

An On-Line Library of Extended High-Temperature Expansions of Basic Observables for the Spin- S Ising Models on Two- and Three-Dimensional Lattices

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We present an on-line library of unprecedented extension for high-temperature expansions of basic observables in the Ising models of general spin S , with nearest-neighbor interactions. We have tabulated through order β^{25} the series for the nearest-neighbor correlation function, the susceptibility and the second correlation moment in two dimensions on the square lattice, and, in three dimensions, on the simple-cubic and the body-centered cubic lattices. The expansion of the second field derivative of the susceptibility is also tabulated through β^{23} for the same lattices. We have thus added several terms (from four up to thirteen) to the series already published for spin $S = 1/2, 1, 3/2, 2, 5/2, 3, 7/2, 4, 5, \infty$.

KEY WORDS: Ising model; critical exponents; universality; hyperscaling; high-temperature expansions.

With the modern developments of the renormalization group theory the understanding of critical phenomena for ordered systems has reached a stage of maturity: the conceptual and computational paradigm has become widely accepted and essentially only more or less important “details” still remain to be worked out.⁽¹⁾ The question of a complete a priori definition of the universality class of critical behavior, the actual computation of the corrections to the scaling behavior, and the accurate determination of the universal and nonuniversal critical parameters are some strictly intertwined examples of these details which must always be faced in the study of specific models. Indeed the identification of the universality class in terms of the

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spatial dimensionality of the system, the number of components and symmetry properties of the order parameter and the range of the interactions is not always unambiguous and ought to be checked in each case. On the other hand the size of the corrections to scaling (and, as a consequence, the size of the asymptotic critical region) may vary strongly among models in the same universality class and unless these corrections can be somehow brought under control, the estimates of the critical parameters and therefore the identification of the universality class may be not very reliable. High-temperature (HT) expansions are a source of valuable numerical benchmarks in the study of spin models and as such are also a good tool to investigate these questions. Therefore it is important to provide easy access to a body of information in the form of exact high-temperature (HT) expansions as extensive as presently possible for a family of models expected to belong to the same universality class such as the Ising models of general spin S . These models have a great historical and conceptual interest: in the past their study⁽²⁾ contributed to shape the modern formulation of the universality hypothesis⁽³⁾ and, still today, they remain the simplest and phenomenologically most useful discrete-state lattice models.⁽⁴⁻⁶⁾ It is worth remarking that in spite of this, for many years, high-temperature series expansions both in two and in three dimensions, have been available only for few observables and have been generally too short to make numerically accurate discussions of these models possible.⁽⁷⁻⁹⁾ For instance, in three dimensions on the simple-cubic (sc) lattice, the expansions of $\chi(\beta; S)$ and of the second moment of the correlation function $\mu_2(\beta; S)$, for spin $S > 1/2$, can be found explicitly in the literature⁽⁸⁾ only up to the order β^{12} . The subsequent work by R. Roskies and P. Sackett⁽¹⁰⁾ who made an extension through β^{15} possible, improved the situation only slightly. On the fcc lattice, the HT series initially derived to order β^{12} in ref. 8, were later extended in ref. 11 to order β^{14} . Only in the case of the body-centered-cubic (bcc) lattice, remarkable progress occurred already two decades ago, with the computation by B. G. Nickel⁽¹²⁾ of expansions for $\chi(\beta; S)$ and $\mu_2(\beta; S)$ through β^{21} . (Exclusively the series for $S = 1/2, 1, 2, \infty$ were published⁽¹³⁾ at the time.)

Also for the second field-derivative of the susceptibility $\chi_4(\beta; S)$ and for the nearest-neighbor correlation function $G(\beta; S)$, the published data are scarce. On the sc lattice, series for $\chi_4(\beta; S)$ could be derived from the data of ref. 14 up to order β^{14} , and, on the bcc lattice, from the data of ref. 15 up to β^{10} . On the fcc lattice, series for $\chi_4(\beta; S)$ are available⁽¹⁶⁾ through β^{13} . For general spin, only expansions^(8,11) of $G(\beta; S)$ up to order β^{14} on the fcc lattice have been published.

In two dimensions the Ising model is (partially) solved only for spin $S = 1/2$ and, by taking advantage of this property, very long series⁽¹²⁾ have

Table I. The Most Extensive HT Data, Published (or Obtainable from Data in the Literature) Before Our Expansions, for the Nearest-Neighbor Correlation, for the Susceptibility χ , for the Second Moment of the Correlation Function μ_2 , and for the Second Field-Derivative of the Susceptibility χ_4 in the Case of the Ising Models with General Spin

Observable	Lattice	Order	Ref.
G	fcc	14	[11]
χ	sq	21	[13]
χ	sc	15	[10]
χ	bcc	21	[13]
χ	fcc	14	[11]
μ_2	sq	21	[13]
μ_2	sc	15	[10]
μ_2	bcc	21	[13]
μ_2	fcc	14	[11]
χ_4	sq	10	[15]
χ_4	sc	14	[14]
χ_4	bcc	10	[15]
χ_4	fcc	13	[16]

been computed for $\chi(\beta; 1/2)$ and $\mu_2(\beta; 1/2)$ on the square (sq) lattice. For $S > 1/2$ the models are not solvable and they even lack any simple duality property. Series up to β^{21} for $\chi(\beta; S)$ and $\mu_2(\beta; S)$ on the sq lattice have been tabulated in ref. 13 for $S = 1, 2$ and ∞ . On the square and the triangular lattices series for $\chi(\beta; S)$, $\mu_2(\beta; S)$ and $\chi_4(\beta; S)$ up to β^{10} can be computed from the data of ref. 15.

A summary of the HT expansions published until now for the Ising models of general spin appears in Table I.

We have long undertaken a systematic project to realize more flexible and efficient algorithms and codes for graphical HT expansions in two-dimensional⁽¹⁷⁾ and in three-dimensional⁽¹⁸⁻²⁰⁾ lattice spin models. By taking advantage also of the steady increase of computer performances in the last decade, we have been able to extend, in successive steps, the HT series for some of the most widely studied spin models, as well as to update their numerical analyses whenever it was possible to improve significantly the determination of the critical parameters. We have now added several terms (from four up to thirteen) to the HT expansions of various observables for the general spin- S Ising models on the sq, the sc and the bcc lattices. In ref. 20 we have already presented an analysis of these series in the three-dimensional case, which adds further support to the validity of hyperscaling and of universality with respect to the lattice structure and to the the value of the spin. Moreover, our extension of the existing computations has

confirmed the remarkably fast convergence properties of the HT expansions on the bcc lattice and has made possible to understand quantitatively how the approach to scaling depends on the spin S . In particular, the spread of the critical exponents estimates as a function of S , already observed long ago in the study of shorter expansions has been simply explained in terms of the pattern of signs and sizes of the leading corrections to scaling and this insight has been used also to improve the determination of the universal critical parameters in the spirit of the suggestions of refs. 21 and 22.

In deriving these data by an appropriately renormalized linked-cluster method,^(14, 15, 23) we have essentially used the same thoroughly tested code which recently produced⁽¹⁹⁾ series through β^{23} for $\chi(\beta; 1/2)$ and $\mu_2(\beta; 1/2)$ on the sc and the bcc lattices. The correctness of our procedures is ensured by numerous internal consistency checks, as well as by their ability to reproduce established results in simpler particular cases, such as the two-dimensional spin 1/2 Ising model or the one-dimensional spin- S Ising models. Of course, we have made sure that our code also reproduces, through β^{21} , the existing computation of ref. 12 for $S = 1, 2, \infty$, on the bcc lattice and, as far as there is overlap, also the recent computation of ref. 24 for $S = 1/2$ on the same lattice.

Our expansions of $G(\beta; S)$, $\chi(\beta; S)$ and $\mu_2(\beta; S)$ to order β^{25} and of $\chi_4(\beta; S)$ up to β^{23} for spin $S = 1/2, 1, 3/2, 2, 5/2, 3, 7/2, 4, 5, \infty$, in two-dimensions for the square lattice case and, in three dimensions, for the simple cubic and the body-centered cubic lattice cases, are now made available in electronic form⁽²⁵⁾ in order to provide a convenient reference for possible future extensions and further work of analysis and phenomenological applications.

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REFERENCES

1. M. E. Fisher, *Rev. Mod. Phys.* **70**:653 (1998).
2. C. Domb and M. F. Sykes, *Phys. Rev.* **128**:168 (1962).
3. M. E. Fisher, *Phys. Rev. Lett.* **16**:11 (1966); L. P. Kadanoff, *Physics* **2**:263 (1966); D. Jasnow and M. Wortis, *Phys. Rev.* **176**:739 (1968); P. G. Watson, *J. Phys. C* **2**:1883 (1969) and *ibid.* **2**:2158 (1969); R. B. Griffiths, *Phys. Rev. Lett.* **24**:1479 (1970); R. B. Griffiths and J. C. Wheeler, *Phys. Rev. A* **2**:1047 (1970); L. P. Kadanoff, Report at the Newport Beach Conference 1970 (unpublished) and in *Proc. E. Fermi 1970 School on Critical Phenomena*, M. S. Green, ed. (Academic, London 1971); C. Domb, in *Statistical Mechanics at the Turn of the Decade*, E. G. D. Cohen, ed. (Dekker, New York, 1971).

4. C. Domb, in *Phase Transitions and critical Phenomena*, C. Domb and M. S. Green, eds., Vol. 3 (Academic, London, 1974).
5. C. Domb, *The Critical Point* (Taylor & Francis, London 1996).
6. M. E. Fisher, *Physica A* **106**:28 (1981).
7. D. M. Saul, M. Wortis, and D. Jasnow, *Phys. Rev. B* **11**, 2571 (1975); J. P. Van Dyke and W. J. Camp, *ibid.* **9**:3121 (1974).
8. W. J. Camp and J. P. Van Dyke, *Phys. Rev. B* **11**:2579 (1975); W. J. Camp, D. M. Saul, J. P. Van Dyke, and M. Wortis, *ibid.* **14**:3990 (1976).
9. D. M. Saul, M. Wortis, and D. Jasnow, *Phys. Rev. B* **11**:2579 (1975).
10. R. Roskies and P. Sackett, *J. Stat. Phys.* **49**:447 (1987).
11. S. McKenzie, *J. Phys. A* **16**:2875 (1983).
12. B. G. Nickel, in *Phase Transitions: Cargese 1980*, M. Levy, J. C. Le Guillou, and J. Zinn-Justin, eds. (Plenum, New York, 1982); S. Gartenhaus and W. Scott Mc Cullough, *Phys. Rev. B* **38**:11688 (1988); W. P. Orrick, B. Nickel, A. J. Guttmann, and J. H. H. Perk, *J. Stat. Phys.* **102**:795–841 (2001). The expansion coefficients computed in this paper to order 323 for the $S=1/2$ susceptibility can be found at the URL: <http://www.ms.unimelb.edu.au/~tonyg/>.
13. B. G. Nickel and J. J. Rehr, *J. Stat. Phys.* **61**:1 (1990).
14. M. Lüscher and P. Weisz, *Nucl. Phys. B* **300**:325 (1988).
15. G. A. Baker and J. M. Kincaid, *J. Stat. Phys.* **24**:469 (1981).
16. S. McKenzie, *J. Phys. A* **16**:3133 (1983).
17. P. Butera, R. Cabassi, M. Comi, and G. Marchesini, *Comp. Phys. Comm.* **44**:143 (1987); P. Butera, M. Comi, and G. Marchesini, *Nucl. Phys. B* **300**:1 (1988); *Phys. Rev. B* **41**:11494 (1990); P. Butera and M. Comi, *Phys. Rev. B* **46**:11141 (1992); *Phys. Rev. B* **47**:11969 (1993); *ibid.* **50**:3052 (1994); *ibid.* **54**:15828 (1996).
18. P. Butera and M. Comi, *Nucl. Phys. B (Proc. Suppl.)* **63**:643 (1998); *Phys. Rev. E* **55**:6391 (1997); *Phys. Rev. B* **52**:6185 (1995); *ibid.* **56**:8212 (1997); *ibid.* **58**:11552 (1998); *ibid.* **60**:6749 (1999); *Ann. Comb.* **3**:277 (1999).
19. P. Butera and M. Comi, *Phys. Rev. B* **62**:14837 (2000).
20. P. Butera and M. Comi, *Phys. Rev. B* **65**:144431 (2002); hep-lat/0112049.
21. J. Zinn-Justin, *J. Physique (France)*, **42**:783 (1981).
22. J. H. Chen, M. E. Fisher, and B. G. Nickel, *Phys. Rev. Lett.* **48**:630 (1982).
23. F. Englert, *Phys. Rev.* **129**:567 (1963); M. Wortis, D. Jasnow, and M. A. Moore, *Phys. Rev.* **185**:805 (1969); M. Wortis, in *Phase Transitions and Critical Phenomena*, C. Domb and M. S. Green, eds., Vol. 3 (Academic, London, 1974); S. McKenzie, in *Phase Transitions Cargese 1980*, M. Levy, J. C. Le Guillou, and J. Zinn Justin, eds. (Plenum, New York, 1982); G. A. Baker, *Quantitative Theory of Critical Phenomena* (Academic, Boston, 1990).
24. M. Campostrini, *J. Stat. Phys.* **103**:369 (2001).
25. P. Butera and M. Comi, hep-lat/0204007.