Critical Loop Gases and Worm Algorithm

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general directions:

- develop efficient MONTE CARLO
- interpret critical phaenomena geometrical
- connected spins = CLUSTERS
- closed loops = LOOP GAS
- closed surfaces = SURFACE GAS

e.g. : VORTEX LOOP PERCOLATION

- a paper in 2000

O(2) symmetry breaking versus vortex loop percolation

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- contains a comment on loop tracing

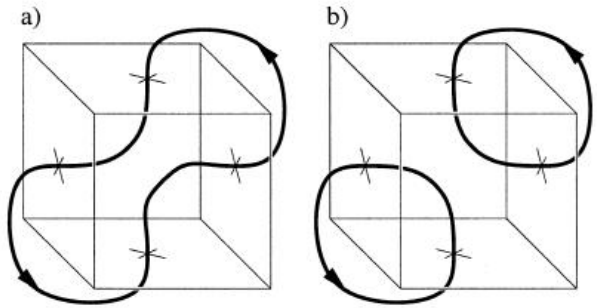


Fig. 1. If two vortices pass through one cell, the vortex tracing algorithm must decide how to connect them, and this leads to an ambiguity in the length distribution.

- finding:

  the loop percolation critical point did not agree with the position of the thermodynamic singularity

- Vortex loop length distribution and LINE TENSION

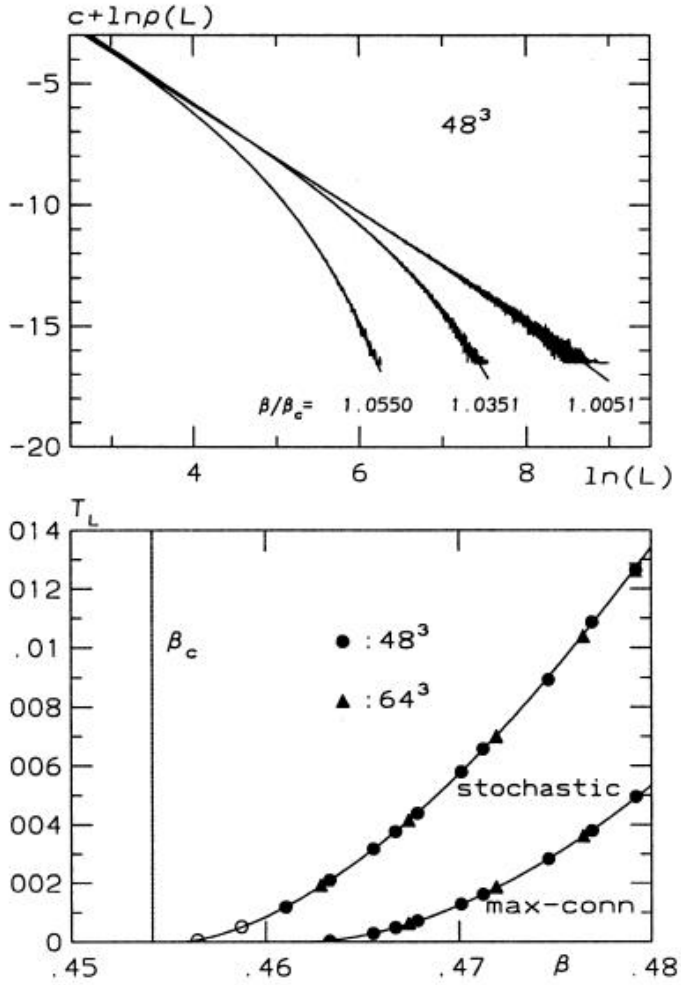


Fig. 5. Upper: The length distribution of vortices at β slightly above β_c with the stochastic definition. Lower: the line tension, determined from the fit in Eq. (4.5) with a free parameter α, with both definitions.

- **Singular Loop Percolation**

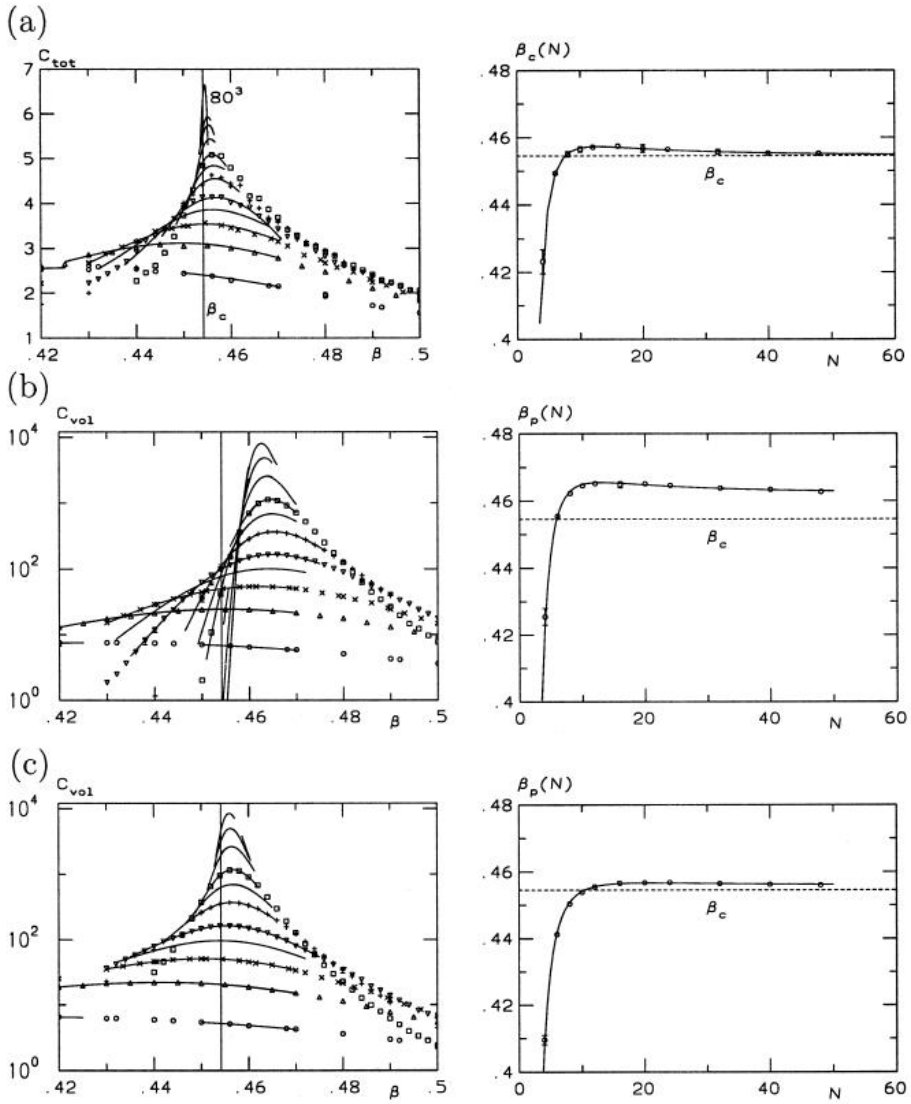


Fig. 2. Left: different susceptibilities, Eq. (3.3), as a function of β; (a) $C_{\rm tot}$, (b) $C_{\rm vol}$ with the maximal connectivity definition, (c) $C_{\rm vol}$ with the stochastic connectivity definition. Right: the location of the apparent critical point determined from the maximum of C. The lines indicate the location of β_c.

Monte Carlo Simulation with CLUSTERS

- Metropolis, $\mathrm{Rosenbluth}^2$ and Teller, J. Chem. Phys. **21** (1953) 1087, spin flips:

$$\mathrm{P}_{\mathrm{acc}} = \min[1, e^{-\beta \Delta H}]$$

- R.H. Swendsen and J.-S. Wang, Phys. Rev. Lett. **58** (1987) 86: non-local updates in the Ising model via the map to a bond-percolated auxiliary system

$$\mathrm{P} = 1 - e^{-K}$$

with dynamical critical exponent $z \approx 0.35 < 2$ ($2d$ Ising)

- Fortuin Kasteleyn representation for the Q state Potts model

$$\mathrm{Z}_{\mathrm{FK}} = \sum_{\mathrm{bonds}} \mathrm{P}^b \, (1 - \mathrm{P})^{B-b} \, \mathrm{Q}^{N_c}$$

DESCENDANTS: Wolff algorithm for $\mathrm{O}(N)$ spin models, but **not** efficient for either frustration, disorder or gauge fields

Monte Carlo Simulation with LOOPS

- N. Prokof'ev and B. Svistunov, "Worm Algorithms for Classical Statistical Models", PRL **87** (2001) 160601 : local updates of wormlike open chains, that are allowed to close and to form a loop gas with dynamical critical exponent $z < 2$
- loop gas representation of 2d $O(N)$ models

$$Z_{\text{loop}} = \sum_{\text{loops}} K^b N^l$$

- critical points on the Honeycomb Lattice, B. Nienhuis, PRL **49** (1982) 1062:

$$K_c = [2 + \sqrt{(2 - N)}]^{-1/2}$$

- ANCESTOR: G. Evertz and M. Marcu, "The Loop-Cluster Algorithm for the full 6 Vertex Model" (1992) DESCENDANTS: directed worm algorithms of F. Alet and E. S. Sorensen (2003)

specific : Worm Algorithm

- samples the graphs of the HTSE i.e., high temperature series expansion of classical spin models directly
- is best suited for Quantum Monte Carlo Simulations where closed loops and open chains $\simeq$ world lines
- at least in $2d$ can deal with frustration, J. S. Wang, PRE **72**, (2005) 036706.
- sign problem for fermions ? , see U. Wolff, “Simulating the All-Order Hopping Expansion. II. Wilson Fermions”, NPB **814**(2009) 549.
- worm algorithm possibly are more flexible, than the cluster algorithms

Ising model examplification

- two point function in the 2d Ising model

$$G(x,y) = \frac{Z(x,y)}{Z(z=z)}$$

- generating partition function with two spin insertions

$$Z(x,y) = \sum_{\text{conf}} e^{-\beta \sum_{\text{nn}} s_i\ s_j}\ s(x)s(y)$$

- is dimerized with dimers $k_l = 0, 1$ on the bonds

$$Z(x,y) = \sum_{\text{dimers}} \Theta(k,x,y)\tanh(\beta)^{\sum_l k_l}$$

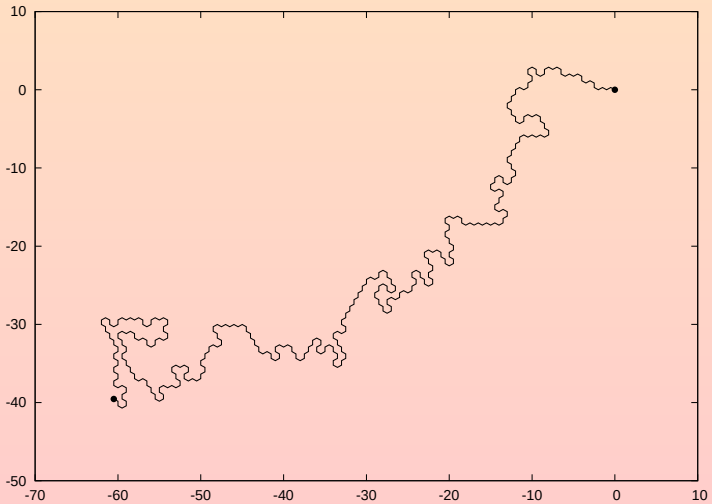
- Θ: even number of dimers for $z \neq x$ and $z \neq y$
- Θ: odd number of dimers for $z = x$ and $z = y$
- dimer chemical potential: μ

$$\mu = -\ln[\tanh(\beta)]$$

$$Z(x,y) = \sum_{\text{Loops,Worm(x,y)}} e^{-\mu \sum_l k_l}$$

Metropolis Algorithm Worm Update

- randomly choose either head or tail of the worm : α or β
- randomly choose a direction : η
- initial dimer value : $k_l = k_{\alpha,\eta}$
- propose a flip : $k_l \to 1 - k_l$
- Metropolis acceptance probability : $P_{\text{accept}} = \min[1, e^{\mu(2k_l-1)}]$
- move the positions of head or tail in case of acceptance
- in case of worm closure: $\alpha = \beta$, KICK $\alpha = \beta$ to any random site [translational invariance] and continue
- Ulli Wolff, Simulating the all-order strong coupling expansion I: Ising model demo, NPB, **810**(2009) 491-502.



Exact versus Monte Carlo

i	$G(1,i)_{\text{exact}}$	$G(1,i)$	$G(1,i)/G(1,i)_{\text{exact}}$	
1	1.0	1.0	1.0	1
2	0.768360	0.768353(30)	0.999991(39)	1
3	0.708394	0.708385(23)	0.999987(33)	1
4	0.708394	0.708342(38)	0.999927(54)	0
5	0.768360	0.768354(32)	0.999993(41)	1
6	0.768360	0.768350(40)	0.999987(52)	1
7	0.722100	0.722082(38)	0.999976(52)	1
8	0.695433	0.695370(33)	0.999910(48)	0
9	0.695433	0.695422(39)	0.999986(56)	1
10	0.722100	0.722175(31)	1.000103(42)	0
11	0.708394	0.708360(35)	0.999952(49)	1
12	0.695433	0.695412(37)	0.999970(53)	1

Examplification : 2D Ising on Honeycomb Lattice

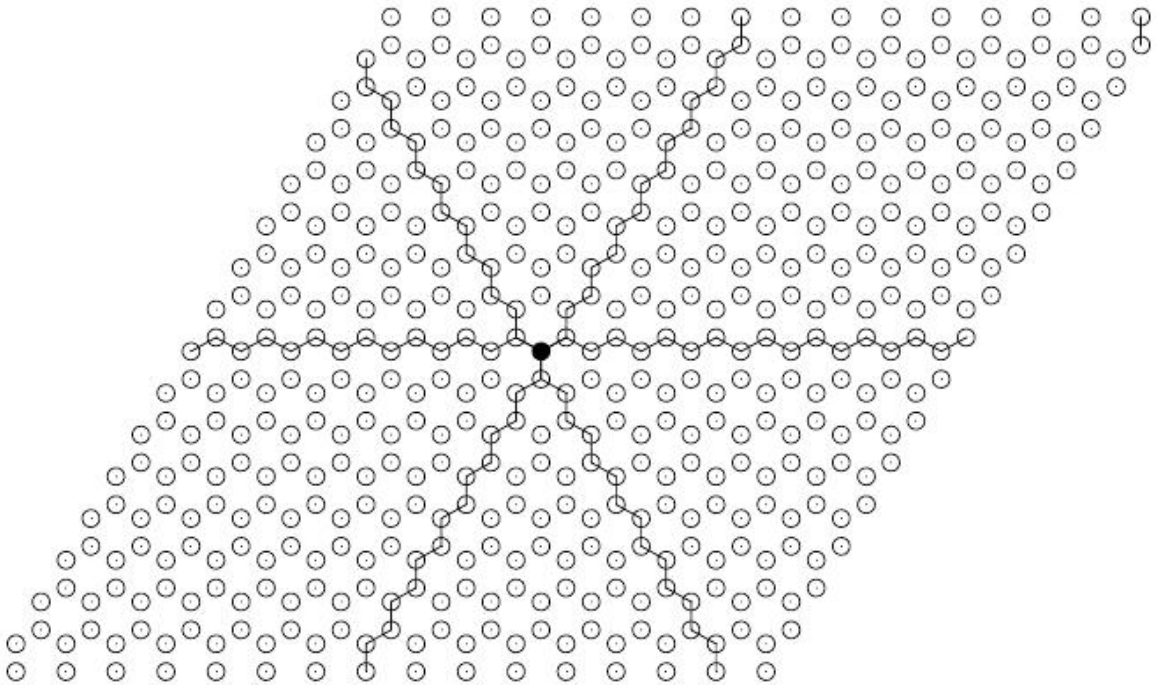


Figure 3: Compact honeycomb lattice with periodicity in three directions. The three operations mapping the site x_i marked by a full circle onto itself through shift operations are indicated by the three polygons, each winding the lattice once. Note the set bond in the upper right corner, which by the periodicity of the lattice belongs to the polygon winding the lattice in the northwest direction.

Wolfhard Janke, Thomas Neuhaus, Adriaan M.J. Schakel, Critical loop gases and the worm algorithm, NPB **829** (2010) 573-599

Loop Gases

PERCOLATION

- small β is mapped to large μ, where loops are suppressed
- large β is mapped to small μ, where loops are abundant
- the $2D$ Ising model is self-dual

$$2\beta_{\mathrm{Dual}} = -\ln[\tanh(\beta)]$$

- as a function of β_{Dual}

loops are Peierls contours for the dual model on the triangular lattice

if the number of loops is even

that are closed on the periodic box

- percolation order parameter

$$I_L(\beta_{\mathrm{Dual}}) = (0[\mathrm{Even}], 1[\mathrm{Odd}])$$

Loop Gases

- the graphs of the HTSE can be characterized by geometrical indices
  at criticality : fractal dimension D
  radius of gyration of loops as well as worms

$$< R_g^2 >=< \frac{1}{n}\sum_{k=1}^{n}(x_k - \bar{x})^2 > \propto n^{2/D}$$

  end to end distance of worms

$$< R_e^2 >=< (x_\alpha - x_\Omega)^2 > \propto n^{2/D}$$

  exact determination of D in $2d$ $O(N)$, Vanderzande, J. Phys. A **25** (1992) at $N = 1$ (Ising)

$$D = \frac{11}{8} = 1.375$$

Loop Gases

- as in polymer physics one can consider the fixed worm length n Ensemble and define the radial end to end distance distribution function $\mathrm{P}_n(r)$ for worms

$$< R_e^2 >= \Omega_d \int_0^\infty r^{d-1} r^2 \mathrm{P}_n(r)$$

algebraic behavior around $r = 0$ is described by $\theta = \frac{3}{8} = 0.375$ (Ising)

$$\mathrm{P}_n(r) \propto r^\theta$$

scaling of $\mathrm{P}_n(r)$

$$\mathrm{P}_n(r) = n^{-d/D} \mathcal{P}(r/n^{1/D})$$

universal scaling function: $\mathcal{P}(t)$ with the suggested form

$$\mathcal{P}(t) = a t^\theta e^{-b t^\delta} \quad \text{Cloizeaux Scaling Form}$$

with $\delta = (1 - \frac{1}{D})^{-1} = \frac{11}{3}$: J. des Cloizeaux, PRA **10** (1974) 1665.

Loop Gases

relations of the standard critical exponents : γ, η and ν
to their geometrical counterparts : D, σ
(line tension scaling exponent) and θ

$$\nu = \frac{1}{\sigma D} \quad ; \quad \eta = 2 - D - \theta \quad ; \quad \gamma = \frac{D + \theta}{\sigma D}$$

the values for $O(N)$ theories in $2d$:

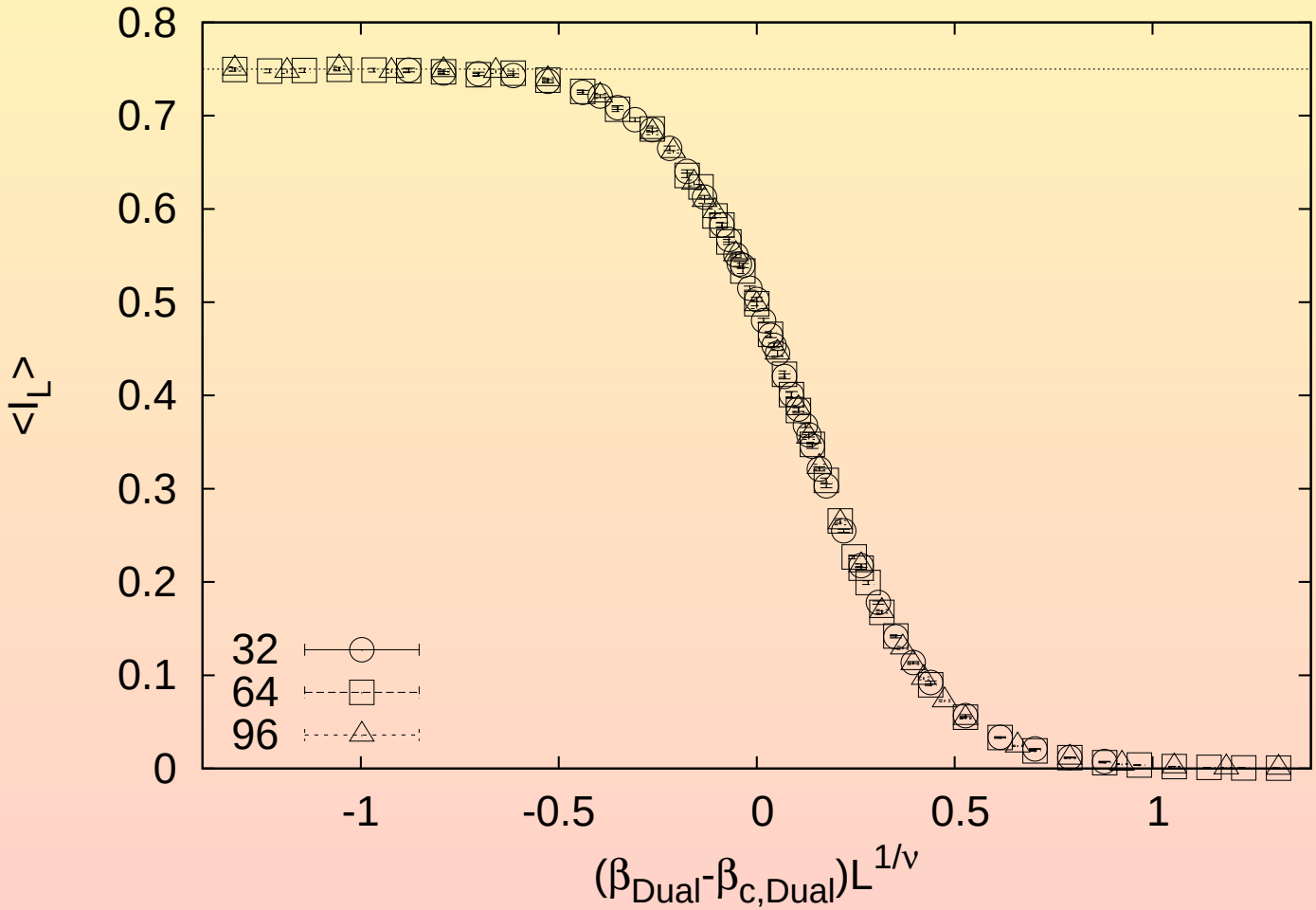
Model	N	γ	η	ν	D	σ	θ
Gaussian	-2	1	0	$\frac{1}{2}$	$\frac{5}{4}$	$\frac{8}{5}$	$\frac{3}{4}$
SAW	0	$\frac{43}{32}$	$\frac{5}{24}$	$\frac{3}{4}$	$\frac{4}{3}$	1	$\frac{11}{24}$
Ising	1	$\frac{7}{4}$	$\frac{1}{4}$	1	$\frac{11}{8}$	$\frac{8}{11}$	$\frac{3}{8}$
XY	2	∞	$\frac{1}{4}$	∞	$\frac{3}{2}$	0	$\frac{1}{4}$
Spherical	∞	∞	0	∞	2	0	0

Numerical Findings

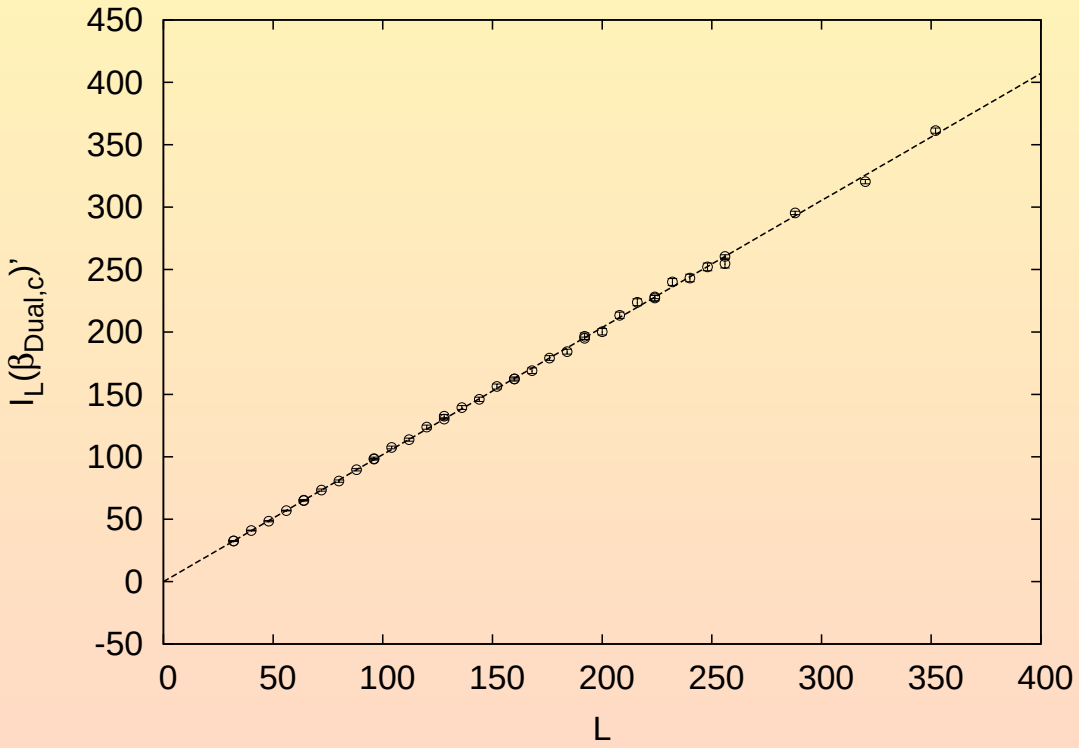
- the loop percolation critical point agrees with the field theoretic one
- the FSS analysis of a loop percolation parameter at criticality yields $\nu^{-1} = 1.0001(15)$
- the fractal dimension is measured to be $D = 1.3752(35)$, compare to $D_{\text{exact}} = 1.375$
  we use analytic scaling corrections in a carefully choosen n window
  $$< R^2_{g,e} >= a n^{\frac{2}{D}} (1 + \frac{b}{n})$$
- the universal end to end distance scaling function: $\mathcal{P}(t)$ is numerically determined and we find a perfect match with the Cloizeaux Scaling Form. The fitted value for the θ exponent value is: $\theta = 0.3769(24)$, compare to to $\theta_{\text{exact}} = 0.375$

percolation order parameter scaled

$$\nu^{-1} = 1.0001(15)$$



Derivative $I_L(\beta_{\mathrm{Dual}})$ with respect to β_{Dual}



$$\nu^{-1} = 1.0001(15)$$

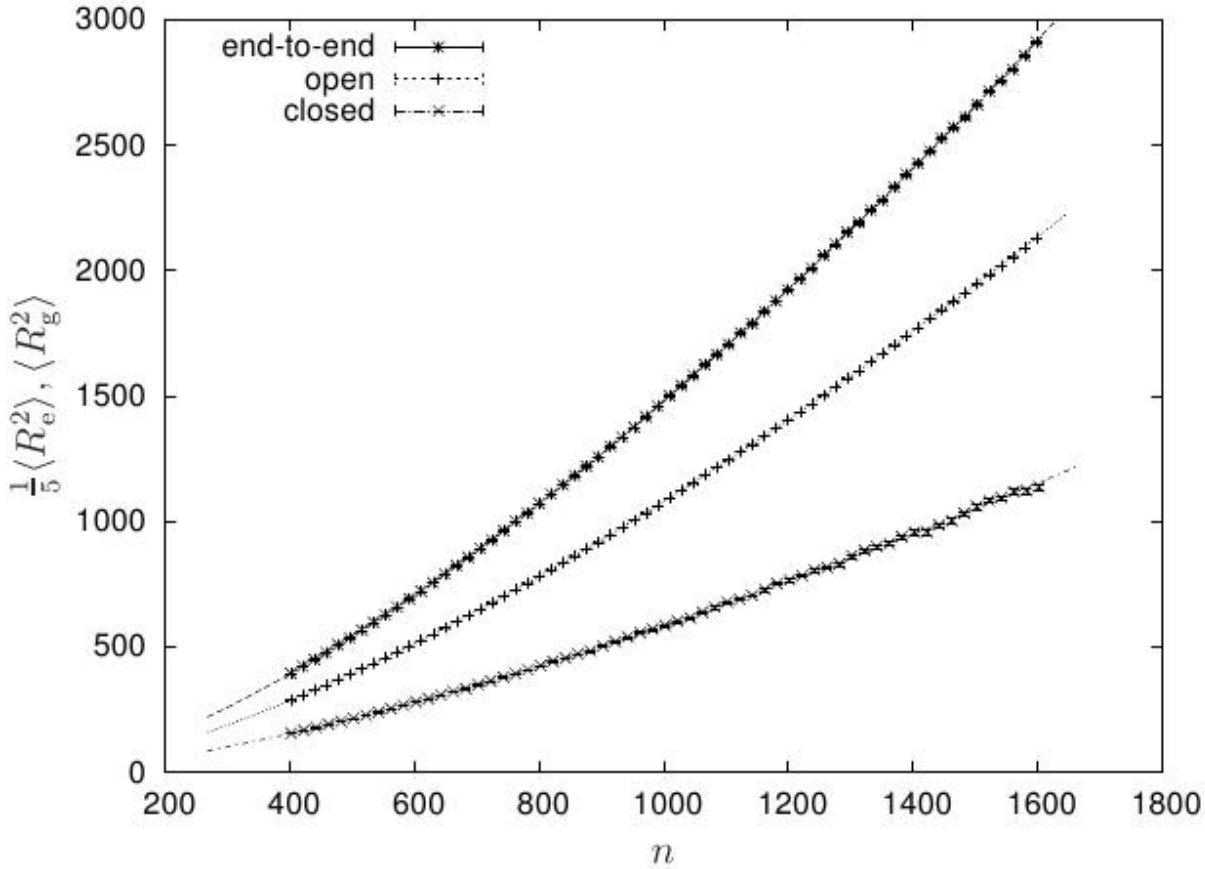


Figure 11: Average square end-to-end distance $\langle R_e^2 \rangle$ (scaled by a factor of five for readability) of open chains, as well as the average square radius of gyration $\langle R_g^2 \rangle$ of open and closed chains, all shown as a function of their length n and measured at the critical point on a lattice of linear size $L = 352$.

fractal dimension

L_{BOX}	χ^2_{dof}	D	$\frac{8D}{11}$
160	0.68198	1.43(14)	1.04(10)
192	0.58752	1.475(46)	1.073(33)
224	0.28772	1.381(16)	1.004(11)
256	0.45341	1.364(12)	0.9924(90)
288	0.62414	1.3733(79)	0.9987(58)
320	0.79112	1.3733(67)	0.9988(49)
352	0.98460	1.3789(55)	1.0028(40)
∞		1.3752(35)	1.0002(25)

polymer end to end distribution

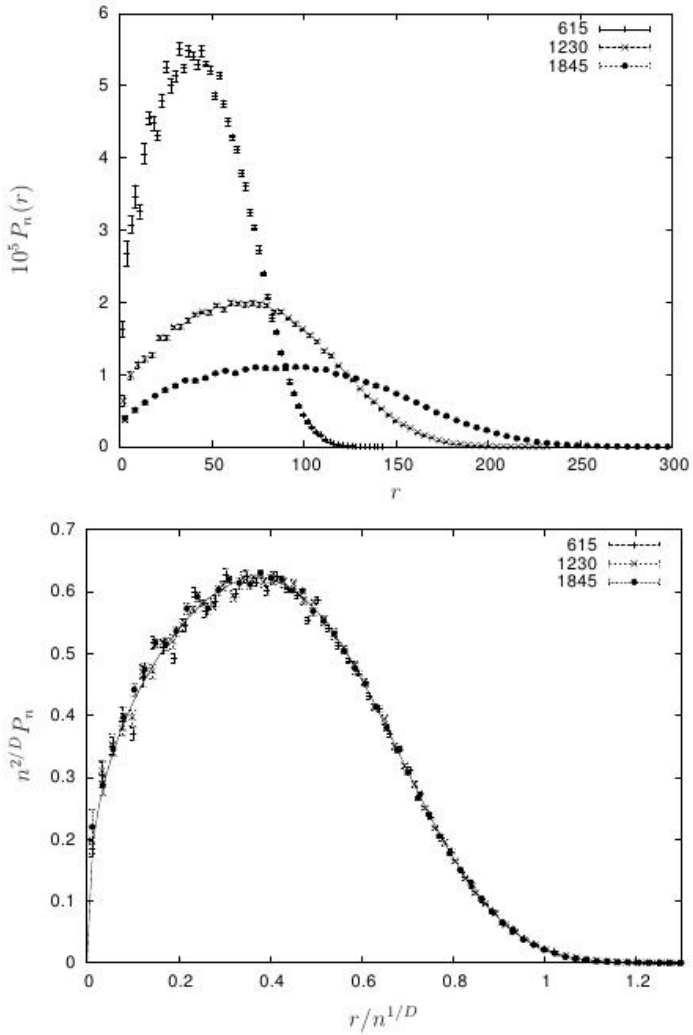


Figure 14: *Top panel*: Distribution $P_n(r)$ (multiplied by a factor of 10^5 for convenience) as a function of the end-to-end distance r for chains of length $n = 615, 1230, 1845$ measured on the largest lattice considered, *viz.* $L = 352$. *Bottom panel*: Rescaled data shown in top panel. The curve through the data points is based on a three-parameter fit to the data using the predicted form (54).

Conlusion

- the field theoretic geoemetric indices of the loop gas at $N = 1$ can be reproduced efficiently
- since then
  Qingquan Liu, Youjin Deng, Timothy M. Garoni, Worm Monte Carlo study of the honeycomb-lattice loop model, NPB **846** (2011) 283-315.
  "We present a Markov-chain Monte Carlo algorithm of worm type that correctly simulates the O(N) loop model on any (finite and connected) bipartite cubic graph, for any real N>0, and any edge weight, including the fully-packed limit of infinite edge weight."

$$N = 0.5, 1.0, 1.5, 2.0$$

- lets do some bread and butter statistical physics, calculate the
- two point function in $3D$ Ising model for the symmetric phase

Evertz and Linden Trick

- H.G. Evertz and W. von der Linden in ”Simulation on Infinite Lattices” PRL 86, 5164 (2001)

Simulations on Infinite-Size Lattices

H. G. Evertz and W. von der Linden

Institut für Theoretische Physik, Technische Universität Graz, 8010 Graz, Austria

(Received 4 August 2000)

We introduce a Monte Carlo method, as a modification of existing cluster algorithms, which allows simulations directly on systems of infinite size, and for quantum models also at $\beta = \infty$. All two-point functions can be obtained, including dynamical information. When the number of iterations is increased, correlation functions at larger distances become available. Limits $q \to 0$ and $\omega \to 0$ can be approached directly. As examples we calculate spectra for the $d = 2$ Ising model and for Heisenberg quantum spin ladders with two and four legs.

Evertz and Linden Trick

- ”infinite hypercubic boxes” an example

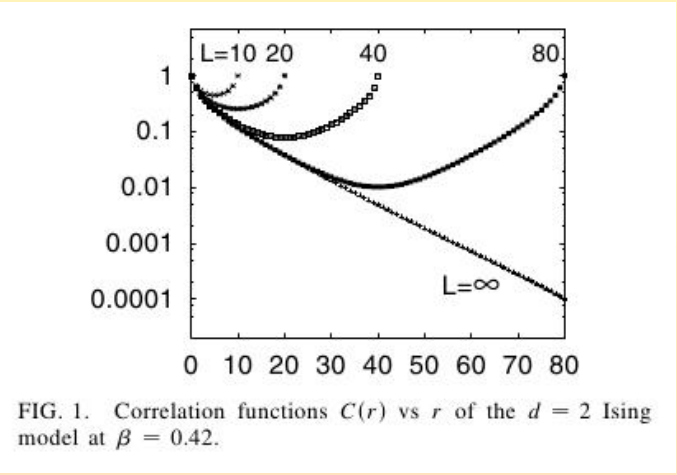


FIG. 1. Correlation functions $C(r)$ vs r of the $d = 2$ Ising model at $\beta = 0.42$.

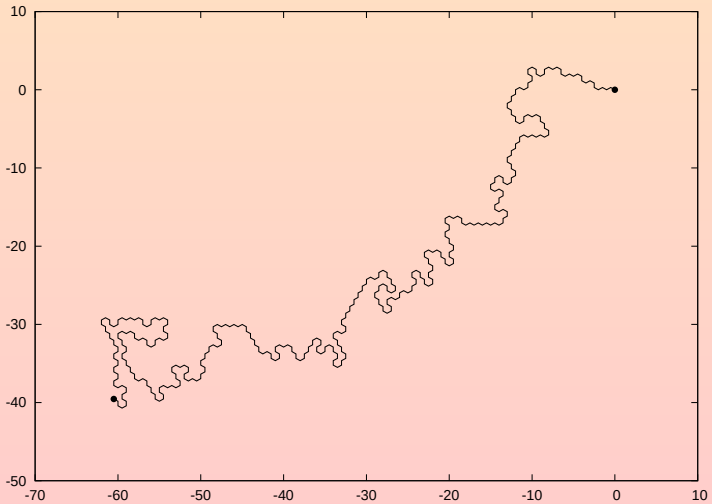
- U. Wolff single cluster update, PRL 1989: a single bond-cluster is flipped, that contains a randomly choosen initial starting site x_0
- E+L:

$$x_0 = \text{const}$$

e.g. : x_0 origin of an Cartesian coordinate system

Metropolis Algorithm Worm Update

- randomly choose either head or tail of the worm : α or β
- randomly choose a direction : η
- initial dimer value : $k_l = k_{\alpha,\eta}$
- propose a flip : $k_l \to 1 - k_l$
- Metropolis acceptance probability : $P_{\text{accept}} = \min[1, e^{\mu(2k_l-1)}]$
- move the positions of head or tail in case of acceptance
- in case of worm closure: $\alpha = \beta$, DO NOT KICK $\alpha = \beta$ to any random site [thus break translational invariance] and continue
- Ulli Wolff, Simulating the all-order strong coupling expansion I: Ising model demo, NPB, **810**(2009) 491-502.



Biased Sampling [Multicanonical] Trick

- biased

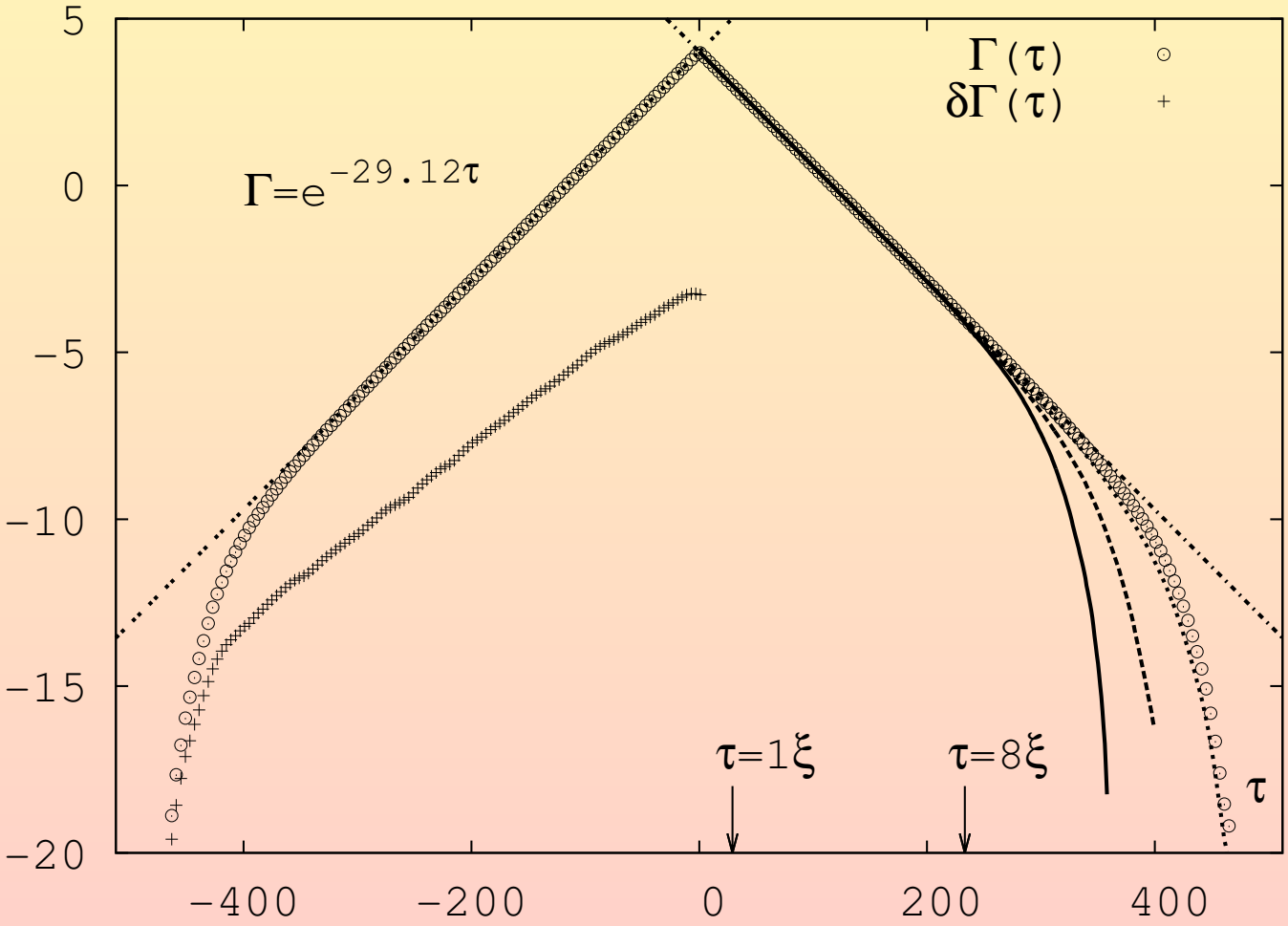
$$Z(u,v,s) = \sum_{Dimers} e^{-\mu \sum_{i,\eta} k_{i,\eta}} \times \delta^1(1 - \mathrm{mod}(\Sigma(u),2)) \times \delta^1(1 - \mathrm{mod}(\Sigma(v),2)) \times \prod_{i \neq u,v} \delta^1(0 - \mathrm{mod}(\Sigma(i),2)) \times e^{+(1-\frac{1}{s})(u_x - v_x)/\xi_{\exp}}$$

$$Z \propto \exp[-\frac{u_x - v_x}{\xi_{\exp}} + (1 - \frac{1}{s})\frac{u_x - v_x}{\xi_{\exp}}] \propto \exp[-\frac{u_x - v_x}{s\xi_{\exp}}]$$

- domain size boost : $s = 1.4$

3D Ising 2 point function

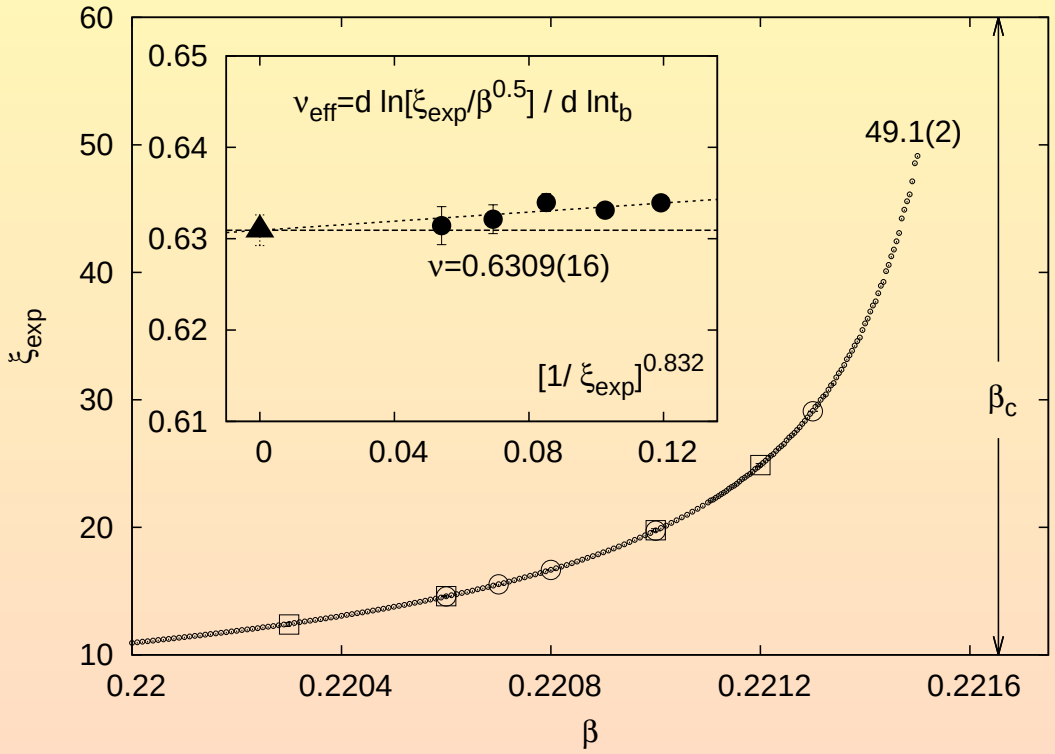
$\beta = 0.22130$ with $\beta_c = 0.22165463(8)$



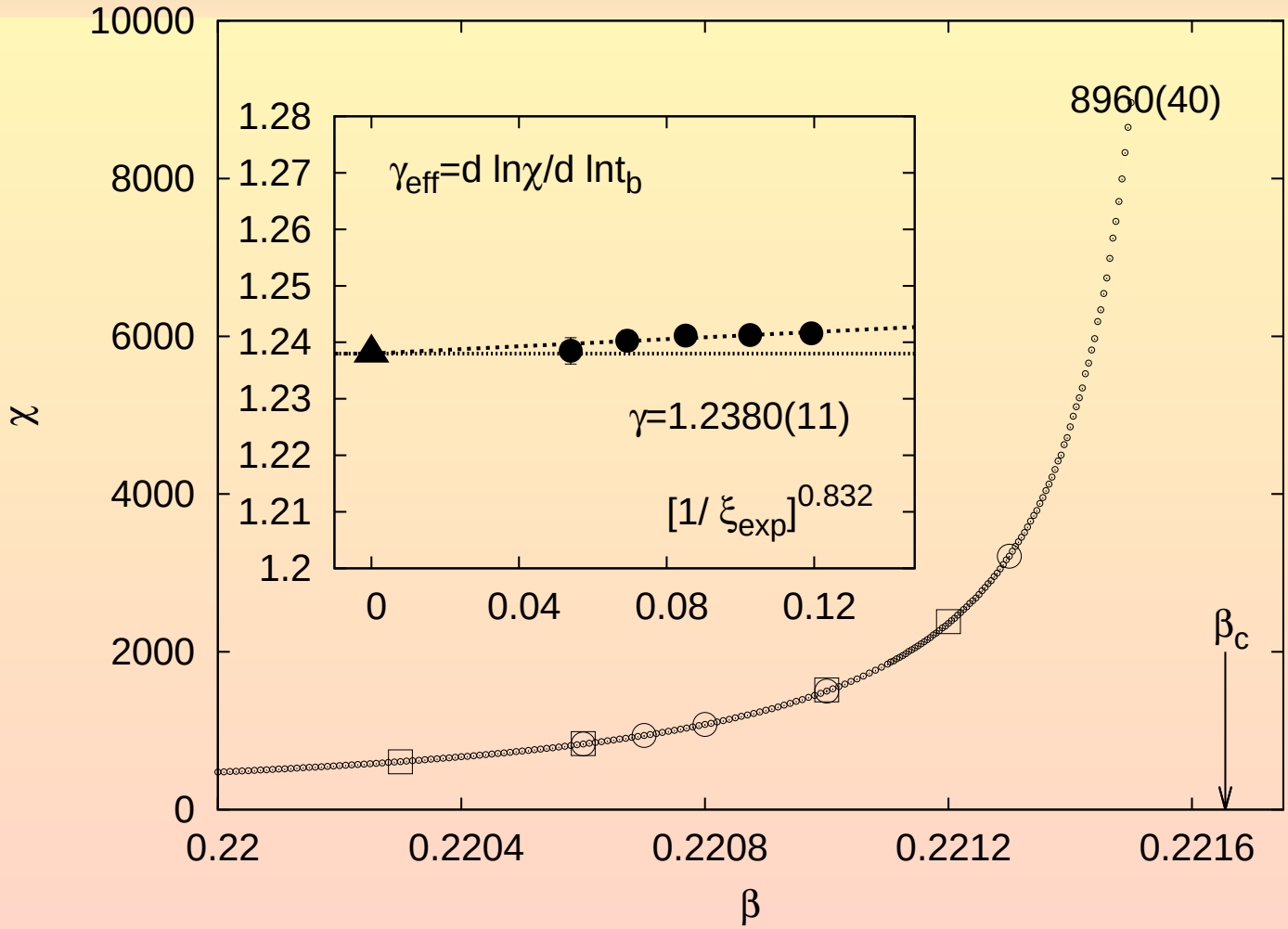
we obtain extremely precise infinite volume data for ξ_{exp} and χ

in the temperature scaling analysis we tend to include scaling corrections as suggested by Campbell

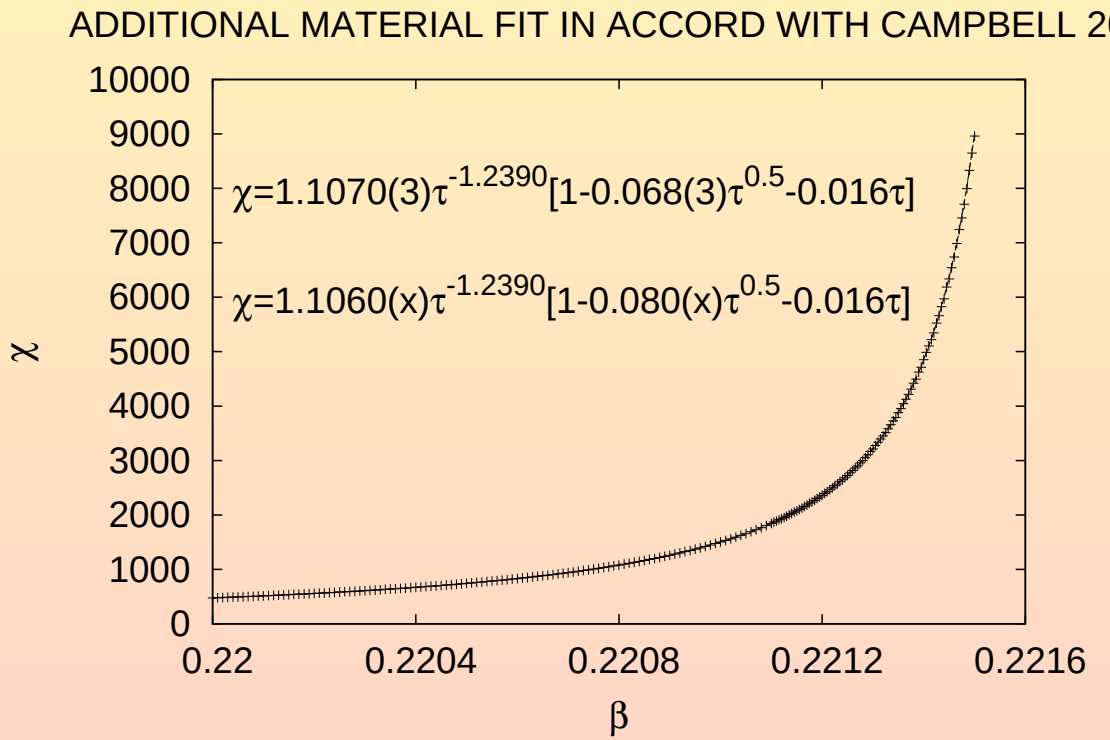
the final exponent values are not yet out

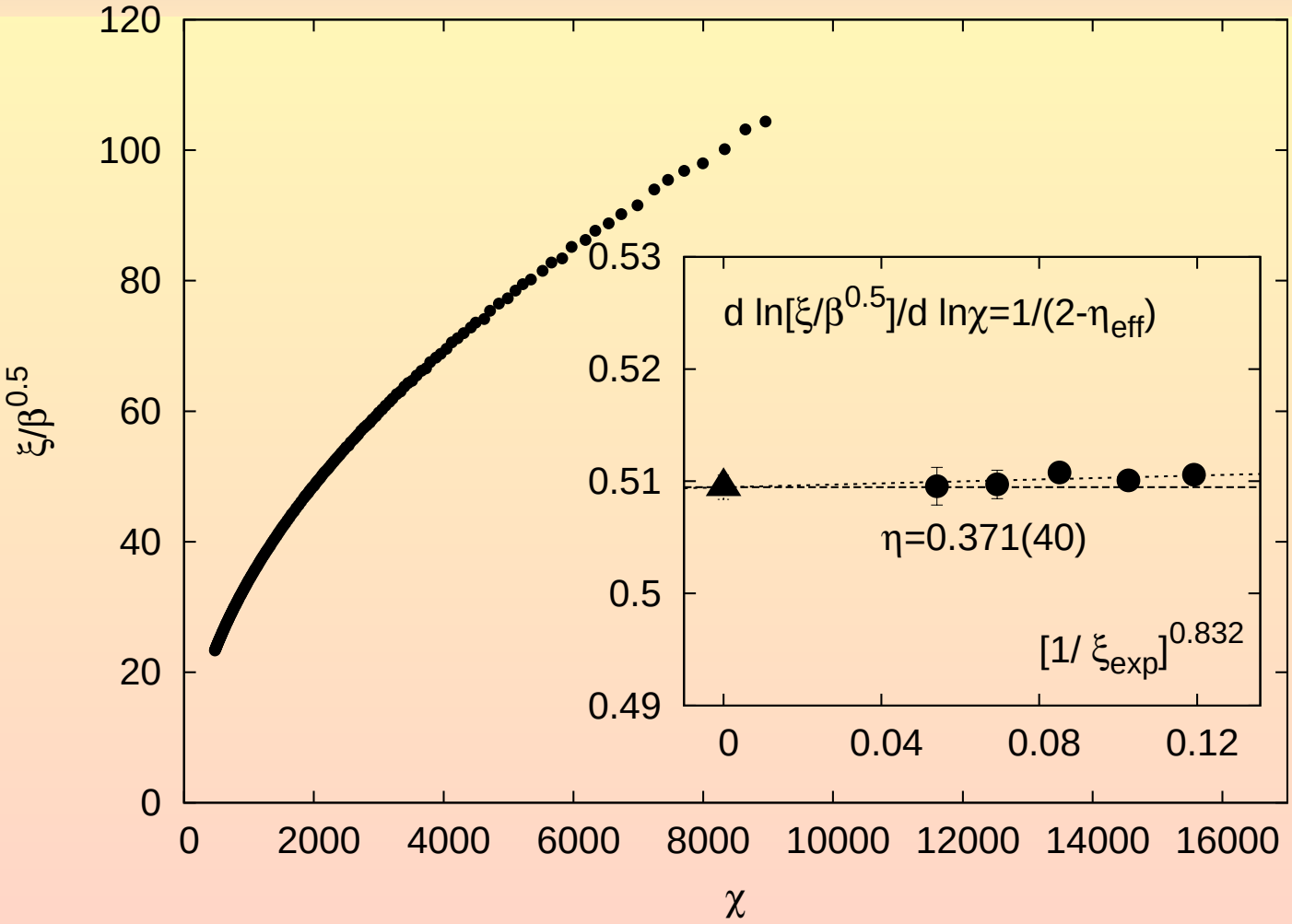


open circles and squares: Kim, Souza, Landau, PRE 1996, Hasenbusch 2012


10000
8000
6000
4000
2000
0
χ
0.22
0.2204
0.2208
0.2212
0.2216
β
8960(40)
β_c
1.28
1.27
1.26
1.25
1.24
1.23
1.22
1.21
1.2
γ_{eff}=d lnχ/d $\ln t_b$
γ=1.2380(11)
$[1/\xi_{exp}]^{0.832}$
0
0.04
0.08
0.12

I.A. Campbell and P.H. Lundow, Extended scaling analysis of the $S = 1/2$ Ising ferromagnet on the simple cubic lattice, PRB **83** (2011) 014411.




120
100
80
60
40
20
0
ξ/β^0.5
0
2000
4000
6000
8000
10000
12000
14000
16000
χ
0.53
0.52
0.51
0.5
0.49
d ln[ξ/β^0.5]/d lnχ=1/(2-η_eff)
η=0.371(40)
[1/ ξ_exp]^0.832
0
0.04
0.08
0.12

Conlusion

- simple straightforward local update for

  two-point function $\Gamma(r)$

  of classical ferromagnets
- it is easy to implement loop updates, without recurrence to Z_{Loop}, for $O(2)$ classical spin models in dimension 2 and 3, in which case Integer Z degrees (Integer valued Currents) circulate the loops
- Quantum Monte Carlo two point functions
- there is no direct access to the magnetization and no Binder cumulant
- observables of loop winding at the percolation threshold have the potential to replace the Binder cumulant [Helicity Modulus in case of O(2)]