5 + \frac{2784992}{18225}\beta^6 + \frac{632918848}{1913625}\beta^7 \\ & + \frac{4075984504}{5740875}\beta^8 + \frac{287925718448}{189448875}\beta^9 + \frac{64384719769312}{19892131875}\beta^{10} + \frac{186782368415874752}{27152760009375}\beta^{11} \\ & + \frac{1186773786369487616}{81458280028125}\beta^{12} + \frac{7528780320376815776}{244374840084375}\beta^{13} + \frac{732954612970918048}{11278838773125}\beta^{14} \\ & + \frac{127972570589148818590048}{934733763322734375}\beta^{15} + \frac{807291210775528531339816}{2804201289968203125}\beta^{16} \\ & + \frac{4736622265468109492081181616}{7832134202881191328125}\beta^{17} + \frac{16393670565274498589242223 63488}{1292302143475396569140625}\beta^{18} \\ & + \frac{5669373833051258567345686140186 88}{21322985367344043390820312 5}\beta^{19} + \dots .\end{aligned}$$

The second correlation moment HT series for the bcc lattice is

$$\begin{aligned}\mu_2^{bcc}(\beta) = {} & \frac{8}{3}\beta + \frac{128}{9}\beta^2 + \frac{784}{15}\beta^3 + \frac{67072}{405}\beta^4 + \frac{4081648}{8505}\beta^5 + \frac{167636864}{127575}\beta^6 + \frac{944026304}{273375}\beta^7 \\ & + \frac{16849951744}{1913625}\beta^8 + \frac{4153759481008}{189448875}\beta^9 + \frac{1065794492624896}{19892131875}\beta^{10} + \frac{1166772237247486528}{9050920003125}\beta^{11} \\ & + \frac{8314233519972990976}{27152760009375}\beta^{12} + \frac{175799675893471696544}{244374840084375}\beta^{13} + \frac{409170117445661176448}{244374840084375}\beta^{14} \\ & + \frac{361305927020036448388 4384}{934733763322734375}\beta^{15} + \frac{1739153605204091866703733 76}{1962940902977742187 5}\beta^{16} \\ & + \frac{3161105847803443673831465 8288}{1566426840576238265625}\beta^{17} + \frac{843832598640540680559633378 6112}{1846145919250566527343 75}\beta^{18} \\ & + \frac{219639404642322325234496716062 61888}{21322985367344043390820312 5}\beta^{19} + \dots .\end{aligned}$$

Let us now comment on our updated estimates for the critical temperatures and the critical exponents γ and ν in the $N = 2, 3, 4, \ldots$ cases, where our new series are significantly longer than those previously available. The main difficulty of the analysis here comes from the expected singular corrections[24] (confluent singularities) to the leading power-law behavior of thermodynamical quantities. For example, the susceptibility should be described, in the vicinity of its critical point β_c, by

$$\chi(N;\beta) \simeq C(N)(\beta_c - \beta)^{-\gamma(N)}\Big(1 + a_\chi(N)(\beta_c - \beta)^{\theta(N)} + \cdots + a'(N)(\beta_c - \beta) + \cdots\Big)$$

with the universal (for each N) exponent $\theta(N) \simeq 0.5$ for small N (Ref. 14) and $\theta(N) = 1 + O(1/N)$ for large N (Ref. 23). The standard ratio and Padé approximant (PA) methods are insufficient to cope with this very unstable double exponential fitting problem. Therefore, we have to resort also to the inhomogeneous differential approximants (DA's) method,[25] a generalization of the PA method better suited to represent functions behaving like $\phi_1(x)(x - x_0)^{-\gamma} + \phi_2(x)$ near a singular point x_0, where $\phi_1(x)$ is a regular function of x and $\phi_2(x)$ may contain a (confluent) singularity of strength smaller than γ. We have essentially followed the protocol of series analysis by the DA's suggested in Ref. 26, which is unbiased for confluent singularities. We have computed β_c and γ from the susceptibility series and have used this estimate of β_c to bias the computation of ν from the series for the square of the (second moment) correlation length ξ^2. The results are reported in Table I along with the previous estimates by other methods. In the sc lattice case our exponent estimates are consistent with the RG ϵ-expansion results,[14,15] but they are slightly larger (by $\simeq 1\%$) than the g-expansion results. In the bcc lattice case the estimates are perfectly compatible with the most recent seventh-order[16] or sixth-order[17] g-expansion results. This is analogous to what is observed in the most accurate unbiased analyses of the $N = 1$ case[26] and suggests that the series for lattices with lower coordination number have a slower convergence[26] and also that unbiased DA's might be unable to account completely for the confluent singularities. For $N > 3$ no elaborate estimates of the exponents by the ϵ-expansion method are available, and only very recently has an extensive computation by the (sixth-order) g-expansion method been published.[17] Unfortunately, no estimates of error for the exponents are given in Ref. 17, but we can safely assume uncertainties of the order of 0.5% for moderate values of N and possibly smaller for $N \geq 8$.

Analyzing our sc series by the simplest biased PA method[27] designed to account explicitly for the confluent singularities, does not significantly alter our DA esti-

TABLE I. A summary of the estimates of critical parameters for various values of N.

N	Method and Ref.	β_c	γ	ν
2	Expt. (Ref. 29)			0.6705(6)
	HT sc	0.45420(6)	1.328(6)	0.679(3)
	HT bcc	0.320434(8)	1.323(2)	0.674(2)
	HT fcc (Ref. 12)	0.2075(1)	1.323(15)	0.670(7)
	RG g expansion (Ref. 16)		1.318(2)	0.6715(15)
	RG ϵ expansion (Ref. 14)		1.315(7)	0.671(5)
	Monte Carlo sc (Ref. 30)	0.45420(2)	1.308(16)	0.662(7)
	Monte Carlo sc (Ref. 31)	0.4542(1)	1.316(5)	0.670(7)
3	HT sc	0.69302(7)	1.403(6)	0.715(3)
	HT bcc	0.48681(2)	1.396(3)	0.711(2)
	HT fcc (Ref. 13)	0.3149(6)	1.40(3)	0.72(1)
	RG g expansion (Ref. 16)		1.3926(20)	0.7096(15)
	RG ϵ expansion (Ref. 14)		1.39(1)	0.710(7)
	Monte Carlo sc (Ref. 32)	0.693035(37)	1.3896(70)	0.7036(23)
	Monte Carlo bcc (Ref. 32)	0.486798(12)	1.385(10)	0.7059(37)
4	HT sc	0.93582(8)	1.471(6)	0.749(4)
	HT bcc	0.65526(3)	1.458(3)	0.742(2)
	RG g expansion (Ref. 34)		1.45(3)	0.74(1)
	RG g expansion (Ref. 17)		1.449	0.738
	Monte Carlo sc (Ref. 33)	0.9360(1)	1.477(18)	0.7479(90)
6	HT sc	1.42838(9)	1.577(6)	0.801(4)
	HT bcc	0.99608(6)	1.564(3)	0.795(2)
	RG g expansion (Ref. 17)		1.556	0.790
8	HT sc	1.9262(3)	1.656(6)	0.840(4)
	HT bcc	1.33976(8)	1.641(3)	0.832(2)
	RG g expansion (Ref. 17)		1.637	0.830
10	HT sc	2.4267(3)	1.712(6)	0.867(4)
	HT bcc	1.6850(2)	1.696(3)	0.859(2)
	RG g expansion (Ref. 17)		1.697	0.859

mates. Therefore, in order to assess with a higher level of precision the influence of these confluent singularities and completely reconcile the series results with those from the RG, further work is required including the computation of even longer series and, as indicated by the experience with the $N = 1$ case, a study of suitable continuous families of models for each universality class.[11,28] The uncertainties we have quoted for our exponent estimates, generously allowing for the scatter of the results in the DA analysis, leave small differences between our central values for the sc lattice, and those from the fixed dimension RG. This suggests that the still insufficient length of the HT series and/or the still incomplete account of the confluent singularities add to some of our estimates a systematic uncertainty twice as large as we have indicated. Even under this conservative proviso, we have significantly improved the precision of the values of the critical parameters from HT series and have not pointed out any serious inconsistency with the estimates either from RG or from stochastic simulations.

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