Critical Phenomena, Finite Size Scaling and Monte Carlo Simulations of Spin Models

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Overview

- Critical phenomena and universality
- Lattice models
- Finite size scaling
- Numerical results
- Improved observables

Collaborators over the last 20 years: S. Meyer, A. Gottlob, K. Pinn, S. Vinti, T. Török, M. Campostrini, A. Pelissetto, P. Rossi, E. Vicari
At a second order phase transition various quantities diverge following power laws. For a magnetic system, vanishing external field $h$:

Magnetisation

$$m \sim B(-t)^\beta$$

Specific heat

$$C_h \sim A_\pm |t|^{-\alpha}$$

Magnetic susceptibility

$$\chi \sim C_\pm |t|^{-\gamma}$$

Correlation length

$$\xi \sim f_\pm |t|^{-\nu}$$

Reduced temperature $t = (T - T_c)/T_c$. At the critical point $t = 0$:

Two-point correlation function

$$G(r) \sim r^{-D-\eta+2}$$

The magnetisation

$$m \sim h^{1/\delta}$$
Critical exponents $\beta$, $\gamma$, $\alpha$, $\nu$, $\eta$, $\delta$ and amplitude ratios ($A_+/A_-$, $f_+/f_-$ ... ) universal

Universality class is characterized by:
Dimension of the system, range of interactions Symmetry of the order parameter; ..., Symmetry breaking pattern; disorder

Scaling and Hyperscaling relations:

$$\alpha = 2 - \frac{d}{y_t} \quad \eta = d + 2 - 2y_h \quad \beta = \frac{d - y_h}{y_t}$$

$$\gamma = \frac{2y_h - d}{y_t} \quad \delta = \frac{y_h}{d - y_h}$$

$y_t$ and $y_h$ RG-exponents
Power laws have corrections:

\[ \chi = C_\pm |t|^{-\gamma} \times (1 + at^\theta + bt + ct^{\theta'} + ... ) \]

- non-analytic (confluent) corrections: 
  \[ at^\theta, ct^{\theta'} \]
  where for the 3D systems discussed here \( \theta \approx 0.5 \) and \( \theta' \approx 1 \)

- analytic (non-confluent) corrections: 
  \[ bt \]
We study a simple cubic lattice with periodic boundary conditions in 3 dimensions. The action

\[ S = -\beta \sum_{x,\mu} \vec{s}_x \vec{s}_{x+\mu} - \vec{h} \sum_x \vec{s}_x \]

where \( \beta = 1/(k_B T) \) is the inverse temperature, \( \vec{h} \) an external field and \( \vec{s}_x \) a real \( N \)-component vector with \( |\vec{s}_x| = 1 \). Special names:

- \( N=1 \) Ising model
- \( N=2 \) XY model
- \( N=3 \) Heisenberg model
N-component $\phi^4$ models:

$$S = -\beta \sum_{x,\mu} \vec{\phi}_x \vec{\phi}_{x+\hat{\mu}} + \sum_x \left[ \vec{\phi}_x^2 + \lambda (\vec{\phi}_x^2 - 1)^2 \right] - \vec{h} \sum_x \vec{\phi}_x$$

where the field variable $\vec{\phi}_x$ is a vector with $N$ real components.

The partition function is given by

$$Z = \left[ \prod_x \prod_{i=1}^N \int d\phi_x^{(i)} \right] \exp(-S)$$

E.g. $N = 2$, $\vec{h} = (0, 0)$
The Monte Carlo Simulations

Single Cluster (Wolff 1989) and Wall Cluster algorithms
(Almost no slowing down)
Cluster does not change $|\vec{\phi}| \Rightarrow$ Local Metropolis updates in addition

Our most recent work: Campostrini et al. XY-universality class:
CPU-time: 20 years of 2 GHz Opteron; (QCD code $\approx 1\text{Gflops}$ on such a CPU; i.e. compares with 20 Gflop years of lattice QCD)

Lattice sizes up to $128^3$ on the largest lattice $O(10^5)$ and for $L \lesssim 20$
$O(10^7)$ statistically independent configurations;
Thermodynamic limit: In practice $L \gtrsim 10\xi$ is needed. Therefore only $|t| \gtrsim (\xi_0/L_{\text{max}})^{1/\nu}$ accessible

$\Rightarrow$ Finite Size Scaling

Dimensionless quantities, Phenomenological couplings:

- **Binder Cumulant** $U_4 = \frac{\langle (\vec{m}^2)^2 \rangle}{\langle (\vec{m}^2) \rangle^2}$
  $U_6 = \frac{\langle (\vec{m}^2)^3 \rangle}{\langle (\vec{m}^2) \rangle^3}$ ...  
  where $\vec{m} = \sum_x \vec{\phi}$

- The second moment correlation length over lattice size $\xi_{2nd}/L$

- Ratio of partition functions $Z_a/Z_p$
  - $a$ antiperiodic boundary conditions
  - $p$ periodic boundary conditions
Dimensionless quantities are functions of $L/\xi$:

$$ R(\beta, L) \sim \tilde{R}(L/\xi(\beta)) \sim \hat{R}(L^{1/\nu} t) $$

⇒ At the critical point ($t = 0$): $R$ does not depend on $L$ (Binder crossing)

⇒

$$ \frac{\partial R(\beta, L)}{\partial \beta} \bigg|_{\beta=\beta_c} = aL^{1/\nu} \times (1 + c_s L^{-\omega} + \ldots) $$

Access to $y_h$:

$$ \chi|_{\beta=\beta_c} = bL^{\gamma/\nu} \times (1 + c_\chi L^{-\omega} + \ldots) $$

$$ \omega \approx 0.8 $$
3D Ising model on the simple cubic lattice $L = 2$ and $L = 3$, exact summation:
Eliminating leading corrections to scaling

In general, correction amplitudes $c_s$, $c_\chi$, \ldots depend on the model parameters; Is there a $\lambda^*$ such that $c_s(\lambda^*) = c_\chi(\lambda^*) = \cdots = 0$?? Renormalization group predicts that, if such a $\lambda^*$ exists, it is the same for all quantities!

A phenomenological $R$ coupling behaves

$$R = R^* + a_r(\beta - \beta_c)L^{1/\nu} + c_rL^{-\omega} + \ldots$$

in the neighbourhood of the critical point. Now we require that $R_1$ assumes a value $R_{1,f}$. (For practical purpose $R_{1,f} \approx R^*$)
This defines $\beta_f(L)$ by

$$R_1(\beta_f(L), L) = R_{1,f}$$
Now we compute $R_2$ at $\beta_f(L)$:

$$\bar{R}_2(L) := R_2(\beta_f(L), L) = \bar{R}_2^* + \bar{c}_2 L^{-\omega} + \ldots$$

with

$$\bar{R}_2^* = R_2^* + \frac{a_{r,2}}{a_{r,1}} (R_{1,f} - R_1^*)$$

and

$$\bar{c}_2 = c_2 - \frac{a_{r,2}}{a_{r,1}} c_1$$

In practice: reweighting or Taylor series (here up to third order)
Ising universality class (Hasenbusch 1999) $\lambda^* = 2.15(5)$
XY universality class (Campostrini et al 2006) $\lambda^* = 2.15(5)$
Is there a $\lambda^*$ for any $N$?

Only possible for $N < 4$

Hasenbusch 2001, Monte Carlo Simulation:
$\lambda^* = 4.4(7)$ for $N = 3$  $\lambda^* = 12.5(4.0)$ for $N = 4$
\( \nu \) from fits of the slope of \( U_4 \) (black) and \( Z_a/Z_p \) (red)
Ising Universality Class

<table>
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<th>Authors</th>
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<th>Method</th>
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XY

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$O(4)$

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Leading corrections to scaling:

\[ U_4(\beta_c) = U_4^* \times (1 + c_4 L^{-\omega} + ...) \]

\[ R_\xi(\beta_c) = R_\xi^* \times (1 + c_\xi L^{-\omega} + ...) \]

\[ \frac{\partial U_4}{\partial \beta} \bigg|_{\beta=\beta_c} = a L^{1/\nu} \times (1 + c_{\text{slope}} L^{-\omega} + ...) \]

\[ \chi(\beta_c) = b L^{2-\eta} \times (1 + c_\chi L^{-\omega} + ...) \]
Ratios of correction amplitudes are universal:
\[ r_\xi = c_\xi / c_4; \quad r_{\text{slope}} = c_{\text{slope}} / c_4; \quad r_\chi = c_\chi / c_4 \]

Then define improved observables

\[
U_4(\beta_c)^{-r_\xi} R_\xi(\beta_c) = (U_4^*)^{-r_\xi} R_\xi^* \times (1 + d_\xi L^{-2\omega} + ...) \]

\[
U_4(\beta_c)^{-r_{\text{slope}}} \left. \frac{\partial U_4}{\partial \beta} \right|_{\beta=\beta_c} = \tilde{a} L^{1/\nu} \times (1 + d_{\text{slope}} L^{-2\omega} + ...) \]

\[
U_4(\beta_c)^{-r_\chi} \chi(\beta_c) = \tilde{b} L^{2-\eta} \times (1 + d_\chi L^{-2\omega} + ...) \]
Determine \( r_\xi = c_\xi / c_4; \quad r_{\text{slope}} = c_{\text{slope}} / c_4; \quad r_\chi = c_\chi / c_4 \)

by simulating e.g. Ising, XY or Heisenberg models;

In practice reduction of leading correction amplitude by factor \( O(10) \) possible

Use these improved observables in simulations of:

- Improved models: leading corrections to scaling can be completely ignored; reduction factors by improving the model and improving the observable multiply (!) I.e. a reduction by a factor of 100 to 400 in the amplitude of the leading correction possible. (comparing with standard observables measured in not improved models)

- New models where the universality class should be verified:
  Faster convergence of the Binder Crossing
  Faster convergence of critical exponents
Conclusion:

Most accurate estimates for critical exponents and amplitude ratios for 3D universality classes are obtained from Monte Carlo simulations and high temperature series expansions of lattice models.