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

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EMMI workshop, 18 February 2009

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

$$m \simeq B(-t)^{\beta}$$

Specific heat

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

Magnetic susceptibility

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

Correlation length

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

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

Two-point correlation function

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

The magnetisation

$$m \simeq h^{1/\delta}$$

Critical exponents β, γ, α, ν, η, δ 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:

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

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

y_t and y_h RG-exponents

Power laws have corrections:

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

- non-analytic (confluent) corrections:
  at^{θ}, $ct^{\theta'}$
  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

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

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:

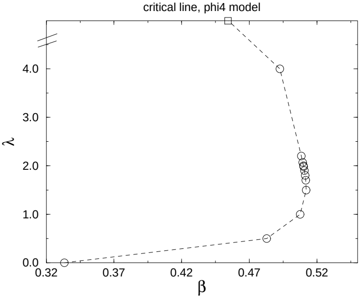
- N=1 Ising model
- N=2 XY model
- N=3 Heisenberg model

N-component ϕ^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.

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



The partition function is given by

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

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 $\approx 1 Gflops$ 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 $L \lessapprox 20$ $O(10^7)$ statistically independent configurations;

Thermodynamic limit: In practice $L \gtrsim 10\xi$ is needed
Therefore only $|t| \gtrsim (\xi_0/L_{max})^{1/\nu}$ accessible

$\Rightarrow$ Finite Size Scaling

Dimensionless quantities, Phenomenological couplings:

- Binder Cumulant $U_4 = \frac{\langle(\vec{m}^2)^2\rangle}{\langle(\vec{m}^2)\rangle^2}$ $\quad U_6 = \frac{\langle(\vec{m}^2)^3\rangle}{\langle(\vec{m}^2)\rangle^3}$ $\quad \ldots$
  where $\vec{m} = \sum_x \vec{\phi}$
- The second moment correlation length over lattice size ξ_{2nd}/L
- Ratio of partition functions Z_a/Z_p
  - a antiperiodic boundary conditions
  - p periodic boundary conditions

Dimensionless quantities are functions of L/ξ:

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

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

$\Rightarrow$

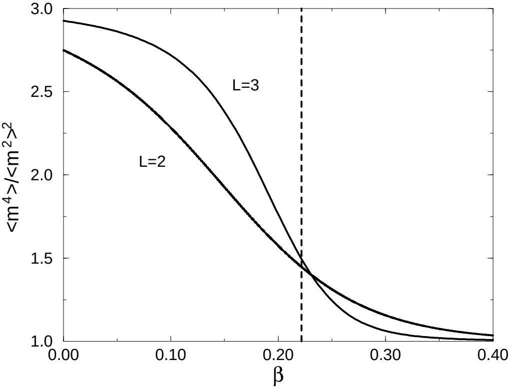
$$\left. \frac{\partial R(\beta, L)}{\partial \beta} \right|_{\beta=\beta_c} = a L^{1/\nu} \times (1 + c_s L^{-\omega} + \ldots)$$

Access to y_h:

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

$\omega \approx 0.8$

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

A phenomenological R coupling behaves

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

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

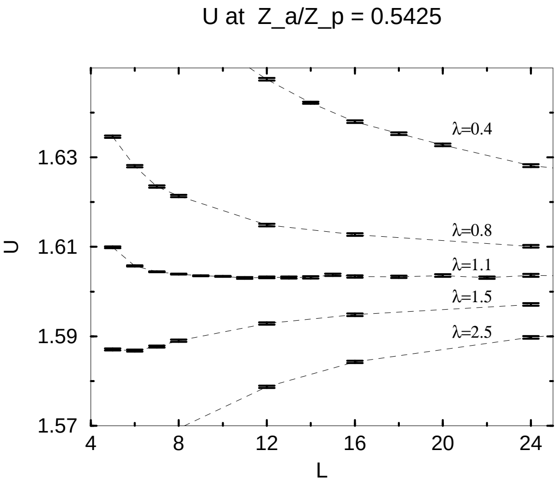
$$\bar{R}_2^* = R_2^* + \frac{a_{r,2}}{a_{r,1}}(R_{1,f} - R_1^*)$$

and

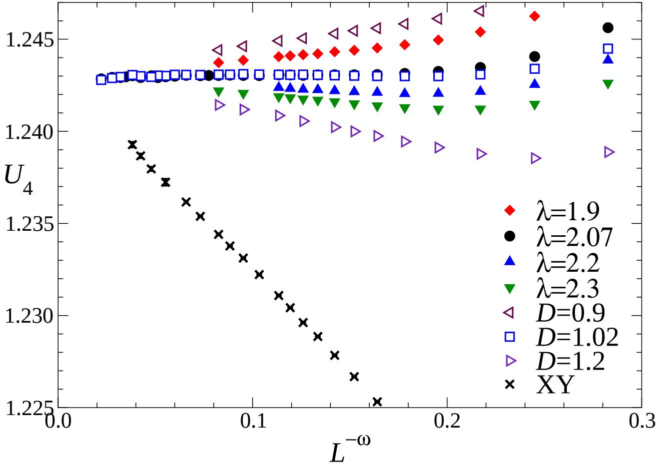
$$\bar{c}_2 = c_2 - \frac{a_{r,2}}{a_{r,1}} c_1$$

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) $\lambda^* = 2.15(5)$

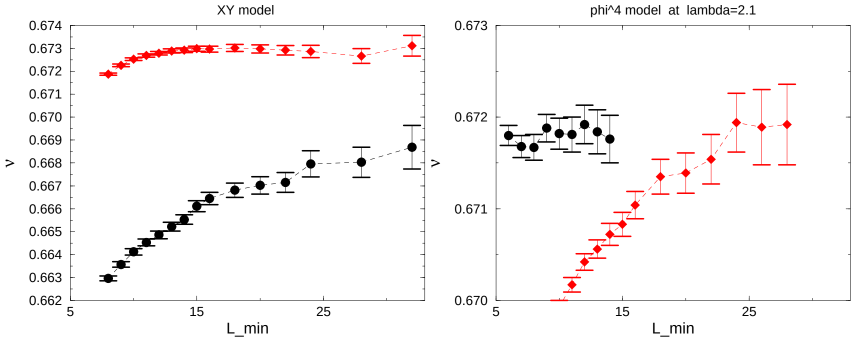


Is there a λ^* for any N?

Campostrini et al (1999) (large N-expansion):
Only possible for $N < 4$

Hasenbusch 2001, Monte Carlo Simulation:
$\lambda^* = 4.4(7)$ for $N = 3$ $\lambda^* = 12.5(4.0)$ for $N = 4$

ν from fits of the slope of U_4 (black) and Z_a/Z_p (red)



Ising Universality Class

Authors	year	Method	ν	η
Deng et al.	2003	MC	0.63020(12)	0.0368(2)
Campostrini et al	2002	IHT	0.63012(16)	0.03639(15)
Butera, Comi	2005	IHT'	0.6299(2)	0.0360(8)*
Guida, Zinn-Justin	1998	3D PT	0.6304(13)	0.0335(25)
Guida, Zinn-Justin	1998	eps	0.6290(25)	0.036(5)
Nickel,Murray	1991	3D PT	0.6301(5)	0.0355(9)
Kleinert	1999	3D PT	0.6305	0.0347(10)

XY

Authors	year	Method	ν	η
Campostrini et al.	2006	MC+IHT	0.6717(1)	0.0381(2)
Campostrini et al.	2001	MC+IHT	0.67155(27)	0.0380(4)
Butera, Comi	1997	HT	0.675(2)	0.037(7)*
Hasenbusch, Török	1999	MC	0.6723(11)	0.0381(4)
Guida,Zinn-Justin	1998	3D PT	0.6703(15)	0.0354(25)
Nickel,Murray	1991	3D PT	0.6715(7)	0.0377(6)
Kleinert	1999	3D PT	0.6710	0.0356(10)
Lipa et al	1997	^{4}He	0.6709(1)	–

Heisenberg

Authors	year	Method	ν	η
Campostrini et al.	2002	MC+IHT	0.7112(5)	0.0375(5)
Hasenbusch	2001	MC	0.710(2)	0.0380(10)
Guida, Zinn-Justin	1998	ϵ-exp	0.7045(55)	0.0375(45)
Guida, Zinn-Justin	1998	3D PT	0.7073(35)	0.0355(25)
Nickel,Murray	1991	3D PT	0.7096(8)	0.0374(4)
Kleinert	1999	3D PT	0.7075	0.0350(5)

O(4)

Hasenbusch	2001	MC	0.749(2)	0.365(10)
Ballesteros et al.	1996	MC	0.7525(10)	0.384(12)
Kanaya, Kaya	1995	MC	0.7479(90)	0.254(38)
Butera, Comi	1997	HT	0.750(3)	0.035(9)*
Guida, Zinn-Justin	1998	3D PT	0.741(6)	0.0350(45)
Guida, Zinn-Justin	1998	ϵ-exp	0.737(8)	0.036(4)

Leading corrections to scaling:

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

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

$$\left.\frac{\partial U_4}{\partial \beta}\right|_{\beta=\beta_c} = aL^{1/\nu} \times (1 + c_{slope} L^{-\omega} + ...)$$

$$\chi(\beta_c) = bL^{2-\eta} \times (1 + c_\chi L^{-\omega} + ...)$$

Ratios of correction amplitudes are universal:

$r_\xi = c_\xi / c_4; \quad r_{slope} = c_{slope} / c_4; \quad r_\chi = c_\chi / c_4$

Then define improved observables

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

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

$$U_4(\beta_c)^{-r_\chi} \chi(\beta_c) = \tilde{b} L^{2-\eta} \times (1 + d_\chi L^{-2\omega} + \dots)$$

Determine $r_\xi = c_\xi / c_4$; $r_{slope} = c_{slope} / c_4$; $r_\chi = c_\chi / c_4$
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.