New Estimates On Various Critical/Universal Quantities of the 3D Ising Model

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We present estimates for the 3D Ising model on the cubic lattice, both regarding interface and bulk properties. We have results for the interface tension, in particular the amplitude $\sigma_0$ in the critical law $\sigma = \sigma_0 t^\nu$, and for the universal combination $R_- = \sigma \xi^2$. Concerning the bulk properties, we estimate the specific heat universal amplitude ratio $A_+ / A_-$, together with the exponent $\alpha$, the nonsingular background of energy and specific heat at criticality, together with the exponent $\nu$. There are also results for the universal combination $f_s \xi^3$, where $f_s$ is the singular part of the free energy. Details can be found in \cite{1} (interface) and \cite{2} (bulk).

1. INTRODUCTION

In this conference contribution, we summarize recent efforts \cite{1,2} to determine various critical quantities of the 3D Ising universality class using the Monte Carlo (MC) method. These efforts are worthwhile for at least three reasons: 1) There are many systems in nature belonging to the Ising universality class. Thus a comparison of theoretical predictions with experimental results is possible. 2) Getting precise estimates is still a challenge, both from the algorithmic side and from a theoretical point of view. MC data with increasing statistical precision put standard assumptions to test and may require more and more refined theoretical modelling. 3) MC precision has now become competitive with, e.g., high/low temperature series expansions, the $\epsilon$-expansion and 3D field theoretic calculations. Comparing the results is interesting and might point out sources of systematic errors in either method.

2. INTERFACE PROPERTIES

Properties of interfaces separating extended domains of different phases are of great interest, both from the experimental and the theoretical point of view. For recent experimental work measuring observables that are related to and can be compared with quantities studied in the present work, see \cite{3,1}.

Figure 1
Lattice geometry

We consider the 3D Ising model on a cubic lattice of size $L \times L \times T$ with spins $s_x = \pm 1$, Hamiltonian $H(s) = -\beta \sum_{\langle x,y \rangle} s_x s_y$, where $\langle xy \rangle$ denotes a pair of nearest neighbour sites on the lattice, and partition function $Z = \sum_s \exp[-H(s)]$. By $Z_p$ we denote the partition function with periodic boundary conditions in all three directions. Antiperiodic boundary conditions in $t$-direction favour the occurrence of interfaces (perpendicular...
to the $t$-axis), see figure 1. The corresponding partition function is denoted by $Z_s$. If we can assume that there is exactly one interface in the system, its free energy is given by

$$F_s = F_a - F_p + \ln T,$$  \hfill (1)

where $\ln T$ takes care of the free motion of the interface in the $t$-direction.

We obtained the interface free energies by integration of the interface energy $E_s = \langle H \rangle_\sigma - \langle H \rangle_p$:

$$F_s = F_s(\beta_o) + \int_{\beta_o}^{\beta} d\beta' E_s(\beta').$$  \hfill (2)

Various state of the art algorithms were employed: the boundary flip cluster algorithm for the determination of $F_s(\beta_0)$, the Wolff single cluster, the Ising interface cluster and the multispin coded demon algorithm for the determination of $E_s$. Detailed descriptions and the appropriate references can be found in [1].

Interface tensions $\sigma$ were then obtained by fitting the free energies with either

$$F_s \simeq C_s + \sigma L^2$$  \hfill (3)

or

$$F_s \simeq C_s + \sigma L^2 + 1/(4\sigma L^2).$$  \hfill (4)

We chose lattice sizes $32^3$, $48^3$, $64^3$ and $96^3$. Data were taken on a dense grid of $\beta$ values in the range $0.223 \ldots 0.23$. In table 1 we quote a few of our fit results for the interface tension. Here, “fit2” la-

Table 1

| Selection of $\sigma$ estimates |
|---------------------------------|
| fit2       | $\beta = 0.2240$ | $\beta = 0.2255$ |
| fit        | 0.004784(9)      | 0.008810(9)      |
| 96vs64     | 0.004799(17)     | 0.008822(18)     |
| fit3       | 0.004782(6)      | 0.008801(6)      |

bels a fit with eq. (3), discarding the $L = 32$ data, under the name of “96vs64” goes a determination of $C_s$ and $\sigma$ from the $L = 64$ and $L = 96$ data alone, and “fit3” refers to a fit of data from all four lattice sizes with eq. (3). The results from the different fit types are fairly consistent.

Our next task was to fit the interface tension results to the critical law

$$\sigma(\beta) \simeq \sigma_0 \mu^\alpha(1 + a_0\mu^\theta + a_1 t).$$  \hfill (5)

Here we included the leading corrections to scaling terms. We compared the results stemming from the two definitions of the reduced temperature, $t_1 = \beta / \beta_c - 1$ and $t_2 = 1 - \beta_c / \beta$. Furthermore, we fixed the following parameters: $\beta_c = 0.2216544(6)$ [3], $\mu = 1.262$, and $\theta = 0.51$ [3]. These were the most precise estimates we could find in the literature. The fit results are quoted in table 2 again for three different fit schemes.

Table 2

| Fit results for $\sigma_0$, $a_\theta$ and $a_1$ |
|-----------------------------------------------|
| fit   | $t$-def | $\sigma_0$ | $a_\theta$ | $a_1$ |
|-------|---------|------------|------------|-------|
| fit2  | $t_1$   | 1.549(11)  | -0.409(72) | 0.01(20) |
|       | $t_2$   | 1.549(11)  | -0.397(76) | 1.13(21) |
| fit3  | $t_1$   | 1.5428(73) | -0.376(49) | -0.06(14) |
|       | $t_2$   | 1.542(73)  | -0.362(51) | 1.06(14) |
| 96vs64| $t_1$   | 1.571(20)  | -0.57(13)  | 0.47(36) |
|       | $t_2$   | 1.571(21)  | -0.56(13)  | 1.61(37) |

Note that the $\sigma_0$ results for the two $t$-definitions are always consistent with each other. $a_1$ should have a jump of $\mu \approx 1.26$ which is obeyed within the errors. Taking into account the various sources of uncertainty (including the variation with the type of fit) we arrive at the final estimate $\sigma_0 = 1.55(5)$. We finally employed our $\sigma$-data in an estimation of the universal ratio $R_-$. Including corrections to scaling, it can be defined through

$$R_- = \sigma(\beta) \xi(\beta)^2 - c \xi^{-\omega},$$  \hfill (6)

where $\beta \rightarrow \beta_c$ from above. $\omega$ is the correction to scaling exponent. We fixed it to 0.81(5) [3]. The $\xi$-data were taken from [6]. Our result is $R_- = 0.1040(8)$, where the error is mainly due to the uncertainty in the exponent $\omega$. A comparison with some results from the literature is given in [3].
3. BULK PROPERTIES

We consider a 3D Ising model on a cubic lattice of size $L^3$, with periodic boundary conditions in all three directions. Important quantities are the free energy per volume

$$f = -1/(3 L^3) \ln Z,$$

the energy, $E = -df/d\beta$ and the specific heat, $C = dE/d\beta$. The quantities are split in a non-singular and a singular part, e.g., $E = E_{\text{ns}} + E_{\text{s}}$. By standard arguments the following finite size scaling laws are expected to hold:

$$E \approx E_{\text{ns}} + \text{const} L^{−d+1/\nu},$$
$$C \approx C_{\text{ns}} + \text{const} C L^{−d+2/\nu},$$

at criticality, and

$$E \approx E_{\text{ns}} - C_{\text{ns}} \beta_c t \mp A_{\pm} \beta_c \frac{|t|^{1-\alpha}}{1 - \alpha},$$

above and below the transition. Using state of the art algorithms we obtained estimates for energy and specific heat at $\beta_c = 0.2216544$ for $L$ ranging from 12 to 112. The relative error of the energy is of order $10^{-5}$ throughout. We then did a combined fit of energy and specific heat to eq. (8).

$\nu$, $E_{\text{ns}}$ and $C_{\text{ns}}$ are given in Table 3. $L_{\text{min}}$ is the smallest lattice size used for the fit, and $X$ denotes $\chi^2$ per degree of freedom.

| $L_{\text{min}}$ | $X$     | $\nu$    | $E_{\text{ns}}$ | $C_{\text{ns}}$ |
|-----------------|---------|----------|-----------------|-----------------|
| 12              | 5.6     | 0.6316(4)| 0.330229(5)     | -12.13(33)      |
| 16              | 2.25    | 0.6315(8)| 0.330218(7)     | -11.83(61)      |
| 20              | 0.75    | 0.6308(10)| 0.330209(8)     | -11.12(76)      |

Our results for $\nu$, $E_{\text{ns}}$ and $C_{\text{ns}}$ are given in Table 3. $L_{\text{min}}$ is the smallest lattice size used for the fit, and $X$ denotes $\chi^2$ per degree of freedom. We find the precision of the $\nu$-estimate of the last line of the table quite remarkable.

In the off critical case, we always aimed at the infinite volume limit of the energy. Our data cover the range from $\beta = 0.21971$ to $\beta = 0.2230$. Lattice sizes up to $L = 128$ were employed. The results of fits with eq. (8) are given in Table 4. Again we used two definitions of $t$, namely $t_1 = 1 - \beta/\beta_c$ and $t_2 = \beta_c/\beta - 1$. There is a slight mismatch of the estimate for $E_{\text{ns}}$ with the estimates from the critical data in Table 3. It is most likely due to corrections to scaling that have not been taken into account.

We finally estimated the universal constant $f_{s} \xi^3$ on both sides of the transition. Estimates for $f_s$ were obtained by integration over $\beta$ of the singular part of the energy, obtained from the approximation $E_s \approx E - E_{\text{ns}} - C_{\text{ns}}(\beta - \beta_c)$. Using our background estimates $E_{\text{ns}}$ and $C_{\text{ns}}$ together with the correlation lengths given in [6], we obtained $f_s \xi^3 = 0.0355(15)$ for $\beta > \beta_c$, and $f_s \xi^3 = 0.0085(2)$ for $\beta < \beta_c$.

4. CONCLUSIONS

For various interface and bulk quantities we could significantly improve on older numerical estimates. Especially interesting is the quite precise determination of $\nu$ from the finite size scaling of the energy and specific heat at criticality.

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