Universal Amplitude Ratios in the 3D Ising Model

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We present a high precision Monte Carlo study of various universal amplitude ratios of the three dimensional Ising spin model. Using state of the art simulation techniques we studied the model close to criticality in both phases. Great care was taken to control systematic errors due to finite size effects and correction to scaling terms. We obtain $C_+/C_- = 4.75(3)$, $f_{+2nd}/f_{-2nd} = 1.95(2)$ and $u^* = 14.3(1)$. Our results are compatible with those obtained by field theoretic methods applied to the $\phi^4$ theory and high and low temperature series expansions of the Ising model.

1. Introduction

In the neighbourhood of a second order phase transition various quantities display a singular behaviour. In this limit microscopic features become irrelevant and models which differ at the microscopic level may share the same singular behaviour. This is the basis of universality. Different models belonging to the same universality class share the same critical indices. However universality has much stronger implications and it is possible to show that for a given universality class the values of particular critical-point amplitude combinations are unique \cite{1}. In the following we shall be interested in the universality class of the 3 dimensional Ising model which has several interesting experimental realizations, ranging from the binary mixtures to the liquid vapour transitions. The action of the Ising model is given by

$$S = -\beta \sum_{<n,m>} s_n s_m , \quad (1)$$

where $s_n \in \{-1,1\}$ is the field variable and $<n,m>$ is a pair of nearest neighbour sites on the lattice. $\beta \equiv \frac{1}{kT}$ is the coupling. The reduced temperature $t$ can be written as $t = \frac{\beta_c - \beta}{\beta_c}$ where $\beta_c$ is the critical coupling. In the following we consider lattices of volume $L^3$ and periodic boundary conditions.

\textsuperscript{*}Talk presented by M.Hasenbusch
puted \( C_+/C_- \), \( f_{+2nd}/f_{-2nd} \), \( 3 \, C_- / f_{+2nd}^3 B^2 \) and \( C_+/f_{+2nd}^3 B^2 \). The finiteness of the last two quantities relies on the scaling (hyper-scaling) relations \( \alpha + 2 \beta + \gamma = 2 \) and \( d \nu = 2 - \alpha \).

2. numerical results

First we simulated the model in the low temperature phase at \( \beta = 0.2391, 0.23142, 0.2275, 0.2260, 0.2240 \) and \( 0.22311 \) on lattices of size \( L = 30 \) up to \( L = 120 \). From finite size tests at the largest \( \beta \) we concluded that \( L > 20 \xi \) is needed to be save of finite size effects. The total number of measurements was about \( 3 \times 10^6 \) for all \( \beta \)'s. We carefully compared our results with IDA’s of low temperature series expansions and Monte Carlo results given in the literature. In general we found good agreement. For details see ref. [14].

Next we simulated the model in the high temperature phase at \( \beta = 0.20421, 0.21189, 0.21581, 0.21731, 0.21931 \) and \( 0.22020 \). In the high temperature phase only \( L > 6 \xi \) is required to be sufficiently close to the thermodynamic limit. The \( \beta \)-values were chosen such that they pair up with a \( \beta \) in the low temperature phase such that \( \beta_{low} + \beta_{high} = 2 \beta_c \).

This choice of \( \beta \)-values allows to compute for example approximations of \( C_+/C_- \) by \( \Gamma_{\chi}(t) = \frac{\chi(t)}{\chi^\prime(-t)} \) with \( t > 0 \). In this way we need not to extract the \( C_\pm \) themselves and the critical exponent \( \gamma \) does not enter into the calculation. The critical limit is then obtained from a fit to the ansatz

\[
\Gamma_{\chi}(t) = \frac{C_+/C_-}{a_0 t^\theta + a_1 t}.
\]

where we have included the leading corrections to scaling. The best known numerical estimate of the correction exponent is \( \theta = 0.51(3) \). The results for the other amplitude ratios and combinations are extracted analogously. In table 1 we have summarised the approximations of \( C_+/C_- \), \( f_{+2nd}/f_{-2nd} \) and \( u^* = 3C_- / f_{+2nd}^3 B^2 \) for finite \( t \). The last line gives our result for the extrapolation to the critical limit. In addition we have \( C_+/f_{+2nd}^3 B^2 = 3.05(5) \) The largest reduced temperature \( t \) is excluded from the fit in all cases. The errors quoted for the critical limit include errors induced by the uncertainty of \( \beta_c \) and \( \theta \). The \( \chi^2/d.o.f. \) was of order 1 for all quantities.

| \( t \) | \( \Gamma_{\chi} \) | \( \Gamma_{\xi} \) | \( u^* \) |
|-------|-----------------|-----------------|--------|
| 0.0787 | 6.044(5)         | 1.902(2)         | 15.00(6)|
| 0.0441 | 5.546(5)         | 1.920(3)         | 14.75(5)|
| 0.0264 | 5.283(3)         | 1.932(3)         | 14.66(6)|
| 0.0196 | 5.182(5)         | 1.939(3)         | 14.64(5)|
| 0.0106 | 5.027(6)         | 1.942(3)         | 14.47(6)|
| 0.0066 | 4.947(6)         | 1.948(3)         | 14.51(7)|
| 0  | 4.75(3)           | 1.95(2)          | 14.3(1) |

Table 1

The various ratios as functions of the reduced temperature \( t \). The last line gives the extrapolation to the critical limit.

| ref. | \( C_+/C_- \) | \( f_{+2nd}/f_{-2nd} \) | \( u^* \) |
|------|----------------|--------------------------|--------|
| 1 | 4.70(10) |  |  |
| 2 | 4.82(10) |  |  |
| 3 | 4.72(17) | 2.013(28) | 14.4(2) |
| 4 | 4.95(15) | 1.96(1) | 14.8(1.0) |
| 5 | 5.18(33) | 2.06(1) | 17.1(1.9) |

Table 2

Results for the amplitude ratios reported in the literature. They are obtained by \( \epsilon \)-expansion [2], perturbation theory in 3 dimensions [2,3], high and low temperature series expansions of the Ising model [4] and Monte Carlo simulations [5].

3. Comparison with theoretical results and experimental data

In table 2 we have summarised the most recent results for amplitude ratios and combinations for the 3D Ising universality class obtained from \( \epsilon \)-expansion [2], perturbation theory in 3 dimensions [2,3], high and low temperature series expansions of the Ising model [4] and a Monte Carlo study of the Ising model [4]. The results for \( C_+/C_- \) of refs. [2,3,4] are in good agreement with our estimate. Our result is however more accurate. For \( f_{2nd,+}/f_{2nd,-} \) our result is compatible with that of ref. [4], the result from perturbation theory in 3 dimensions [3] is larger then our estimate, however still within a 2\( \sigma \) deviation. There is however a clear discrepancy with the Monte Carlo result of ref. [4]. Their value is much larger...
then our one. For \( u^* \) and \( \frac{C_+}{f_{+2nd}B^2} \), our result is consistent with the other methods. In both cases we could reduce the errors considerably.

The experimental data reported in tab.3 refer to the three most important experimental realizations of the Ising universality class, namely binary mixtures (bm), liquid-vapour transitions (lvt) and uniaxial anti-ferromagnetic systems (af). It is important to notice that these realizations are not on the same ground. Antiferromagnetic systems are particularly apt to measure the \( C_+/C_- \) and \( f_{+2nd}/f_{-2nd} \) ratios, while for the liquid-vapour transitions the \( \Gamma_c \equiv R_c^2/R_0^2 \) combination is more easily accessible. Finally, in the case of binary mixture all the three ratios can be rather easily evaluated. The common attitude is to assume that the above systematic errors are randomly distributed and to take the weighted mean of the various experimental results. The numbers are taken from ref. [1], where more details on the experiments and the averaging procedure can be found.

Table 3
Experimental estimates for some amplitude ratios. (bm) refers to binary mixtures, (lvt) to liquid-vapour transitions and (af) to uniaxial anti-ferromagnetic systems. (all of them) gives an weighted average.

| exp. setup | \( C_+/C_- \) | \( f_{+2nd}/f_{-2nd} \) | \( \frac{C_+}{f_{+2nd}B^2} \) |
|------------|----------------|----------------|----------------|
| (bm)       | 4.8(4)         | 1.93(7)        | 3.01(50)       |
| (lvt)      | 4.9(2)         | 2.83(31)       |                |
| (af)       | 5.1(6)         | 1.92(15)       |                |
| (all of them) | 4.86(46)     | 1.93(12)       | 2.93(41)       |

In the case of the \( f_{+2nd}/f_{-2nd} \) ratio (for which, as we have seen, some of the present theoretical or Monte Carlo estimates disagree) we have listed, for a more detailed comparison, all the available experimental data in tab.17. In this table we denote with “N-H” the nitrobenzene – n-hexane binary mixture, and with “I-W” the one obtained by mixing isobutryric acid and water. A much more detailed account of the various experimental estimates can be found in [1].

A detailed account of our work can be found in ref. [10].

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