RECENT RESULTS OF MULTIMAGNETICAL SIMULATIONS OF THE ISING MODEL

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ABSTRACT

To investigate order-order interfaces, we perform multimagnetical Monte Carlo simulations of the 2D and 3D Ising model. Stringent tests of the numerical methods are performed by reproducing with high precision exact 2D results. In the physically more interesting 3D case we estimate the amplitude $F_{s0}$ of the critical interfacial tension.

Keywords: Monte Carlo Simulations; Ising model; Interfaces; Surface tension.

1. Introduction

Since long, there has been continuous interest in the properties of interfaces in Ising models. Past numerical studies were, however, hampered by a problem of principle. The surface tension per unit area $F^*$ between different states has a finite value. Thus in the canonical ensemble, where one samples with the Boltzmann weights $P^{B} \propto e^{-\beta H}$, configurations containing interfaces with an area $A$ are suppressed by exponential factors $e^{-AF^*}$. Corresponding there is an exponentially fast increase of the tunneling time between pure phases when the system is simulated with local Monte Carlo (MC) algorithms. Recently this difficulty was overcome by the proposal to perform the MC simulation for a multimagnetical ensemble, a natural extension of the multicanonical ensemble introduced in (Ref. 2). The original canonical ensemble is then obtained by re-weighting, while the slowing down becomes reduced to a power law close to $\sim V^2$.

For our models, spins $s_i = \pm 1$ are defined on sites of a square lattice of volume $V = L^D$ with periodic boundary conditions and the symbol $<i,j>$ is used to denote nearest neighbors. The partition function of the Ising model is given by

$$Z = \sum_{\text{configurations}} \exp(-\beta H).$$

(1.1)

The Ising Hamiltonian $H$

$$H = H_I - h M \quad \text{with} \quad H_I = -\sum_{<i,j>} s_i s_j \quad \text{and} \quad M = \sum_i s_i$$

(1.2)

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contains the nearest neighbor interaction term $H_I$ and a term which couples the external magnetic field $h$ to the magnetization. In our case is $h = 0$. In the broken region $\beta > \beta_c$ the magnetic probability densities $P_L(M)$ are double peaked and $P_L(M) = P_L(-M)$, as the model is globally $Z(2)$ symmetric. The positions of the maxima are $\pm M_L^{\text{max}}$ and the distribution takes its minimum at $P_L^{\text{min}} = P_L(0)$.

The surface tension $F^s$ is the free energy per unit area of the interface between coexisting phases. Here we consider order-order interfaces in the broken region $\beta > \beta_c$. The magnetic probability densities $P_L(M)$ are double peaked and $P_L(M) = P_L(-M)$, as the model is globally $Z(2)$ symmetric. The positions of the maxima are $\pm M_L^{\text{max}}$ and the distribution takes its minimum at $P_L^{\text{min}} = P_L(0)$.

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The function $\alpha_L(M)$ is then defined by the recursion relation
\[
\alpha_L(M + 2) = \alpha_L(M) + \beta [h_L(M) - h_L(M + 2)] (M + 2), \quad \alpha_L(-M_{L}^{\text{max}}) = 0. \tag{2.3}
\]
Once $h_L(M)$ is given, $\alpha_L(M)$ follows automatically. With this choice the resulting multimagnetical probability density will be approximately flat:
\[
P_{L}^{\text{mm}}(M) = n(M) P_{L}^{\text{mm}}(M) \approx \text{const.} \tag{2.4}
\]
Here $n(M)$ is the magnetical density of of states (for fixed temperature $\beta^{-1}$). The standard Markov process is well-suited to generate configurations which are in equilibrium with respect to this multimagnetical distribution. The canonical probability density $P_L(M)$ is obtained from $P_{L}^{\text{mm}}(M)$ by re-weighting\textsuperscript{3,4}:
\[
P_L(M) = c P_{L}^{\text{mm}}(M) \exp(-\alpha_L(M) - h_L(M)\beta M). \tag{2.5}
\]
The constant $c$ is obtained by imposing the appropriate normalization on $P_L(M)$.

For small systems $P_L(M)$ can be calculated by performing standard MC simulations, and $h_L(M)$ follows directly from “Eq. 2.2”. On larger systems we get $h_L(M)$ by making every time a FSS prediction of $P_L(M)$ from the already controlled smaller systems.

To compare the efficiency of our method with standard MC we measured for the 2D Ising model with $\beta = 0.5$ the tunneling time $\tau_L^t$. As before\textsuperscript{1,2} we define the tunneling time $\tau_L^t$ as the average number of updates needed to get from a
configuration with $M = M_{\text{min}} = -M_{\text{max}}$ to a configuration with $M = M_{L}^{\text{max}}$ and back. In figure 2 we display on a log-log scale both the tunneling times for the multimagnetical MC and the heatbath algorithm. While there is an exponential fast increase of $\tau^{L}_{t}$ for the heatbath algorithm, the increase of $\tau^{L}_{t}$ is for the multimagnetical MC of the type of a power law divergence. The ratio

$$R = \tau^{L}_{t}(\text{heatbath})/\tau^{L}_{t}(\text{multicanonical})$$

is a direct measure for the improvement due to our method. $R$ increases from a factor 4 for the smallest lattice ($L = 2$) up to $R \approx 450$ for $L = 16$, the largest lattice size where it was with our statistics possible to get data from standard MC. The extrapolation to $L = 100$ yields $R \approx 6.1 \times 10^{15}$, i.e. an improvement by more than fifteen orders of magnitude.

3. Numerical Results

For the two dimensional Ising model we performed multimagnetical simulations at the critical temperature $\beta = \beta_{c} = \ln(1 + \sqrt{2})/2 = 0.44068...$, at $\beta = 0.47$ and 0.5 with at least $4 \times 10^{6}$ sweeps per lattice size. In each run additional 200,000 initial sweeps without measurements were performed for reaching equilibrium with respect to the multimagnetical distribution. We compared our $L = \infty$ estimates of the tension with the exact values which follow from Onsager’s equation

$$F^{s} = 2\beta - \ln \left[ \frac{1 + e^{-2\beta}}{1 - e^{-2\beta}} \right], \ (\beta \geq \beta_{c}).$$
Both are collected in table 1. Good agreement is found in all cases.

Table 1. Surface tensions $F^s$ for the 2D Ising model

| $\beta$  | $F^s_{\text{mm}}$ | $F^s_{\text{exact}}$ |
|----------|------------------|----------------------|
| $\beta_c$| 0.00033(34)      | 0                    |
| 0.47     | 0.11526(80)      | 0.11492...           |
| 0.5      | 0.2281(5)        | 0.22806...           |

In the case of the 3D Ising model we performed simulations at $\beta = 0.227$, 0.232 and 0.2439 with at least $4 \times 10^6$ sweeps for every lattice size. As in the 2D case 200,000 additional, initial sweeps were performed in each run for reaching equilibrium. In figure 4 we display the effective tensions as functions of the lattice size together with asymptotic fits. We notice that finite size effects play a more important role in three dimensions than two and are more complicated, too. The non-monotone behaviour shows that it is necessary to use large enough lattices to estimate the interface tension.

The value $\beta = 0.232$ was chosen, because it enables a comparison with the recent literature. In (Ref. 8) cluster improved estimators were used to calculate correlations for $L = 8 - 14$ in a cylindrical geometry. Fitting the obtained tunneling mass gaps yields $F^s = 0.03034 \pm 0.00015$ for the surface tension, when systematic errors are admitted, this is consistent with our value. All our $F^s$ (see table 2) values
are much higher than the old estimates of (Ref. 6), which had to rely on far too small lattices. Our estimates are also consistent with the values presented by Münster and Potvin in other talks on this workshop.

Table 2. Surface tensions $F^*$ and the amplitude $F_0^*$ for the 3D Ising model

| $\beta$ | $F^*$     | $F_0^*$   |
|---------|-----------|-----------|
| 0.227   | 0.01293(17) | 1.455(9)  |
| 0.232   | 0.03140(14) | 1.581(7)  |
| 0.2439  | 0.07403(30) | 1.513(6)  |

Of particular interest in the 3D Ising model are amplitude ratios which involve the amplitude $F_0^*$ of the critical 3D interfacial tension, because they can be compared with a variety of experimental results for fluids which are supposed to populate the Ising model universality class. The other amplitudes are fairly accurately known, and the uncertainty in the ratios stems mainly from $F_0^*$. Old estimates of $F_0^*$ (Ref. 6) led to amplitude ratios which are in disagreement with the experimental results, whereas Mon obtained consistency by calculating the excess energy between a system with an interface imposed by an antiperiodic boundary condition and a system without such an interface and with periodic boundary conditions.
The asymptotic behaviour of the interface tension for $\beta \to \beta_c$ is

$$F^s = F^s_0 t^\mu, \quad (3.2)$$

where $t = (1 - \beta_c/\beta)$ is the reduced temperature and $\mu = 1.26$ in 3D. Our $t$-values are small enough to apply this formula. The results for the amplitude are included in table 2. By averaging over our three values we get

$$F^s_0 = 1.52 \pm 0.05, \quad (3.3)$$

cmpared to Mon’s value $F^s_0 = 1.58 \pm 0.05$ (Ref. 15).

4. Conclusion

Multimagnetical simulations allow to study the magnetic probability density in the broken region with a hitherto unreached precision. Our numerical calculations for the 2D Ising model agree well with the exact results. For the 3D Ising model we obtain new surface tension estimates, which agree reasonably with (Ref. 8, 9, 10), and for our amplitude good agreement is found with Mon (Ref. 15).

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