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# Series and Monte Carlo Study of High-Dimensional Ising Models

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Ising models in high dimensions are used to compare high-temperature series expansions with Monte Carlo simulations. Simulations of the magnetization on four-, six-, and seven-dimensional hypercubic lattices give consistent values of the critical temperature from both equilibrium and nonequilibrium data for $d=6$ and 7. We tabulate 15 terms of series expansions for the susceptibility for general $d$ and give $J/k_B T_c = 0.092295$ (3) and 0.077706 (2) for $d=6$ and 7. In contrast to five dimensions, where earlier series found nonanalytic scaling corrections, for $d=6$ and 7 the leading scaling correction may be analytic in $T-T_c$. In most cases these expansions gave more accurate results than these simulations.

**KEY WORDS:** Series expansions; Monte Carlo simulation; Ising models; corrections to scaling.

## 1. INTRODUCTION

Series expansions and Monte Carlo simulations are the two standard numerical methods to investigate collective phenomena in discrete models of statistical physics. Here we compare them for high-dimensional Ising models where the critical exponents are known. Modern computers allow the simulation of Ising models with hundreds of millions of spins, and thus make studies of dimensionalities above four much easier. There we know the leading critical exponents, which are those of mean field theory, and

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thus we can check better how reliable our methods are. Eleventh-order series expansions were generated[1] for dimensions below 7 in 1964, and we have now extended these to 15th order in general dimensionality $d$. Thus we can compare the accuracy of series versus Monte Carlo methods for high dimensions.

In particular, we want to find out if we can extract from these numerical data the leading scaling correction factor const $+ (T_c - T)^{\Delta_1}$; theoretically[2] we expect the leading correction to have $\Delta_1 = 1/2$ in five and to be analytic in six and more dimensions. The exact form for these corrections is given in ref. 2, where the general result $\Delta_1 = (d-4)/2$ is quoted, but according to Guttmann[2] at $d = 6$ the analytic correction is modified by a logarithmic factor, and at $d = 7$ we expect additional analytic corrections to possibly overwhelm the $\Delta_1 = 3/2$. Since for Monte Carlo simulation we have developed programs which work in several dimensions (possible for series expansions for some time), we want to compare the accuracy achieved with these two methods[3,4] for a case that should be free of some of the complications of previous comparisons. Apart from obtaining answers for methodological comparisons from the high-dimensional programming methods, these new algorithms may be of practical use in other problems, such as high-dimensional shape space in immunology.[5] We present results for simulations in $d = 4$, 6, and 7 and for analysis for series in $d = 6$ and 7. The series are quoted in general dimensions.

## 2. SIMULATIONS

To simulate $L^d$ spins in $d$ dimensions, mostly we use a usual multispin coding program[6] with four bits per spin to sum up easily the 14 neighbors in up to seven dimensions. After the calculation we compress four words into one to save memory, and in a slight improvement over ref. 4 we need only three lattice lines of length $L$ in the expanded form of four bits per site. Our program is written for workstations and Intel 860-based parallel computers and it is not vectorized.[7] [Each Intel 860 (i860) chip is comparable in speed with an IBM RS/6000 320 workstation if programmed in Fortran; the Intel Hypercube at KFA Jülich allows one to use up to 32 such processors in parallel.] Thus it is suited for slow simulations of large lattices, whereas other programs[8] are better for fast simulations of smaller lattices. Each i860 processor needed a few microseconds to update a spin in Glauber kinetics (heat bath). Our largest lattice sizes are $L^d = 224^4$, $31^6$, and $16^7$, larger than other simulations known to us for the same dimensionalities.[9] A 256M IBM RISC/6000 560 was used for the $31^6$ sample. We started with all spins up and watched how the magnetization then relaxed toward its equilibrium value.

Above four dimensions the critical exponents for the leading behavior are those of mean field theory.[10] Thus the magnetization at the critical temperature relaxes toward zero with time $t$ as $t^{-1/z} = t^{-1/2}$, whereas its equilibrium behavior below $T_c$ is

$$M = B(1 - T/T_c)^{1/2}[1 + O(T_c - T)^{\Delta_1}] \tag{1}$$

An effective kinetic exponent $z$ can be determined from consecutive magnetization values and is plotted versus $1/t$ in Fig. 1 for $K = J/k_B T =$ 0.09225, 0.09230, and 0.09235 and $d = 6$. We see that the middle temperature gives a good extrapolation to the correct $z = 2$, whereas the two other temperatures are plausible upper and lower error limits. Figure 2 shows analogous data in seven dimensions for $K = 0.07769$, 0.07771, and 0.,07776; similarly we conclude that the correct $z = 2$ is obtained for $K =$ $0.07772 \pm 0.00003$. Figure 3 shows that this method fails in four dimensions, where at the presumed[10] critical point $K = 0.14966$ the data first seem to suggest a much higher $z$ value and only for longer times might turn downward to $z = 2$. The method[4,8] of looking at large lattices for rather short times thus has been tested for two to seven dimensions and was found to work in all except for four dimensions, where logarithmic correction factors[10] are expected.

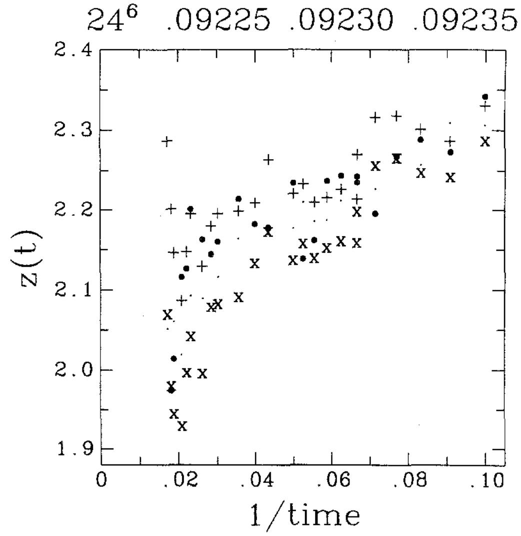


Fig. 1. Effective exponent $z(t)$ versus reciprocal time for six dimensions, for $K = 0.09225$ ($\times$), 0.09230 (dots), and 0.09235 (+). The correct intercept should be $z = 2$. Data for $16^6$ spins agreed with these data for $24^6$ spins. The small dots refer to $32^2 \times 30^4$ spins.

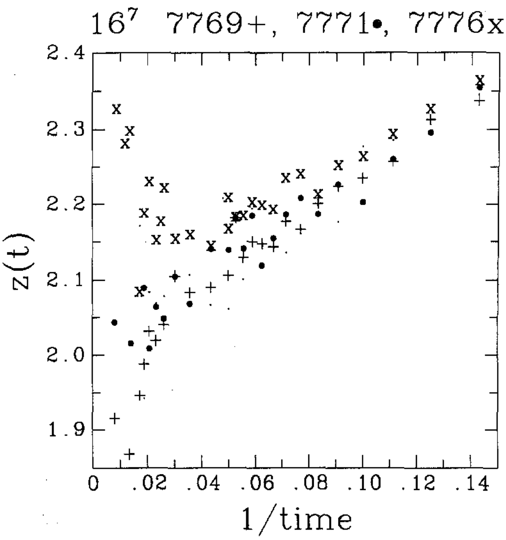


Fig. 2. As for Fig. 1, for $16^7$ spins at $K=0.07769$ (+), 0.07771 (dots), and 0.07776 (×); the small dots refer to $11^7$ sites.

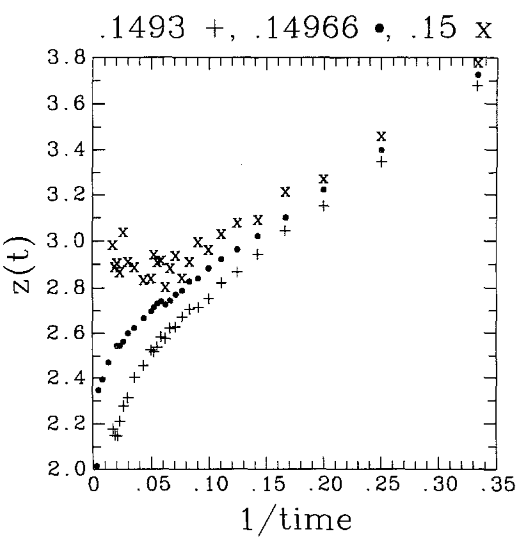


Fig. 3. As for Fig. 1, for $112^4$ spins at $K=0.14930$ (+), $224^4$ at 0.14966 (dots), and $104^4$ at 0.15000 (×).

We also looked at the spontaneous magnetizations in six and seven dimensions and found them to vanish at about the same critical temperatures as found in the above dynamical method. When $K$ approaches its critical value, the slopes $dM^2/dK$ increase toward a finite value related to the critical amplitude $B$, thus confirming $\beta = 1/2$. This increase seems asymptotically linear in $K - K_c$ and is thus consistent with $\Delta_1 = 1$, i.e., with analytic corrections to scaling. However, we found the same behavior also from the five-dimensional data used in ref. 4, where $\Delta_1 = 1/2$ is expected. For $d = 6$ and 7 we found $B = 2.0$ for the amplitude of the spontaneous magnetization, Eq. (1). (Ref. 4 claimed Monte Carlo evidence in favor of $\Delta_1 < 1/2$, but that was based on a wrong interpretation of Fig. 3 there.)

Thus the Monte Carlo simulations gave good values for the critical point and the leading behavior of the spontaneous magnetization, but no clear evidence for a change from nonanalytic to analytic corrections.

## 3. SERIES EXPANSIONS

New 15th-order series have recently been obtained[11] for the susceptibility $\chi$ of the Ising model on hypercubic lattices in general dimension. This is an extension by four terms of the previous enumeration[1] in dimensions below 7 and presumably the first published enumeration for 7 and higher dimensions. The series were generated in the framework of a project to study the Ising model in a random field, and are based on the No-Free-End graph enumerations of Harris.[12] Details of the generation for both the zero-field and the random-field cases are given in ref. 11, but the series for the special case of the zero-field Ising model are presented in this paper in Table I. Some results of the analysis for the five-dimensional case were presented in ref. 4 and we discuss below the results for dimensions six and seven.

Previous series analysis[2] using ratio methods for the six-dimensional 11-term series gave $K_c = 0.092294 \pm 0.000007$ with an imposed $\gamma = 1$ and a deduced quoted $\Delta_1 = 1.02 \pm 0.05$.

The present analysis is based on the expectation that these series will have the general form

$$\chi \propto (K_c - K)^{-\gamma} [1 + a(K_c - K)^{\Delta_1} + b(K - K_c) + \cdots] \qquad (2)$$

where $\gamma = 1$ and $\Delta_1 = (d-4)/2$ for $d > 4$. The logarithmic modification at $d = 6$ is not explicitly handled, and we expect it will lead to a lowering of the effective $\Delta_1$. We have estimated the location of the critical point and both the dominant and correction exponents, $\gamma$ and $\Delta_1$, respectively. Our analysis is carried out with no prior assumptions regarding exponent values. We have studied the series in the $K$ variable with two methods, commonly known as M1 and M2. These have been used and are discussed in refs. 13–15 and a version including three-dimensional visualization is currently being prepared for publication.[16] In both these methods the series are suitably transformed, and Padé approximants to the transformed series should intersect in a three-dimensional ($K_c$, $\gamma$, $\Delta_1$) parameter space.

The $d=6$ series give optimal convergence for both M1 and M2 near $K_c = 0.092295$. The M1 graph for this analysis is given in Fig. 4 for a range of temperatures centered on the above. Note the gaps between the approximants seen at the temperatures 0.092290 and 0.092300, indicating

**Table I. Coefficients $a(n)$ of Our High-Temperature Series for the Susceptibility in Powers of $K$, for General Dimensionality $d$**

$$a(0)=1$$
$$a(1)=2d$$
$$a(2)=-2d+4d^2$$
$$a(3)=2d-8d^2+8d^3$$
$$a(4)=2d+8d^2-24d^3+16d^4$$
$$a(5)=-6d+8d^2+32d^3-64d^4+32d^5$$
$$a(6)=-46d+48d^2-16d^3+112d^4-160d^5+64d^6$$
$$a(7)=122d-352d^2+264d^3-128d^4+352d^5-384d^6+128d^7$$
$$a(8)=1626d-2608d^2+616d^3+528d^4-544d^5+1024d^6-896d^7+256d^8$$
$$a(9)=-(12290/3)d+(42376/3)d^2-(44608/3)d^3+(12512/3)d^4+1312d^5 -1920d^6+2816d^7-2048d^8+512d^9$$
$$a(10)=-91674d+(564500/3)d^2-(331232/3)d^3+(18112/3)d^4+(19040/3)d^5 +3840d^6-6144d^7+7424d^8-4608d^9+1024d^{10}$$
$$a(11)=210594d-(2514440/3)d^2+1125208d^3-(1798528/3)d^4+89312d^5 +8192d^6+12032d^7-18432d^8+18944d^9-10240d^{10}+2048d^{11}$$
$$a(12)=7443926d-(53279924/3)d^2+(43455704/3)d^3-(12613760/3)d^4 -141216d^5+(474304/3)d^6+(14080/3)d^7+37888d^8-52736d^9+47104d^{10} -22528d^{11}+4096d^{12}$$
$$a(13)=-15843566d+(209490208/3)d^2-109272848d^3+77249728d^4 -(72585056/3)d^5+(5765632/3)d^6+(865280/3)d^7-(71168/3)d^8+116736d^9 -145408d^{10}+114688d^{11}-49152d^{12}+8192d^{13}$$
$$a(14)=-829492286d+(6573743096/3)d^2-2155450632d^3+(2865993728/3)d^4 -(456250912/3)d^5-(40569088/3)d^6+(10250752/3)d^7+553728d^8 -144384d^9+349184d^{10}-389120d^{11}+274432d^{12}-106496d^{13}+16384d^{14}$$
$$a(15)=(5091593302/3)d-(39892107016/5)d^2+(41414984488/3)d^3 -(34685058272/3)d^4+(14984743328/3)d^5-(5042989184/5)d^6+44514432d^7 +6060544d^8+(3442688/3)d^9-(1718272/3)d^{10}+1013760d^{11}-1015808d^{12} +647168d^{13}-229376d^{14}+32768d^{15}$$

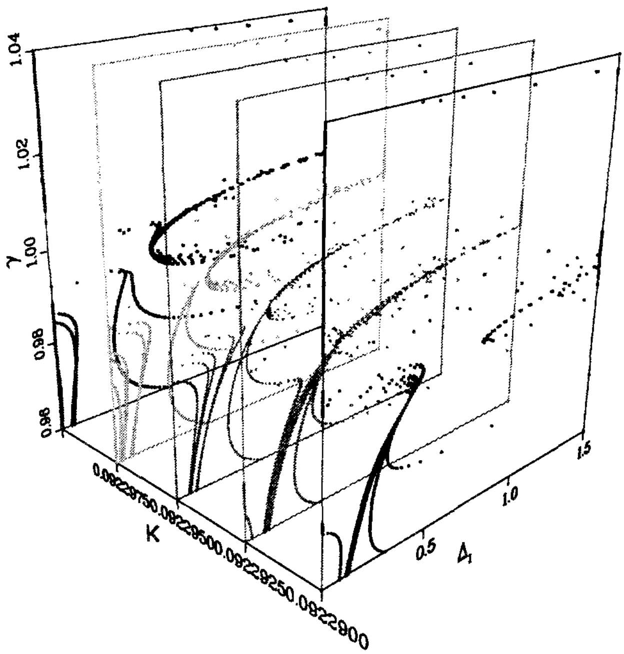


Fig. 4. Three-dimensional plot of approximants to the critical exponent $\gamma$ (known to be 1) as functions of inverse temperature $K$ and correction exponent, for the M1 analysis at $d=6$. Critical parameters correspond to optimal intersection for different curves.

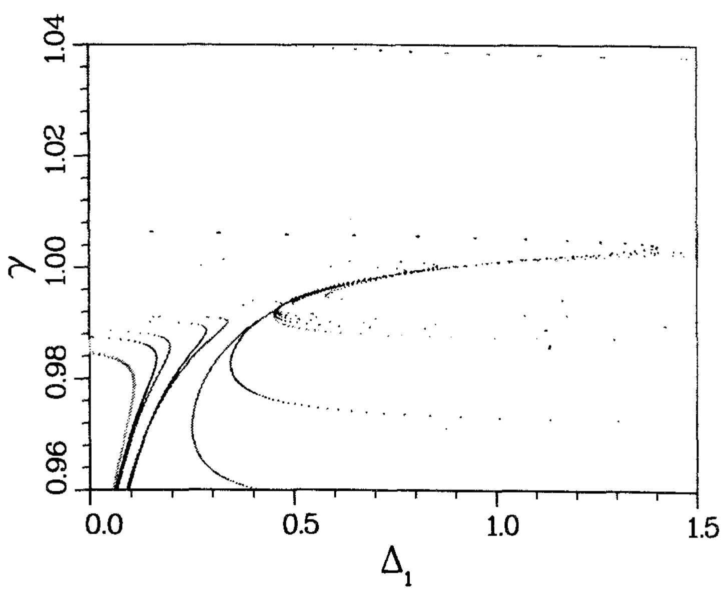


Fig. 5. Two-dimensional plot of approximants to the critical exponent $\gamma$ as functions of the correction exponent, at fixed $K_c = 0.092295$ in $d=6$ for the M1 analysis.

that convergence is found within the three central planes, which is equivalent to quoting $K_c = 0.092295 \pm 0.000003$. The M1 graph for the central temperature is shown in Fig. 5, where we see a nice convergence of approximants for $\Delta_1 = 1.0 \pm 0.3$, with $\gamma = 1.000$ within the limit of reading. The M2 graphs indicate the same $K_c$ choice, but optimal convergence is seen for $\gamma = 0.996$ and near $\Delta_1 \approx 0.75$. We suspect that the latter might represent an effect of the logarithmic correction to the analytic value of $\Delta_1$.

In $d = 7$, convergence was also better in M1, and we present the three-dimensional graph in Fig. 6, leading to a temperature range of $K_c = 0.077706 \pm 0.000002$. From the graph at the central temperature in Fig. 7, we quote $\gamma = 1.00 \pm 0.02$ and $\Delta_1 = 0.8 \pm 0.2$.

Our estimates for the critical point can also be compared with the $1/d$ expansion[1] estimates, which are quoted as $K_c = 0.113789$ and 0.092253 for $d = 5$ and 6. This expansion can be summed to give $K_c = 0.077693$ for $d = 7$. We find the differences to decrease rapidly as $d$ increases from 5 to 7; for 6 and 7 dimensions the discrepancy with the $1/d$ extrapolation is already of the order of our Monte Carlo error.

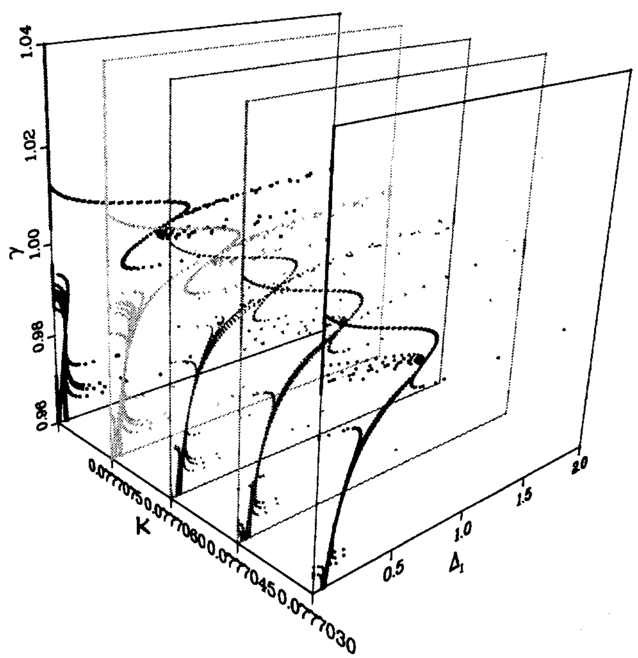


Fig. 6. Three-dimensional plot of approximants to the critical exponent $\gamma$ (known to be 1) as functions of the inverse temperature $K$ and correction exponent, for $d = 7$ for the M1 analysis. Critical parameters correspond to optimal intersection for different curves.

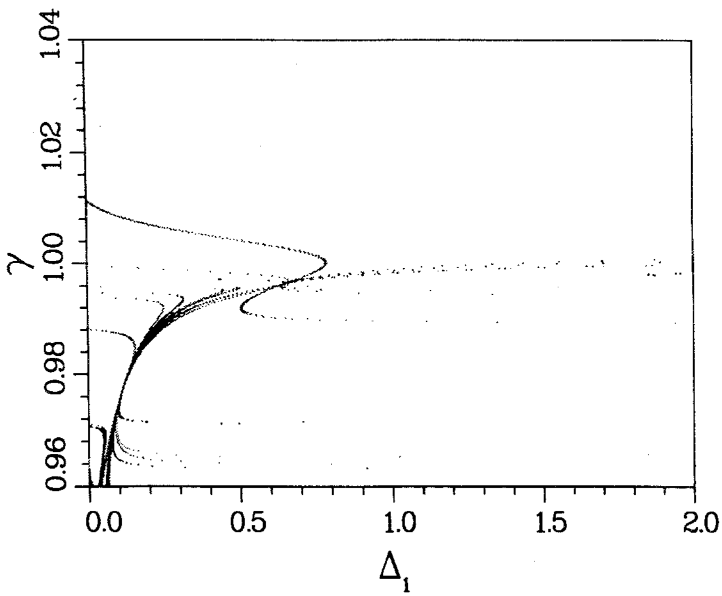


Fig. 7. Two-dimensional plot of approximants to the critical exponent $\gamma$ as functions of the correction exponent, at fixed $K_c = 0.0777060$ in $d = 7$ for the M1 analysis.

In conclusion, for both $d = 6$ and 7, series expansions gave more accurate critical points than Monte Carlo simulations, and the letter gave critical amplitudes for the spontaneous magnetization. Series expansion showed indications of the expected corrections to scaling, while simulations for rather short times yielded estimates of the critical temperature from the behavior of the kinetic exponent $z$. Our techniques can be used to generate series expansions for higher-order susceptibilities and associated universal amplitude ratios, as will be discussed elsewhere.

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