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The high-temperature specific heat exponent of the 3D Ising model

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Abstract. We have extended the high-temperature specific heat series of the three-dimensional spin-$\frac{1}{2}$ Ising model to $O(v^{26})$. Analysis of the new series gives $\alpha = 0.101 \pm 0.004$.

In an earlier paper [1], we gave series to order v^{22} for the high-temperature expansion of the zero-field partition function of the three-dimensional Ising model. More precisely, we gave the coefficients a_n, $n = 0, 22$, defined by

$$Z = 2[\cosh(J/kT)]^3 \Phi(v) \qquad \text{with } \Phi(v) = \sum_n a_n v^n.$$

The series were obtained by the finite-lattice method. One difficulty with the finite-lattice method for this problem is its voracious appetite for computer memory. Our earlier computation, in fact, calculated the series to two further terms—to order v^{26}—but due to addressing limitations, we were unable to retain the intermediate information. This particular calculation requires 2.08 GB of memory, and we were unable to address more than 2 GB, due to operating system limitations. We have now been able to rerun our program under a different operating system that permits us to address this large address space.

The program was run on an IBM 3090/400J with 500 MB of memory and 2 GB of extended storage—a slower type of memory. The use of the MVS operating system allowed the large address space to be used. Even so, two-byte integers were used, and the program was run twice *modulo* two different primes. The results were combined using the Chinese remainder theorem, and provided the least significant digits of the new coefficients; the most significant digits were obtained by differential approximants. The final results were then compared by running with a third prime. Each run took 150 hours.

As a result, we have obtained two further non-zero terms (the partition function being an even function has vanishing odd-order coefficients). We have also obtained the six most significant digits of the $O(v^{28})$ coefficient, by the method of differential approximants. In our earlier paper, we obtained the coefficient of the $O(v^{24})$ coefficient by this method and claimed the coefficient to be $a_{24} = 27\,337 \times 10^7$. The present calculation gives the coefficient as $a_{24} = 273\,374\,177\,222$, verifying our prediction. The subsequent coefficients are found to be $a_{26} = 4\,539\,862\,959\,852$ and $a_{28} = 7\,474\,452 \times 10^7 \pm 5 \times 10^7$, where the last coefficient is obtained by differential approximants. (The approximate coefficient was not used in the

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subsequent analysis, as differential approximants require more accurate coefficients. It is nevertheless useful for ratio-type methods of analysis.)

As we were completing this work, we received a preprint [2] in which a variant of the finite-lattice method, using helical boundary conditions, was used to obtain one further coefficient than we had previously obtained. This work also confirmed our predicted coefficient, and agrees with our exact coefficient. (Note that they give the free-energy series and we give the partition function series). They also predicted a_{26}, and our exact coefficient confirms their predicted value.

We have analysed the new series using several methods. The series is now, for the first time, sufficiently long that the method of differential approximants can be used with some confidence. For our initial analysis, we used unbiased approximants, but for maximum precision we used biased approximants. This requires a knowledge of the critical temperature which has been accurately estimated from the more readily analysed high-temperature susceptibility series, as well as from a variety of Monte Carlo estimates. The series estimates are reviewed in [3] and we use the best estimate given there, $v_c = 0.218093$, which is in good agreement with the most recent high-precision Monte Carlo estimate of $v_c = 0.2180992 \pm 0.0000026$ [4].

Our method of analysis is fully described in [5], and provides a weighted mean of critical exponent estimates from inhomogeneous first-and second-order differential approximants, with one estimate obtained for each order of the series. Our analysis was carried out on the coefficients of the partition function itself. Our unbiased estimates are

$$v_c^2 = 0.04756 \pm 0.00003 \text{ and } 2-\alpha = 1.905 \pm 0.016 \text{ with } K = 1$$

$$v_c^2 = 0.04756 \pm 0.00002 \text{ and } 2-\alpha = 1.897 \pm 0.012 \text{ with } K = 2.$$

In the above, $K = 1, 2$ refers to first- and second-order differential approximants, respectively. The unbiased estimates are seen to be in excellent agreement with the susceptibility series estimate $v_c^2 = 0.0475646$, while an estimate of $\alpha = 0.10 \pm 0.01$ can be made. A biased analysis yields the following estimate:

$$2-\alpha = 1.899 \pm 0.004 \qquad K = 1 \text{ and } 2-\alpha = 1.900 \pm 0.006 \qquad K = 2.$$

Thus, we find from this analysis $\alpha = 0.101 \pm 0.004$. This is substantially more precise than our earlier analysis, using two fewer series coefficients, of $\alpha = 0.104 \pm 0.018$. It is consistent with the analysis of [2] who find $\alpha = 0.104 \pm 0.004$, though, as can be seen, we favour a rather lower value. Note that second-order differential approximants implicitly take correction-to-scaling terms into account. The agreement between first- and second-order differential approximants suggests that correction-to-scaling exponents are weak. A subsequent analysis provides numerical confirmation of this.

Ratio techniques can also be used with this series. We have analysed the free-energy series by a variety of extrapolation methods, based on the observation that if the free-energy $\Psi/kT \sim A(1 - v^2/v_c^2)^{2-\alpha}$, then the ratio of successive coefficients in the series expansion of Ψ/kT behaves like

$$\frac{1}{v_c^2}\left(1 + \frac{\alpha - 3}{n}\right)$$

with higher-order corrections from correction-to-scaling exponents, as well as corrections due to analytic terms. In any event, the sequence of ratios can obviously be rearranged to give a sequence that will converge to α. Neville extrapolation (which takes into account only analytic correction terms), gives $\alpha = 0.103 \pm 0.006$. Other extrapolation methods, such as Levin's u-transform and Brezinski's θ-algorithm, are less accurate, allowing only the estimate $\alpha = 0.10 \pm 0.03$.

In our previous analysis, we also studied the amplitude of the 'correction-to-scaling' term a_θ, where the specific heat is defined to have the scaling form $C \sim A|t|^{-\alpha}[1 + a_\theta|t|^\theta + a_1|t| + \cdots]$, where $t = (T - T_c)/T_c$ and $\theta \approx 0.52$ [6]. In [7], it was argued that a_θ should be negative and our earlier analysis [1] seemed to confirm this, in that we found $a_\theta \approx -0.04$. This can be seen from the behaviour of the ratios of successive coefficients as follows. We first write $C(v) = \sum c_n v^{2n}$, since the expansion we obtain is in terms of the usual high-temperature variable $v = \tanh(J/kT)$. Note that, to leading order, $t = (T - T_c)/T_c = B(v - v_c)/v_c$, where B is a positive constant. It, therefore, follows that the correction-to-scaling amplitude of the specific-heat series expanded in the variable v^2 should also be of negative sign. Writing

$$C(v) = \sum c_n v^{2n} = A(1 - v^2/v_c^2)^{-\alpha}(1 + b(1 - v^2/v_c^2)^\theta + \cdots)$$

it follows that

$$c_n = \frac{A\Gamma(\alpha + n)}{\Gamma(\alpha)\Gamma(n+1)v_c^{2n}}\left[1 + \frac{b\Gamma(\alpha)\Gamma(\alpha + n - \theta)}{\Gamma(\alpha - \theta)\Gamma(\alpha + n)} + \cdots\right].$$

Hence

$$\frac{c_n}{c_{n-1}} = \frac{1}{v_c^2}\left[1 + \frac{\alpha - 1}{n} - \frac{b\Gamma(\alpha)\theta}{\Gamma(\alpha - \theta)n^{\theta+1}} + \mathrm{O}\left(\frac{1}{n^2}\right)\right].$$

Taking $\alpha \approx 0.1$ and $\theta \approx 0.5$, it follows that the above equation can be rewritten as

$$\frac{c_n}{c_{n-1}} = \frac{1}{v_c^2}\left[1 + \frac{\alpha - 1}{n} + \frac{1.28..b}{n^{\theta+1}} + \mathrm{O}\left(\frac{1}{n^2}\right)\right].$$

Hence, we find that

$$\left(\frac{c_n}{c_{n-1}}v_c^2 - 1\right)n + 1 \sim \alpha + \frac{1.28..b}{n^\theta} + \mathrm{O}\left(\frac{1}{n}\right).$$

This means that if $b < 0$, estimators of α, given by the left-hand side of the above equation, should approach α *from below*. In fact, we find the approach to be from above, but a simple n-shift of 1 makes the approach change to an approach from below! Even an analysis taking into account the analytic correction term does not alter this behaviour. To be more precise, we have repeated the above analysis with an additional analytic correction-to-scaling term present and found that the numerical value of b changes sign with an n-shift of just 1. In all cases, the estimate of b is numerically rather small and we conclude that this analysis is not sensitive enough to distinguish b from zero. A similar conclusion, based on a somewhat different analysis, was obtained in [2].

Our estimate of α is rather lower than the field-theory estimate [8] of $\alpha = 0.110 \pm 0.0045$, but the field-theory and series estimates are both (separately) consistent with the hyperscaling relation $d\nu = 2 - \alpha$. Our best series estimate of $\nu = 0.632^{+0.002}_{-0.003}$ implies $\alpha = 0.104^{+0.006}_{-0.009}$, while the best field-theory estimate [6] is $\nu = 0.630$, which implies $\alpha = 0.110$, a value at the centre of the field-theory estimates.

We summarize the various estimates of α in table 1.

Table 1. Summary of α estimates.

α estimate	Method	Reference
0.101(4)	series	this work
0.104(4)	series	[2]
0.1100(45)	field theory	[8]
$0.104^{+0.006}_{-0.009}$	series and hyperscaling	[5]
0.110	field theory and hyperscaling	[6]

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References

[1] Guttmann A J and Enting I G 1993 *J. Phys. A: Math. Gen.* **26** 807–21
[2] Bhanot G, Creutz M, Glässner U and Schilling K 1994 *Phys. Rev.* B **49** 2909
[3] Guttmann A J 1987 *J. Phys. A: Math. Gen.* **21** 1855–63
[4] Ferrenberg A M and Landau D P 1991 *Phys. Rev.* B **44** 5081–91
[5] Guttmann A J 1987 *J. Phys. A: Math. Gen.* **21** 1839–54
[6] Nickel B G 1991 *Physica* **177A** 189–96
[7] Liu A J and Fisher M E 1990 *J. Stat. Phys.* **58** 431
[8] Le Guillou J C and Zinn-Justin J 1980 *Phys. Rev.* B **21** 3976