Monte Carlo study of improved lattice models in three dimensions

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The Galileo Institute for Theoretical Physics, Firenze,
Bootstrapping Nature: Non-perturbative Approaches to Critical Phenomena,
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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. Hasenbusch 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

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).

Plan of the talk

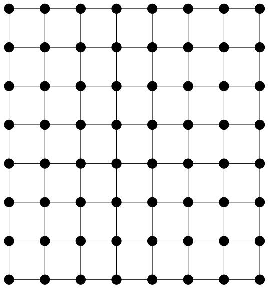
- lattice models
- algorithms (very briefly)
- RG and finite size scaling
- Results for critical exponents
- Work in progress

Lattice model can be seen either as

- discretisation of a field theory in the continuum
- microscopic model of an experimental system, e.g. a magnet

d-dimensional regular lattice; here simple cubic

periodic boundary conditions: Reduce deviations of the finite system from thermodynamic limit; translational invariance



x: site , (x, μ): link;
where μ gives the direction

(Field) variables live on the sites and sometimes on the links.

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:

$$H(\{s\}) = -J \sum_{x,\mu} s_x s_{x+\hat{\mu}} - h \sum_x s_x$$

$\hat{\mu}$: unit vector in μ-direction
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.

Computational methods

- Mean-field
- Lattice perturbation theory
- High/low temperature series expansions
- Transfermatrix (exact/numerical); mainly two dimensions
- Tensor-Network methods
- Monte Carlo simulation

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

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

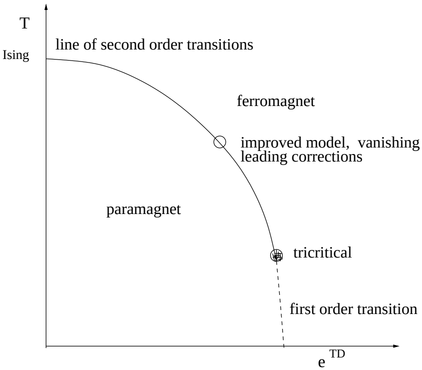
where $\vec{\phi} \in \mathbb{R}^N$. Partition function $Z = \int \mathrm{D}[\phi] \exp\left(-\mathcal{H}(\{\vec{\phi}\})\right)$

Universality (symmetry of the order parameter, range of the interaction, dimension of space)

- $N = 1$: Ising universality class; binary mixtures, bipolar magnets
- $N = 2$: XY universality class; λ-transition of ^{4}He
- $N = 3$: Heisenberg universality class; magnetic systems

The Blume-Capel model on a simple cubic lattice.
The reduced Hamiltonian

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

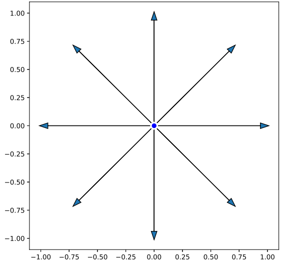


$N = 2$, XY-universality class

Generalization of the q-state clock model. The field assumes one of the following values

$$\vec{s}_x \in \{(0,0), (\cos(2\pi m/q), \sin(2\pi m/q))\} \ , \quad m \in \{1, ..., q\}$$

$$q = 8$$



In the program, we store $\vec{s}_x$ as $m = 0, 1, 2, ..., q$ using an 8 bit char variable.

$N = 3$, Heisenberg universality class

Similar to the XY case:
Field variable assumes one of twelve vectors of unit length which are given by the normalized vertices of the icosahedron as value. Similar to the Blume-Capel model, we add in the generalized model $(0, 0, 0)$ as allowed value.

Regular convex polyhedra:

tetrahedron is selfdual
octahedron is dual to the cube
dodecahedron dual to the icosahedron

We study a simple cubic lattice with periodic/anti-periodic boundary conditions. The reduced Hamiltonian of the $(q+1)$-state clock model

$$\mathcal{H} = -\beta \sum_{\langle xy \rangle} \vec{s}_x \cdot \vec{s}_y - D \sum_x \vec{s}_x^{\,2} - \vec{H} \sum_x \vec{s}_x \, ,$$

Partition function

$$Z = \sum_{\{\vec{s}\}} \prod_x w(\vec{s}_x) \; \exp(-\mathcal{H}) \, ,$$

where

$$w(\vec{s}_x) = \delta_{0,\vec{s}_x^{\,2}} + \frac{1}{q} \delta_{1,\vec{s}_x^{\,2}} = \delta_{0,m_x} + \frac{1}{q} \sum_{n=1}^{q} \delta_{n,m_x}$$

Algorithms

Hybrid of local updates and cluster updates

local updates

- Metropolis
- Overrelaxation
- Toda-Suwa (does not fulfil detail balance)

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

M. P. Nightingale,
Scaling Theory and Finite Systems, Physica 83A, 561 (1976)

K. Binder,
Finite Size Scaling Analysis of Ising Model Block Distribution Functions, Z. Phys. B: Condens. Matter **43**, 119 (1981).

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

Dimensionless quantities R used in finite size scaling study

Binder cumulant

$$U_4 = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$$

Second moment correlation length over lattice size

$$\frac{\xi_{2nd}}{L}$$

Ratio of partition functions

$$\frac{Z_a}{Z_p}$$

with periodic boundary conditions in all d directions (p) and antiperiodic in one and periodic in the remaining (a)

General Hamiltonian with infinitely many terms with some hierarchy

$$H = -\sum_{\alpha} K_{\alpha} \sum_{x} S_{\alpha,x}$$

A blockspin transformation with a scale factor b defines a mapping in the space of coupling constants

$$\vec{K}' = \mathcal{R}(\vec{K})$$

linearize in the neighbourhood of a fixed point $\vec{K}^*$

$$\delta\vec{K}' = T\delta\vec{K}$$

where $\delta\vec{K} = \vec{K} - \vec{K}^*$ and the matrix T is not symmetric in general.
Left eigenvectors, values $\vec{\phi}_j T = \lambda_j \vec{\phi}_j$, RG-exponents $y_j = \frac{\log(\lambda_j)}{\log(b)}$

Scaling field $u_j = \vec{\phi}_j \delta\vec{K}$ transforms as $u_j' = \vec{\phi}_j \delta\vec{K}' = \vec{\phi}_j T \delta\vec{K} = \lambda_j u_j$

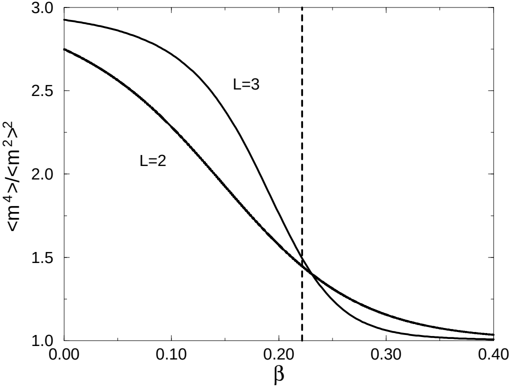
Our starting point, derived using basic ideas of the RG, see textbooks, reviews (For vanishing external field):

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

The scaling fields $u_t(\lambda, t)$=O(t), $u_j(\lambda, t)$ are analytic functions of the model parameter λ, and the reduced temperature $t = \beta - \beta_c(\lambda)$. In particular, there is no singular behaviour at the transition.

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

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



$$\left.\frac{\partial R_i(\beta,\lambda,L)}{\partial \beta}\right|_{\beta=\beta_c} = \left.\frac{\partial R_i(u_t L^{y_t},\{u_j L^{y_j}\})}{\partial t}\right|_{t=0}$$

$$= \left.\frac{\partial R_i(u_t L^{y_t},\{u_j(\lambda,0) L^{y_j}\})}{\partial u_t L^{y_t}}\right|_{u_t L^{y_t}=0} \left.\frac{\partial u_t}{\partial t}\right|_{t=0} L^{y_t}$$

$$+ \sum_j \left.\frac{\partial R_i(0,\{u_j(\lambda,t) L^{y_j}\})}{\partial u_j L^{y_j}}\right|_{u_j L^{y_j}=0} \left.\frac{\partial u_j}{\partial t}\right|_{t=0} L^{y_j}$$

Taylor-expansion:

$$= \left.\frac{\partial R_i(u_t L^{y_t},\{u_j=0\})}{\partial u_t L^{y_t}}\right|_{u_t L^{y_t}=0} \left(1+\sum_j c_{ij} L^{y_j} + \ldots\right) L^{y_t} + \sum_j d_{ij} L^{y_j}$$

$$= a_i \left(1+\sum_j c_{ij} u_j(\lambda,0) L^{y_j} + \ldots\right) L^{y_t} + \sum_j d_{ij} L^{y_j}$$

Improved models

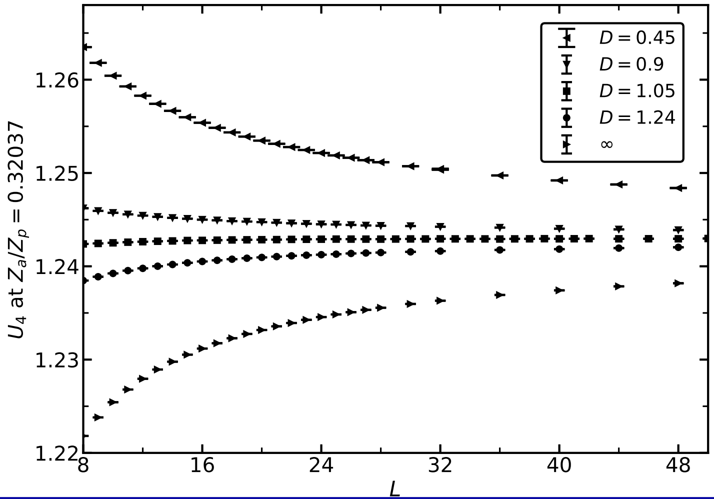
Find value λ^* of the parameter λ such that $u_3(\lambda^*, 0) = 0$

Use U_4 at a given value of Z_a/Z_p or ξ_{2nd}/L:

Find value β_f of β such that Z_a/Z_p or ξ_{2nd}/L assumes the desired value.
Then evaluate U_4 at β_f.

Technically: In the simulation we determine the Taylor-coefficient up to third order around the simulation point $\beta_s \approx \beta_f \approx \beta_c$.

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



Critical exponents are obtained by fitting

Magnetic susceptibility at criticality

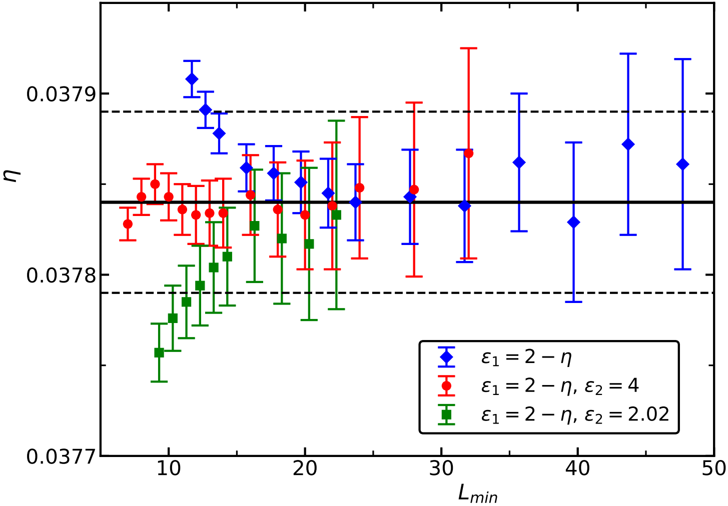
$$\chi \propto L^{2-\eta}$$

The slope of dimensionless quantities at criticality

$$\frac{\partial R}{\partial \beta} \propto L^{1/\nu}$$

and more or less correction terms added (not the leading one)

Fitting data for χ at $Z_a/Z_p = 0.19477$, improved icosahedral model:



Ising universality class

method	year	ν	η	ω
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)
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)
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)		

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)	-
NRG	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]

Work in progress: Cubic perturbation

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

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

Generalization of the improvement to a two-parameter theory!
Here mandatory since there is a correction with $0 < \omega_2 \ll 1$
Peliminary results very encouraging, clearly more accurate than field-theoretic results.

Thank you for your attention!

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