New extended high temperature series for the $N$-vector spin models on three-dimensional bipartite lattices

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Abstract

Abstract: 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 $\beta^{19}$ for arbitrary $N$. For $N = 2, 3, 4, \ldots$ we present revised estimates of the critical parameters from the newly computed coefficients.

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There has been a resurgence of interest in series expansions for the Statistical Mechanics of lattice models witnessed by the recent publication of several new remarkably long high-temperature (HT) and low-temperature (LT) series, in particular for the $N$-vector model with $N = 0$ (the self-avoiding walk model) [1], 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 $O(\beta^{21})$ respectively for $N = 0$, to $O(\beta^{19})$ and $O(\beta^{15})$ respectively for $N = 1$, to $O(\beta^{17})$ for $N = 2$ and to $O(\beta^{14})$ for any other $N$. On the bcc lattice, $\chi$ and $\mu_2$ have been computed to $O(\beta^{16})$ for $N = 0$ [5], to $O(\beta^{21})$ for $N = 1$ [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 $\epsilon$–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 extends substantially
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
M. Luescher and P. Weisz (LW) [8], devoted to the model, the \( O(N) \) symmetric \( P(\vec{\varphi}^2) \) lattice
field theory, described by the partition function

\[
Z = \int \prod \mu(\vec{\varphi}_i^2) \exp[\beta \sum_{\langle i,j \rangle} \vec{\varphi}_i \cdot \vec{\varphi}_j],
\]

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 \( \chi, \mu_2, \chi^{(4)} \) 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 \( 2 \cdot 10^6 \) graphs
enter into the evaluation of \( \chi \) and \( \mu_2 \) through \( O(\beta^{19}) \). This should be compared with the
corresponding figure: \( 1.1 \cdot 10^4 \), 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
a single procedure, we produce numbers in agreement with all expansion coefficients already
available for \( N = 0,1,2,3 \) and \( \infty \) (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 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. [8,13].

The susceptibility HT series for the sc lattice is:

\[
\chi^{sc}(\beta) = 1 + 2\beta + \frac{10}{3}\beta^2 + \frac{244}{45}\beta^3 + \frac{230}{27}\beta^4 + \frac{37612}{2835}\beta^5 + \frac{864788}{42525}\beta^6 + \frac{19773464}{637875}\beta^7 + \\
\frac{89686514}{1913625}\beta^8 + \frac{25478812}{360855}\beta^9 + \frac{140348301868}{1326142125}\beta^{10} + \frac{477383158731608}{3016973334375}\beta^{11} + \\
\frac{426768736125964}{1810184000625}\beta^{12} + \frac{28560817226680664}{81458280028125}\beta^{13} + \frac{775988604270248}{1491909890625}\beta^{14} + \\
\frac{16004552656617124832}{2077186140717875}\beta^{15} + \frac{354950851980427607594}{31157792110758125}\beta^{16} + \\
\frac{1464128352813955096312676}{870237133653465703125}\beta^{17} + \frac{1068764655864454858376417828}{430767381158465523046875}\beta^{18} + \\
\frac{259814093690188797550933157144}{71076617891146871302734375}\beta^{19} \ldots
\]

The second correlation moment HT series for the sc lattice is:

\[
\mu_{2}^{sc}(\beta) = 2\beta + 8\beta^2 + \frac{964}{45}\beta^3 + \frac{2192}{45}\beta^4 + \frac{57116}{567}\beta^5 + \frac{8340368}{42525}\beta^6 + \frac{33324872}{91125}\beta^7 + \frac{1263947744}{1913625}\beta^8 + \\
\frac{73478278372}{63149625}\beta^9 + \frac{13325285538064}{6630710625}\beta^{10} + \frac{3434294378983784}{1005657778125}\beta^{11} + \frac{51819882101501984}{9050920003125}\beta^{12} + \\
\frac{773005999283909656}{81458280028125}\beta^{13} + \frac{19031243835736702816}{1221874200421875}\beta^{14} + \frac{225650609227937809568}{890226317359375}\beta^{15} + \ldots
\]
\[
\chi_{\text{bcc}}(\beta) = 1 + \frac{8}{3} \beta + \frac{56}{9} \beta^2 + \frac{1936}{135} \beta^3 + \frac{12904}{405} \beta^4 + \frac{119600}{1701} \beta^5 + \frac{2784992}{18225} \beta^6 + \frac{632918848}{1913625} \beta^7 + \\
\frac{4075984504}{5740875} \beta^8 + \frac{287925718448}{189448875} \beta^9 + \frac{64384719769312}{19892131875} \beta^{10} + \frac{186782368415874752}{27152760009375} \beta^{11} + \\
\frac{1186773786369487616}{81458280028125} \beta^{12} + \frac{7528780320376815776}{244374840084375} \beta^{13} + \frac{732954612970918048}{11278838773125} \beta^{14} + \\
\frac{12797257058914881859048}{93473376332734375} \beta^{15} + \frac{807291210775528531339816}{2804201289968203125} \beta^{16} + \\
\frac{4736622265468109492081181616}{7832134202881191328125} \beta^{17} + \frac{1639367056527449858924222363488}{1292302143475396569140625} \beta^{18} + \\
\frac{566937383305125856734568614018688}{213229853673440433908203125} \beta^{19} \ldots
\]

The second correlation moment HT series for the bcc lattice is:

\[
\mu_{\text{bcc}}^2(\beta) = \frac{8}{3} \beta + \frac{128}{9} \beta^2 + \frac{784}{15} \beta^3 + \frac{67072}{405} \beta^4 + \frac{4081648}{8505} \beta^5 + \frac{167636864}{127575} \beta^6 + \frac{944026304}{273375} \beta^7 + \\
\frac{16849951744}{1913625} \beta^8 + \frac{4153759481008}{189448875} \beta^9 + \frac{1065794492624896}{19892131875} \beta^{10} + \frac{1166772237247486528}{9050920003125} \beta^{11} + \\
\frac{8314233519972990976}{27152760009375} \beta^{12} + \frac{175799675893471696544}{244374840084375} \beta^{13} + \frac{409170117445661176448}{244374840084375} \beta^{14} + \\
\frac{3613059270200364483884384}{934733763322734375} \beta^{15} + \frac{173915360520409186670373376}{1962940902977421875} \beta^{16} + \\
\frac{31611058478034436738314658288}{1566426840576238265625} \beta^{17} + \frac{8438325986405406805596333786112}{184614591925056652734375} \beta^{18}+
\]

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Let us now comment on our updated estimates for the critical temperatures and the critical exponents $\gamma$ and $\nu$ in the $N = 2, 3, 4...$ 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 $\beta_c$, by

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

with the universal (for each N) exponent $\theta(N) \simeq 0.5$ for small $N$ [14] and $\theta(N) = 1 + O(1/N)$ for large $N$ [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) 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 $\gamma$. We have essentially followed the protocol of series analysis by DA’s suggested in Ref. [26] which is unbiased for confluent singularities. We have computed $\beta_c$ and $\gamma$ from the susceptibility series and have used this estimate of $\beta_c$ to bias the computation of $\nu$ from the series for the square of the (second moment) correlation length $\xi^2$. 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 $\epsilon$—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 [14] 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 $\epsilon$—expansion method are available...
and only very recently an extensive computation by the (sixth order) $g$–expansion method has 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 $N \geq 8$.

Analysing our sc series by the simplest biased PA method [27] designed to account explicitly for the confluent singularities, does not significantly alter our DA estimates. 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 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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REFERENCES

[1] H.E. Stanley, Phys. Rev. Lett. 20,589 (1968).

[2] D. MacDonald et al., J. Phys. A25, 1429 (1992); A. R. Conway, I. G. Enting, A. J. Guttmann, J. Phys. A26, 1519 (1993).

[3] G. Bhanot, M. Creutz and J. Lacki, Phys. Rev. Lett. 69,1841 (1992); C. Vohwinkel, Phys. Lett. B301, 208 (1993); A. J. Guttmann and I. G. Enting, J. Phys. A26, 807 (1993); I. G. Enting, A. J. Guttmann and I. Jensen, Melbourne Univ. preprint October 1994.

[4] P. Butera and M. Comi, Phys. Rev. B47, 11969 (1993); P. Butera, M. Comi and A. Guttmann, Phys. Rev. B48,13987 (1993).

[5] A. J. Guttmann, J. Phys. A22, 2807 (1989).

[6] D.S. Gaunt and M.F. Sykes, J. Phys. A12, 425 (1979).

[7] R. Roskies, Phys. Rev. B23,6037 (1981).

[8] M. Luescher and P. Weisz Nucl. Phys. B300,325 (1988). See also M. Klomfass, Nucl. Phys. B412, 621 (1994).

[9] P. Butera, M. Comi, and G. Marchesini, Phys.Rev. B41,11494 (1990). See also: P. Butera, M. Comi and G. Marchesini, Nucl. Phys. B300,1 (1988).

[10] B.G.Nickel, in Phase Transitions: Cargese 1980, Edited by M. Levy, J. C. Le Guillou and J. Zinn-Justin; Plenum Press, New York 1982.

[11] B.G.Nickel and J.J. Rehr, J. Stat. Phys. 61,1 (1990).

[12] M. Ferer, M. A. Moore and M. Wortis, Phys. Rev. B8, 5205 (1973).

[13] S. McKenzie, C. Domb and D.L. Hunter, J. Phys. A15,3899 (1982); M. Ferer and A. Hamid-Aidinejed, Phys. Rev. B34, 6481 (1986).
[14] J. Zinn Justin, *Quantum field theory and critical phenomena*, Clarendon Press, Oxford 1992.

[15] G.A. Baker, B. G. Nickel and D. I. Meiron, Phys. Rev. B17, 1365 (1978); J. C. Le Guillou and J. Zinn Justin, Phys. Rev. B21, 3976 (1980); J. C. Le Guillou and J. Zinn Justin, J. Physique Lett. 45, 137 (1985).

[16] D.B. Murray and B.G. Nickel, *Revised estimates for critical exponents for the continuum N-vector model in 3 dimensions*, Unpublished Guelph University report (1991).

[17] S. A. Antonenko and A. I. Sokolov, Phys. Rev. 51E, 1894 (1995).

[18] M. Wortis, in *Phase Transitions and critical Phenomena* Vol. 3, C Domb and M.S. Green Eds., (Academic Press, London, 1974); S. McKenzie, in *Phase Transitions Cargese 1980*, M. Levy, J. C. Le Guillou and J. Zinn Justin eds., Plenum Press, New York 1982.

[19] W. J. Camp and J. P. van Dyke, Phys. Rev. Lett. 35, 323 (1975).

[20] G. A. Baker and J. M. Kincaid, J. Stat. Phys. 24, 469 (1981).

[21] R. Z. Roskies and P. D. Sackett, J. Stat. Phys. 49, 447 (1987).

[22] We have corrected some very small numerical mistakes in the last few coefficients for the $N = 2$ model series of Ref. [4] both in 2 and in 3 dimensions. However the conclusions of the series analyses do not change.

[23] S. K. Ma, Phys. Rev. A10, 1818 (1974);

[24] F. Wegner, Phys. Rev. B5, 4529 (1972).

[25] A. J. Guttmann, in *Phase Transitions and critical Phenomena*, C. Domb and J. Lebowitz Eds. Vol. 13; Academic Press, New York 1989.

[26] A. J. Guttmann, J. Phys. A20, 1839, 1855 (1987).

[27] J. Adler, C. Holm and W. Janke, Physica A201, 581 (1993).
[28] J.H. Chen, M. E. Fisher and B. G. Nickel, Phys. Rev. Lett. 48, 259 (1982).

[29] L.S. Goldner and G. Ahlers, Phys. Rev. B45, 13129 (1992).

[30] M. Hasenbusch and S. Meyer, Phys. Lett. B241, 238 (1990); A. P. Gottlob and M. Hasenbusch, Physica A201, 593 (1993).

[31] W. Janke, Phys. Lett. A143, 306 (1990).

[32] K. Chen, A. M. Ferrenberg and D.P. Landau, Phys. Rev. B48, 3249 (1993); C. Holm and W. Janke, Phys. Lett. A173, 8 (1993) and Phys. Rev. B48, 936 (1993).

[33] K. Kanaya and S. Kaya, *Critical exponents of a three dimensional O(4) spin model*, Tsukuba University Preprint UTHEP-284 September 1994.

[34] For other estimates of the exponents in the $N = 4$ case we can also refer either to a private communication from B. G. Nickel quoted in: G. Malmstrom and D. J. W. Geldart, Phys. Rev. B21, 1133 (1980) and in F. Wilczek, Int. J. Mod. Phys. A7, 3911 (1992), which we have reported in this table, or to a private communication by J. C. Le Guillou, quoted in: P. Azaria, B. Delamotte, T. Jolicour, Phys. Rev. Lett. 64, 3175 (1990) stating that $\gamma \simeq 1.47$ and $\nu \simeq 0.74$, with no indication of error.
### TABLE I. A summary of the estimates of critical parameters for various values of $N$

| $N$ | Method and Ref. | $\beta_c$ | $\gamma$ | $\nu$  |
|-----|----------------|-----------|---------|--------|
| 2   | Exper. [29]    | 0.6705(6) | 1.328(6) | 0.679(3) |
|     | HTE sc         | 0.45420(6) | 1.323(2) | 0.674(2) |
|     | HTE bcc        | 0.32043(8) | 1.324(15)| 0.670(7) |
|     | HTE fcc [12]   | 0.2075(1)  | 1.318(2) | 0.671(5) |
|     | R.G. g-exp. [10]| 0.4542(1) | 1.315(7) | 0.671(7) |
|     | R.G. $\epsilon$ exp. [14] | 1.3926(20) | 0.7096(15) |
|     | MonteCarlo sc [30] | 0.45420(2) | 1.308(16) | 0.662(7) |
|     | MonteCarlo sc [31] | 0.45421(1) | 1.316(5) | 0.670(7) |
|     | 3              |           |         |        |
|     | HTE sc         | 0.69302(7) | 1.403(6) | 0.715(3) |
|     | HTE bcc        | 0.48681(2) | 1.396(3) | 0.711(2) |
|     | HTE fcc [13]   | 0.3149(6)  | 1.40(3)  | 0.72(1) |
|     | R.G. g-exp. [10]| 0.4545(3) | 1.3926(20)| 0.7096(15) |
|     | R.G. $\epsilon$ exp. [14] | 1.39(1) | 0.710(7) |
|     | MonteCarlo sc [32] | 0.693035(37) | 1.3896(70) | 0.7036(23) |
|     | MonteCarlo bcc [32] | 0.486798(12)| 1.385(10)| 0.7059(37)|
|     | 4              |           |         |        |
|     | HTE sc         | 0.93582(8) | 1.471(6) | 0.749(4) |
|     | HTE bcc        | 0.65526(3) | 1.458(3) | 0.742(2) |
|     | R.G. g-exp. [14]| 1.45(3) | 0.74(1) |
|     | R.G. $\epsilon$ exp. [17] | 1.449 | 0.738 |
|     | MonteCarlo sc [33] | 0.9360(1) | 1.477(18) | 0.7479(90) |
|     | MonteCarlo sc [31] | 0.8014(1) | 1.577(6) | 0.801(4) |
|     | 6              |           |         |        |
|     | HTE sc         | 1.42838(9) | 1.577(6) | 0.801(4) |
|     | HTE bcc        | 0.99160(6) | 1.564(3) | 0.795(2) |
|     | R.G. g-exp. [17] | 1.556 | 0.790 |
|     | 8              |           |         |        |
|     | HTE sc         | 1.9262(3)  | 1.656(6) | 0.840(4) |
|     | HTE bcc        | 1.33976(8) | 1.641(3) | 0.832(2) |
|     | R.G. g-exp. [17] | 1.637 | 0.830 |
|     | 10             |           |         |        |
|     | HTE sc         | 2.4267(3)  | 1.712(6) | 0.867(4) |
|     | HTE bcc        | 1.6850(2)  | 1.696(3) | 0.859(2) |
|     | R.G. g-exp. [17] | 1.697 | 0.859 |