Monte Carlo study of improved lattice models in three dimensions

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CompPhys24, 28 November 2024

Plan of the talk

- improved models
- algorithms
- Renormalization Group and Finite Size Scaling
- How to find the improved model
- Results for critical exponents

General idea:
- Study families of models with an extra parameter
- Tune this parameter such that leading corrections to scaling vanish

Talk based on

M. H., K. Pinn, S. Vinti, Critical Exponents of the 3D Ising Universality Class From Finite Size Scaling With Standard and Improved Actions, Phys.Rev.B 59 (1999) 11471

M. H. and T. Török, High precision Monte Carlo study of the 3D XY-universality class, J.Phys.A 32 (1999) 6361

... some more ...

M. Campostrini, M. H., A. Pelissetto, P. Rossi, E. Vicari, Critical behavior of the three-dimensional XY universality class, Phys. Rev. B 63, 214503 (2001)

... several more ...

M. H., Monte Carlo study of a generalized icosahedral model on the simple cubic lattice, Phys. Rev. B 102, 024406 (2020)

The idea goes back to (using High temperature series expansion)

J. H. Chen, M. E. Fisher and B. G. Nickel, *Unbiased Estimation of Corrections to Scaling by Partial Differential Approximants*, Phys. Rev. Lett. **48**, 630 (1982).

M. E. Fisher and J. H. Chen, *The validity of hyperscaling in three dimensions for scalar spin systems*, J. Physique (Paris) **46**, 1645 (1985).

With Monte Carlo simulations:

H. W. J. Blöte, E. Luijten and J. R. Heringa, *Ising universality in three dimensions: a Monte Carlo study*, J. Phys. A: Math. Gen. **28**, 6289 (1995).

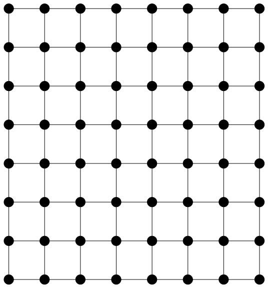
H. G. Ballesteros, L. A. Fernández, V. Martín-Mayor, and A. Muñoz Sudupe, *Finite Size Scaling and "perfect" actions: the three dimensional Ising model*, Phys. Lett. B **441**, 330 (1998).

Lattice model can be seen either as

- discretisation of a field theory in the continuum,
  Representative of universality class of universality class
- (accurate) model of an experimental system, e.g. a magnet

d-dimensional regular lattice; here square, simple cubic

Finite linear lattice size L, periodic boundary conditions: Reduce deviations from thermodynamic limit; translational invariance



x site, $< xy >$ link,
nearest neighbor pair

lattice spacing $a = 1$

(Field) variables live on the sites

Statistical physics:

More or less accurate model of a real world system

Prototype:
Ising model: $s_x \in \{-1, 1\}$ (Lenz/Ising 1924)

Classical Hamiltonian:

$$H(\{s\}) = -J \sum_{<xy>} s_x s_y - h \sum_x s_x$$

$< xy >$: pair of nearest neighbor sites.
Partition function

$$Z = \sum_{\{s\}} \exp\left(-\beta H(\{s\})\right)$$

Note that there are 2^V summands, where V is the number of sites.

ϕ^4-theory on the lattice; reduced Hamiltonian:

$$\mathcal{H}(\{\vec{\phi}\}) = -\beta \sum_{<xy>} \vec{\phi}_x \cdot \vec{\phi}_y + \sum_x \left[\vec{\phi}_x^2 + \lambda(\vec{\phi}_x^2 - 1)^2 + \vec{h} \cdot \vec{\phi}_x\right]$$

where $\vec{\phi} \in \mathbb{R}^N$. Partition function $Z = \int D[\phi] \exp\left(-\mathcal{H}(\{\vec{\phi}\})\right)$

$\lambda = 0$: Gaussian model $\quad \lambda \to \infty$: $|\vec{\phi}_x| = 1$

$\lambda > 0$: second order phase transition

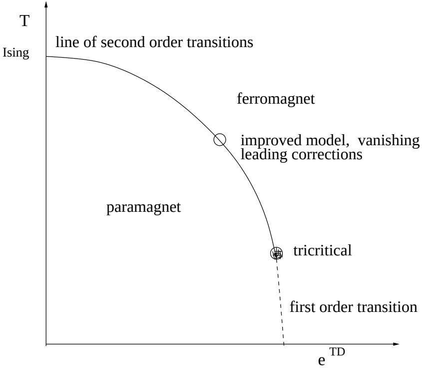
Universality class is the same for all $\lambda > 0$: same symmetry of the order parameter, range of the interaction, dimension of space

$N = 1, 2, 3$: Ising, XY, Heisenberg universality classes

The Blume-Capel model on a simple cubic lattice.

The reduced Hamiltonian

$$\mathcal{H} = -\beta \sum_{\langle xy \rangle} s_x s_y + D \sum_x s_x^2 - H \sum_x s_x \; , \quad \text{where} \;\; s_x \in \{-1, 0, 1\}$$



Algorithms

local Metropolis update

- Proposal (Ising model): $s'_x = -s_x$ for one site x
- Accept with Prop. $\min[1, \exp(-\mathcal{H}(X') + \mathcal{H}(X))]$

critical slowing down cured by cluster algorithms:

R.H. Swendsen and J.-S. Wang, *Nonuniversal critical dynamics in Monte Carlo simulations*, Phys. Rev. Lett. **58**, 86 (1987).

U. Wolff, *Collective Monte Carlo Updating for Spin Systems*, Phys. Rev. Lett. **62**, 361 (1989).

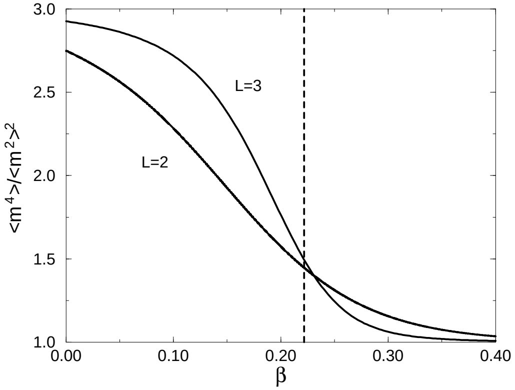
Finite Size Scaling (with dimensionless quantities)

M. P. Nightingale,
Scaling Theory and Finite Systems, Physica 83A, 561 (1976)
Correlation length over linear lattice size: $\frac{\xi}{L}$

K. Binder,
Finite Size Scaling Analysis of Ising Model Block Distribution Functions, Z. Phys. B: Condens. Matter **43**, 119 (1981)
$U_4 = \frac{\langle((\vec{m}^2)^2\rangle}{\langle\vec{m}^2\rangle^2}$ where $\vec{m} = \sum_x \vec{\phi}_x$.

M. N. Barber,
Finite-size Scaling in *Phase Transitions and Critical Phenomena, Vol. 8*, eds. C. Domb and J. L. Lebowitz, (Academic Press, 1983)

Ising model on the simple cubic lattice, summation over all configurations



Our starting point, derived using basic ideas of the RG, see textbooks, reviews (For vanishing external field $h = 0$):

renormalized couplings at scale L

$$\downarrow \qquad \downarrow$$

$$R_i(\beta, \lambda, L) = R_i(u_t(\beta, \lambda) L^{y_t}, \{u_i(\beta, \lambda) L^{y_i}\})$$

for a dimensionless quantity.

The scaling fields $u_t(t, \lambda)$=O(t), $u_j(t, \lambda)$ are analytic functions of the model parameter λ and the reduced temperature $t = \beta - \beta_c(\lambda)$.

Thermal RG-exponent $y_t = 1/\nu > 0$ relevant.
RG-exponents $y_j = d - \Delta_j < 0$ for $j = 3, 4, ...$ irrelevant
Correction exponent $\omega = -y_3 \approx 0.8$, for $-2 \gtrapprox y_j$ for $j \geq 4$.

Improved models

Find value λ^* of the parameter λ such that $u_3(0, \lambda^*) = 0$

Define $\beta_f(\lambda, L)$ such that $[Z_a/Z_p](\beta_f, \lambda, L)$ or $[\xi_{2nd}/L](\beta_f, \lambda, L)$ assumes the fixed value $[Z_a/Z_p]_f$ or $[\xi_{2nd}/L]_f$

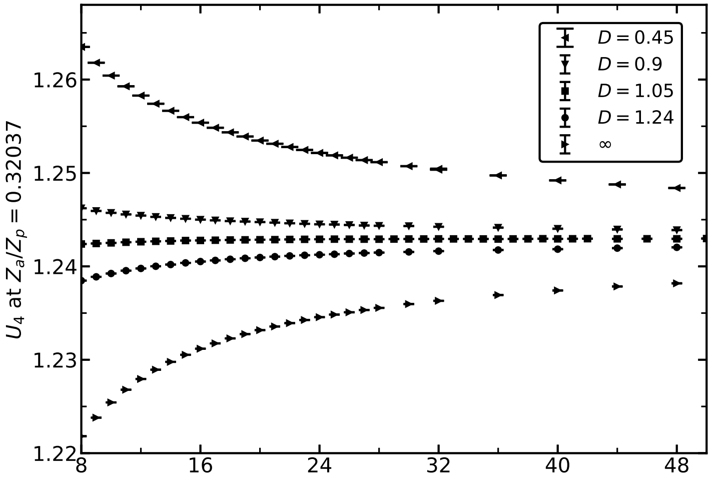
Note that $\lim_{L\to\infty} \beta_f(\lambda, L) = \beta_c(\lambda)$

Then

$$\bar{U}_4(\lambda, L) = U_4(\beta = \beta_f, \lambda, L)$$

XY universality class, generalized clock model

$$\bar{U}_4 = \bar{U}_4^* + b(D)L^{-\omega} + cb^2(D)L^{-2\omega} + d(D)L^{\omega'} + \dots$$



Computing the RG-exponents:

Slopes of dimensionless quantities

$$S_i(\lambda, L) = \left. \frac{\partial R_i(\beta, \lambda, L)}{\partial \beta} \right|_{\beta=\beta_c} = a_i(\lambda) L^{y_t} \left(1 + \sum_j d_{ij}(\lambda) L^{y_j} + \ldots \right)$$

magnetic susceptibility

$$\chi(L, \lambda, \beta = \beta_c) = a_\chi(\lambda) L^{2y_h - d} (1 + d_{\chi,j}(\lambda) L^{y_j} + \ldots) + b(\lambda) + \ldots$$

where $\chi = \frac{1}{L^d} \left\langle \left(\sum_x \vec{\phi}_x \right)^2 \right\rangle$

- Generate data for some range of linear lattice sizes L

- Perform least square fits using various Ansätze, taking more and more corrections into account:

$$S_i(L) = a_i L^{y_t}$$

$$S_i(L) = a_i L^{y_t}(1 + b_i L^{-\omega})$$

$$S_i(L) = a_i L^{y_t}(1 + b_i L^{-\omega} + c_i L^{-2\omega} + d_i L^{-\omega_{NR}})$$

where $\omega \approx 0.8$, $\omega_{NR} \approx 2$

Ising model
simple cubic lattice

magnetic
susceptibility

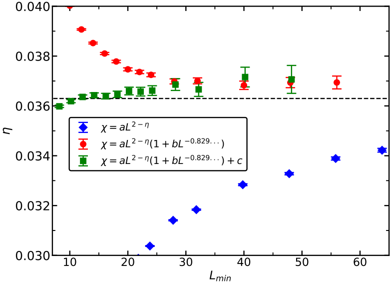
at criticality
$Z_a/Z_p = 0.5425$

Phys. Rev. B 82, 174433 (2010)

New: L=80, 140
About one year on one CPU core

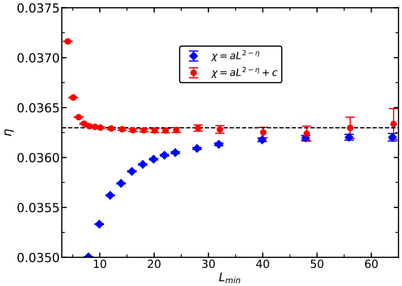
L	chi	error
8	89.053643	0.000483
10	139.069841	0.001090
12	199.856729	0.001608
14	271.344892	0.001989
16	353.474468	0.002898
18	446.210014	0.003371
20	549.505106	0.005417
22	663.299314	0.005123
24	787.579346	0.005908
28	1067.476456	0.013649
32	1388.858443	0.016168
36	1751.692254	0.023604
40	2155.684487	0.045664
48	3086.516434	0.060237
56	4180.457758	0.145556
64	5436.792642	0.173595
80	8432.106069	0.328889
96	12068.067988	0.639970
140	25338.255645	2.375325
400	199253.709891	36.513797

Ising model



L_min	chi^2/DOF	p
12	1.246	0.2330
14	1.213	0.2618
24	2.626	0.0049
28	1.033	0.4082
64	27.724	0.0000

Improved Blume-Capel model with nearest and next-to-next-to nearest neighbour coupling



L_min	chi^2/DOF	p
7	3.082	0.0000
8	1.161	0.2414
9	0.992	0.4795
10	0.928	0.5784
28	3.839	0.0000
32	1.983	0.0129
40	1.033	0.4155

Ising universality class

method	year	ν	η	ω
CB	2024	0.62997097(12)	0.036297612(48)	
CB	2016	0.6299709(40)	0.0362978(20)	0.82968(23
ϵ-exp., 6-loop	2017	0.6292(5)	0.0362(6)	0.820(7)
FRG	2020	0.63012(16)	0.0361(11)	0.832(14)
MC, Ising	1991	0.6289(8)	0.030(11)	≈ 1
HT, var	2002	0.63012(16)	0.03639(15)	0.825(50)
MC, var	2003	0.63020(12)	0.0368(2)	0.821(5)
MC, BC	2010	0.63002(10)	0.03627(10)	0.832(6)
MC, Ising	2018	0.629912(86)	0.03610(45)	
MC, BC, iso	2021	0.62998(5)	0.036284(40)	0.825(20)

taken from Table VI of M. H., *Restoring isotropy in a three-dimensional lattice model: The Ising universality class*, arXiv:2105.09781, Phys. Rev. B 104, 014426 (2021)

XY universality class

method	year	ν	η	ω
ϵ-exp. 5l	1998	0.6680(35)	0.0380(50)	0.802(18)
ϵ-exp. 6l	2017	0.6690(10)	0.0380(6)	0.804(3)
3D-expansion	1998	0.6703(15)	0.0354(25)	0.789(11)
FRG	2020	0.6716(6)	0.0380(13)	0.791(8)
MC+HT	2006	0.6717(1)	0.0381(2)	0.785(20)
MC	2019	0.67183(18)	0.03853(48)	0.77(13)
CB	2016	0.6719(11)	0.03852(64)	
CB	2020	0.67175(10)	0.038176(44)	0.794(8)
MC	2019	0.67169(7)	0.03810(8)	0.789(4)
^{4}He experiment	1996	0.6709(1)		

M.H.: [arXiv:1910.05916], Phys. Rev. B 100, 224517

Shai M. Chester, Walter Landry, Junyu Liu, David Poland, David Simmons-Duffin, Ning Sue and Alessandro Vichi: JHEP06(2020)142 [arXiv:2011.14647]

Heisenberg universality class

method	year	ν	η	ω
3D-exp.	1998	0.7073(35)	0.0355(25)	0.782(13)
ϵ-exp. 5l	1998	0.7045(55)	0.0375(45)	0.794(18)
ϵ-exp. 6l	2017	0.7059(20)	0.0378(5)	0.795(7)
CB	2016	0.7121(28)	0.03856(124)	-
CB	2021	0.71168(41)	0.037872(134)	-
FRG	2020	0.7114(9)	0.0376(13)	0.769(11)
MC	2001	0.710(2)	0.0380(10)	-
MC+HT	2002	0.7112(5)	0.0375(5)	-
MC+HT	2002	0.7117(5)	0.0378(5)	-
MC	2011	0.7116(10)	0.0378(3)	-
MC, icosahedral	2020	0.71164(10)	0.03784(5)	0.759(2)

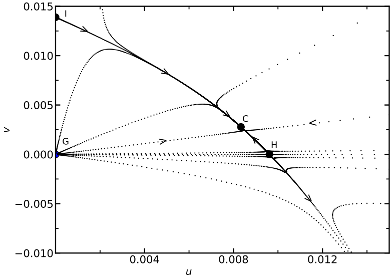
Bootstrapping Heisenberg Magnets and their Cubic Instability, Shai M. Chester, ..., Phys. Rev. D 104, 105013, Editors' Suggestion, (2021) [arXiv:2011.14647]

Recent work: Cubic perturbation

$$\mathcal{H}(\{\vec{\phi}\}) = -\beta \sum_{<xy>} \vec{\phi}_x \cdot \vec{\phi}_y$$

$$+ \sum_x \left[\vec{\phi}_x^{\,2} + \lambda(\vec{\phi}_x^{\,2} - 1)^2 + \mu \left(\sum_a \phi_{x,a}^4 - \frac{3}{N+2} \left(\vec{\phi}_x^{\,2} \right)^2 \right) \right]$$

RG-flow from ϵ-expansion



Generalization of the improvement to a two-parameter theory!

Here mandatory since correction with $0 < \omega_2 \ll 1$

Results are clearly more accurate than field-theoretic ones.

$N = 3$:

$y_{t,cubic} - y_{t,O(N)} = 0.00124(12)$
$Y_4 = 0.0141(10)$, $Y_4 - \omega_2 = 0.00081(7)$

Other universality classes

- $O(4)$, For $N \geq 5$, λ^* does not exist. (For the particular Hamiltonian and the simple cubic lattice)
  Most recent: M.H., Phys. Rev. B 105, 054428 (2020), [arXiv:2112.03783].
- Diluted Ising
  quenched dilution; Harris criterion relevant perturbation of the Ising fixed point;
  $\omega = 0.33(3)$ and $\omega_2 = 0.82(8)$.
  The universality class of 3D site-diluted and bond-diluted Ising systems, M H, F Parisen Toldin, A Pelissetto, E Vicari, Journal of Statistical Mechanics: Theory and Experiment 2007 (02), P02016
- Selfavoiding walk

Applications other than critical exponents:

Universal amplitude ratios, e.g. f_+/f_- , B_+/B_-, A_+/A_- :
In the thermodynamic limit:

$$\xi(t) = f_{\pm} t^{-\nu} (1 + b_{+,-} t^{\Delta} + ...)$$

$$\chi(t) = C_{\pm} t^{-\gamma} (1 + c_{+,-} t^{\Delta} + ...)$$

$$C_h(t) = A_{\pm} t^{-\alpha} (1 + d_{+,-} t^{\Delta} + ...)$$

$\pm$: high and low temperature phase, $t = (T - T_c)/T$ reduce temperature, $\Delta = \omega\nu$.

- Dynamical critical behaviour

- thin films, thermodynamic Casimir Force

- surface/boundary physics:
very recent work by Francesco Parisen Toldin, Max Metlitski:
Boundary Criticality of the 3D O(N): From Normal to Extraordinary
Phys. Rev. Lett. 128, 215701 (2022)

Summary and conclusions

Improved models are useful when studying universal features

There are one or two irrelevant scaling fields with $0 > y_i \gtrapprox -2$

Finite size scaling of RG-invariant quantities used to determine improved parameters

Little computational overhead compared with Ising model or $O(N)$-vector models

Accurate estimates of universal quantities have been obtained for various universality classes

Thank you for your attention!

The work is supported by the DFG under the grants No HA 3150/5-1, HA 3150/5-2, HA 3150/5-3.