Interface tension and the cluster exchange algorithm

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Plan of the talk

- 3D Ising and Blume-Capel model
- Anti-periodic boundary conditions
- Exchange cluster algorithm
- Numerical results
- Conclusions

M. H., *The interface tension in the improved Blume-Capel model*, arXiv:1707.05665, Phys. Rev. E 96, 032803 (2017)

We study a simple cubic lattice with periodic boundary conditions in 3 dimensions. The reduced Hamiltonian of the Ising model

$$H = -\beta \sum_{x,\mu} J_{x,\mu} s_x s_{x+\hat{\mu}}$$

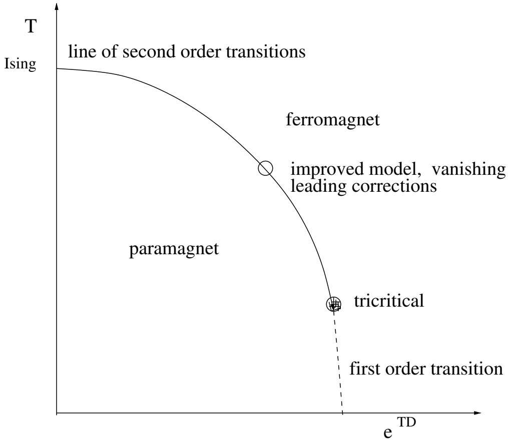
$x_i \in \{0, 1, 2, ..., L_i - 1\}$, $\mu = 0, 1, 2$, $\hat{\mu}$ unit-vector in μ-direction $s_x \in \{-1, 1\}$ and $J_{x,\mu} \in \{-1, 1\}$ quenched variable; $J_{x,\mu} = 1$, if not specified otherwise; $\beta = 1/kT$; $Z = \sum_{\{s\}} \exp(-H[\{s\}])$

In our context: simplified model of a binary liquid mixture or solid in equilibrium with its vapor.

Generalization: Blume-Capel model

$$H = -\beta \sum_{x,\mu} J_{x,\mu} s_x s_{x+\hat{\mu}} + D \sum_x s_x^2 \quad , \quad s_x \in \{-1, 0, 1\}$$

Phase diagram of the Blume-Capel model



MH 2010

$D^* = 0.656(20)$

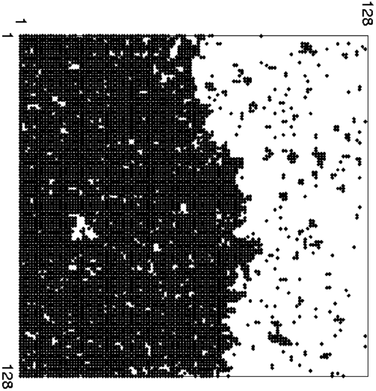
Deng,Blöte 2004

$D_{tri} = 2.0313(4)$

Anti-periodic boundary conditions

Set $J_{x,\mu} = -1$ for $x_0 = L_0 - 1$ and $\mu = 0$

$\Longrightarrow$ Translational invariance in 0-direction



Interface free energy for anti-periodic boundary conditions

$$F_s = -\ln(Z_a/Z_p) + \ln L_0$$

periodic/anti-periodic boundary conditions: no/one interface

Alternatives:
- different ensemble; E.g. fixing magnetisation $m = 0$
- Histogram method (pioneered by Binder) , Multicanonical simulations;

Monte Carlo Simulations

boundary-flip cluster algorithm (M.H. 1993) that allows to directly compute $Z_{\mathrm{a}}/Z_{\mathrm{p}}$
Rough idea: Simulate an ensemble with the type of the boundary condition b as variable; $Z = Z_a + Z_p$. Clusters are constructed as for the Swendsen-Wang cluster algorithm. If there is no cluster that wraps around the torus, the boundary conditions can be flipped along with the cluster update.

$$\frac{Z_a}{Z_p} = \frac{\langle \delta_{b,a} \rangle}{\langle \delta_{b,p} \rangle}$$

Efficient as long as $\frac{Z_a}{Z_p}$ is not too small

For large σA: Integration over β (very old idea)

$$F_s(\beta) = F_s(\beta_0) + \int_{\beta_0}^{\beta} \mathrm{d}\tilde{\beta} \;\; E_s(\tilde{\beta})$$

where $E_s = E_a - E_p$

$$E = -\frac{\partial \ln Z(\beta)}{\partial \beta} = \frac{\sum_{\{s\}} \exp[-\beta H(\{s\})] \, H(\{s\})}{\sum_{\{s\}} \exp[-\beta H(\{s\})]} = \left\langle \sum_{x,\mu} J_{x,\mu} s_x s_{x+\hat{\mu}} \right\rangle$$

In practice: simulate at $O(100)$ values of β and perform numerical integration by using e.g. the trapezoidal rule.

Variance reduced estimator for $E_s = E_a - E_p$ based on the exchange cluster algorithm (Redner, Machta, and Chayes 1998)

swap spins between two systems; here periodic and anti-periodic

$$\begin{aligned} s'_{a,x} &= s_{p,x} \\ s'_{p,x} &= s_{a,x} \end{aligned}$$

Probability to delete link $p_{d,<xy>} = \min[1, \exp(-2\beta_{embed,<xy>})]$

$$\beta_{embed,<xy>} = \beta \frac{J_{p,<xy>} + J_{a,<xy>}}{4} (s_{p,x} - s_{a,x})(s_{p,y} - s_{a,y})$$

Hence

$$\beta_{embed,<xy>\in B} = 0 \quad \text{and} \quad \beta_{embed,<xy>\notin B} = \frac{\beta}{2}(s_{p,x} - s_{a,x})(s_{p,y} - s_{a,y})$$

where B is set of pairs $< xy >$ with $x_0 = 0$ and $y_0 = L_0 - 1$

For $J_{p,<xy>} \neq J_{a,<xy>}$ external field:

$$h_{embed,x,<xy>} = \beta \frac{J_{p,<xy>} - J_{a,<xy>}}{4} (s_{p,x} - s_{a,x})(s_{p,y} + s_{a,y})$$

At B:

$$h_{x,<xy>,embed} = \frac{\beta}{2} (s_{p,x} - s_{a,x})(s_{p,y} + s_{a,y})$$

$$p_{d,h} = \min[1, \exp(-2h_{x,embed})]$$

Alignment of configurations

- Translate the configurations such that the physical interface is located at $x_0 = 0, L_0 - 1$
- Change sign of the spins such that the magnetisation of both systems is the same

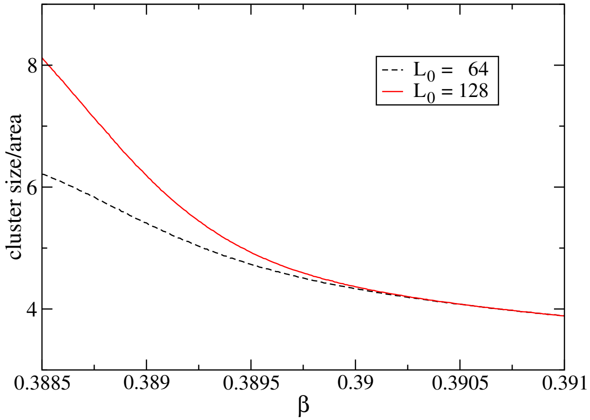
Idea: Swap as many spins as possible

Variance reduction: contributions to observables from swapped clusters exactly cancel

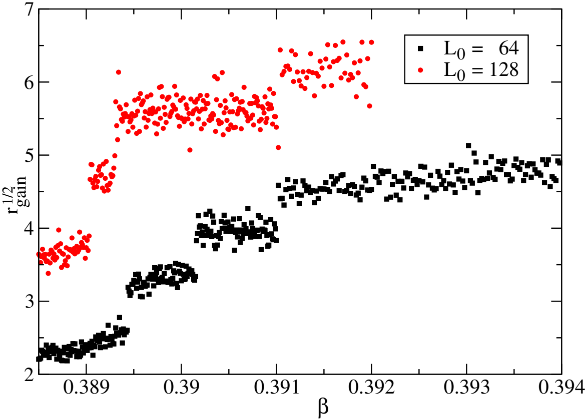
Update/measurement cycle:

- Align configurations
- Construct exchange clusters; Start with magnetic field at the boundary; perform the measurement
- Unalign: random shift; random overall sign

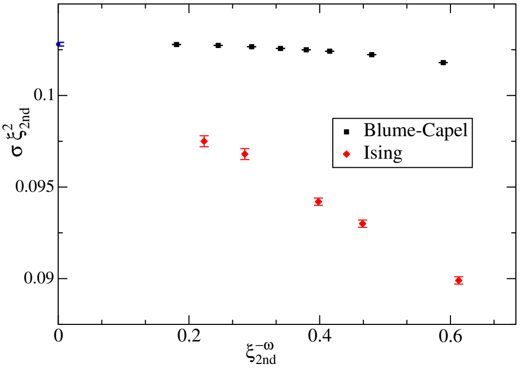
Size of the frozen clusters per area



Improvement achieved by the variance reduced estimator, $L = 64$



$$\sigma = \sigma_0(-t)^{\mu}(1+a_{\sigma}(-t)^{\theta}+ct\ldots) \quad , \quad \mu = 2\nu$$



$$R_{2nd,+} = \sigma_0 f^2_{2nd,+} = 0.3863(6), \; R_{2nd,-} = \sigma_0 f^2_{2nd,-} = 0.1028(1),$$
$$R_{exp,-} = \sigma_0 f^2_{exp,-} = 0.1077(3)$$

Summary of experimental results for various binary liquid mixtures:
M. R. Moldover, Interfacial tension of fluids near critical points and two-scale-factor universality, Phys. Rev. A **31**, 1022 (1985)

$$R_+ = 0.386$$

study of a cyclohexane-aniline mixture:
T. Mainzer and D. Woermann, (1996)

$$R_+ = 0.41(4)$$

Brézin and Feng (1984) to order ϵ^2, $R_{2nd,-} =\approx 0.051$ up to ≈ 0.057

Münster, semiclassical calculation at one-loop level (1990);
P. Hoppe and G. Münster, two-loop level (1998)

$$R_{2nd,-} = 0.1088(2)$$

Conclusions and outlook

Universal amplitude ratios $R = \sigma_0 f^2$ computed to high precision

Cluster exchange algorithm:

- Thermodynamic Casimir effect
- Correlation function for Z_2 symmetry breaking

Further applications of the variance reduced estimator based on the exchange cluster algorithm? Defect properties

Thanks for your attention!

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Alternate: Define a family of systems that interpolate between periodic and anti-periodic boundary conditions

$$J_b = \frac{2i}{N_r} - 1 \quad , \quad i \in \{0, 1, ..., N_r\}$$

then

$$\frac{Z_a}{Z_p} = \prod_{i=1}^{N_r} \frac{Z_{i-1}}{Z_i}$$

Defining

$$H_R = -\beta \sum_{x_1,x_2} s_{0,x_1,x_2} s_{L_0-1,x_1,x_2}$$

we get

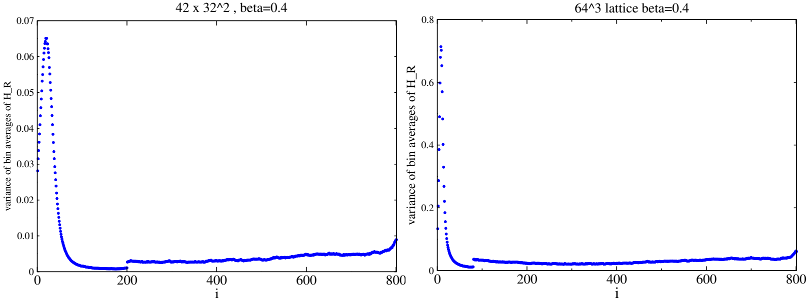
$$F_s^{(1)} = \ln L_0 - \ln \frac{Z_a}{Z_p} = \ln L_0 - \int_{-1}^{1} \mathrm{d}J_b \, \langle H_R \rangle_{J_b}$$

Difficulty for J_b slightly larger than -1:

the entropy gain of the interface moving freely along the lattice and the energetic advantage of sitting at $x_0 = L_0 - 1/2$ compete.

$\Longrightarrow$ large variance of H_R and large autocorrelation times

Parallel tempering simulation; making use of the translational invariance at $J_b = -1$ should eliminate the problem of large autocorrelation times



Running the 64^3 system one month with 42 copies

$$F_s = 118.61255(37)$$