Exploring Random-Graph Ensembles with Worms

Wolfhard Janke

Computational Quantum Field Theory
Institut für Theoretische Physik
Universität Leipzig, Germany

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Outline

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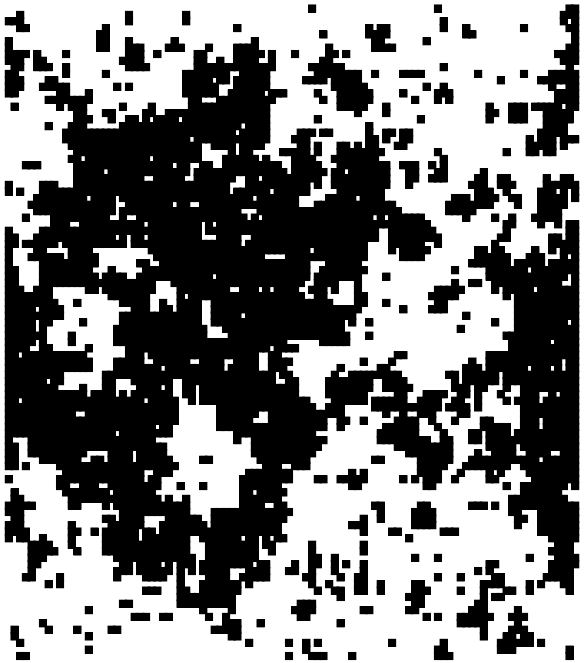
Motivation

- Geometrical picture of phase transitions and critical phenomena in terms of clusters or boundaries of clusters $=$ loops in 2d

WJ & A.M.J. Schakel, Nucl. Phys. B **700** (2004) 385; Phys. Rev. E **71** (2005) 036703; Phys. Rev. Lett. **95** (2005) 135702

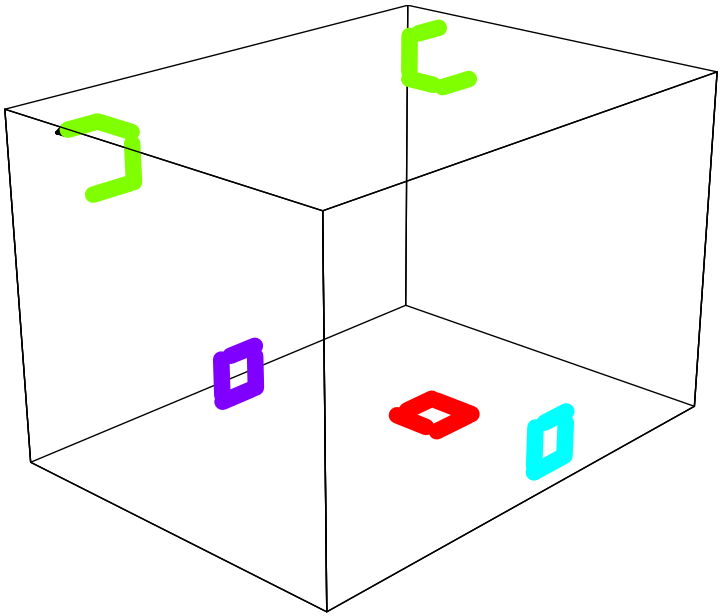
100×100 Ising model: black = spin “up”, white = spin “down”



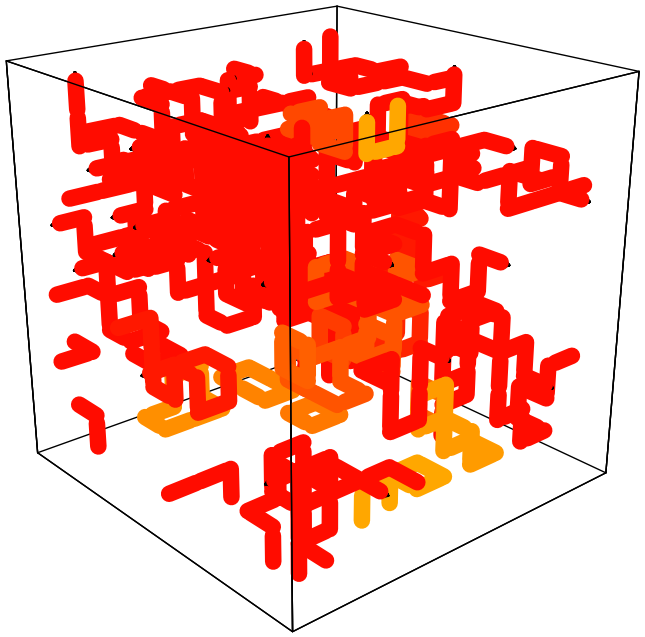
CRITICAL

$T = 1.02\, T_c$

Vortex loops in 3D $|\phi|^4$ theory



$T < T_c$



$T > T_c$

F. Winter, WJ, A.M.J. Schakel, Phys. Rev. E **77** (2008) 061108

Motivation

- Geometrical picture of phase transitions and critical phenomena in terms of clusters or boundaries of clusters $=$ loops in 2d
- Or vice versa, e.g., polymer or surface properties in terms of field theories or spin models
- At criticality, thermodynamic critical exponents can be related to the fractal dimension of the geometrical objects
- Worm update: Combines naturally loops ($=$ energetic sector) and (open) chains ($=$ magnetic sector)

Theory I: Basic scaling properties of loop gases

Distribution of line length n, similar to percolation:

$$\ell_n \sim n^{-d/D-1} e^{-\theta n}\,, \qquad \theta \propto (K - K_c)^{1/\sigma}\,.$$

Given: Tuning parameter K and dimension d (here $d = 2$)

Measured: Fractal dimension D and exponent σ, governing approach to criticality at K_c

At criticality: Radius of gyration R_g, end-to-end distance R_e (for open chains):

$$\langle R_g^2 \rangle \propto \langle R_e^2 \rangle \sim n^{2/D}$$

Fractal dimension D for 2d models:

$$D = 1 + 1/2\overline{\kappa}$$

(SLE classification, Coulomb gas, conformal field theory)

2d Ising: $\overline{\kappa} = 4/3 \longrightarrow D = 11/8 = 1.375$

Parameter σ:

$$\sigma = \frac{1}{\nu D}$$

2d Ising: $\nu = 1 \longrightarrow \sigma = 8/11 = 0.727272\ldots$

Theory II: High-temperature expansion of the Ising model

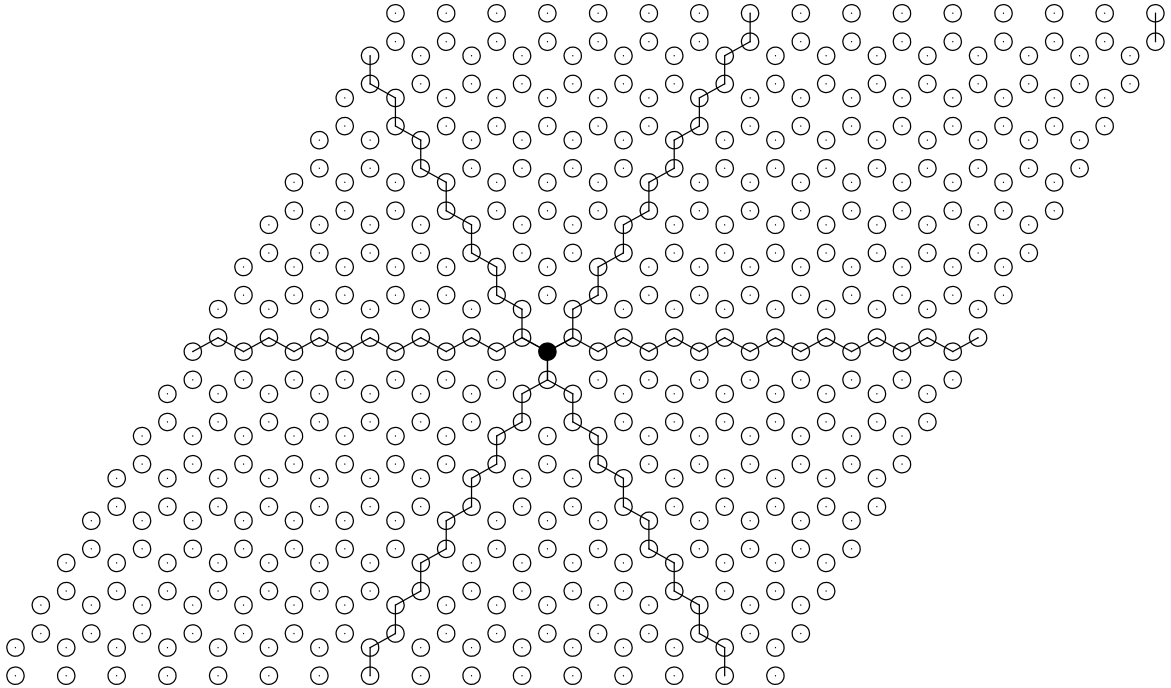
- Leads automatically to a loop gas with fugacity parameter $K = \tanh\beta$ (in arbitrary d)
- Contains in general intersection points ("knots")
- Pure loop gas on 2d honeycomb lattice with coordination number $z = 3$ as used here:

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

  b: number of occupied bonds, l: number of loops,
  N: number of loop colors for O(N) model ($N = 1$ for Ising)
- Critical parameter:

$$K_c = \left[2 + (2-N)^{1/2}\right]^{-1/2} = 1/\sqrt{3} \;\; (N = 1)$$

Compact honeycomb lattice with periodicity in three directions



Monte Carlo Simulations: Worm update

Qualitative description:

- Move one end of (open) chain through background of loops
- Connects loop and chain sector by reopening existing loops or creating new ones by self-closing or a “back bite”, leaving a loop behind

Quantitative update prescription ($R_e > 1$):

1. choose randomly either endpoint of the chain
2. choose randomly any of the links attached
3. update $b_l \longrightarrow b_l' = 1 - b_l$ with acceptance probability

$$P_{\text{accept}} = \min\left(1, K^{1-2b_l}\right)$$

(in effect: $P_{\text{accept}} = K < 1$ for bond creation, and bond deletion always accepted)

If $R_e = 1$, mixed loop/chain configuration can be turned into a pure loop gas – possible switch between magnetic and energetic sector:

We always attempt to close the chain and, if accepted, proceed by randomly choosing a new link among all links of the lattice. The bond variable on that link is accepted/rejected as usual.

Slightly different from Prokof'ev/Svistunov's original proposal [PRL 87 (2001) 160 601], but close to Wolff's version [NPB 810 (2009) 491].

Numerical tests

Critical slowing down greatly reduced.

Correlation function $G(x_1, x_i)$: Comparison with exact enumeration on a 5×5 square lattice with periodic boundary conditions:

- Overall agreement better than 0.01%
- For example, on-axis distance 2 and 3:
  0.708 385(23), 0.708 342(38) vs 0.708 394 . . .
  0.999 987(33), 0.999 927(54) $= G/G_{\text{exact}}$

Exploiting duality

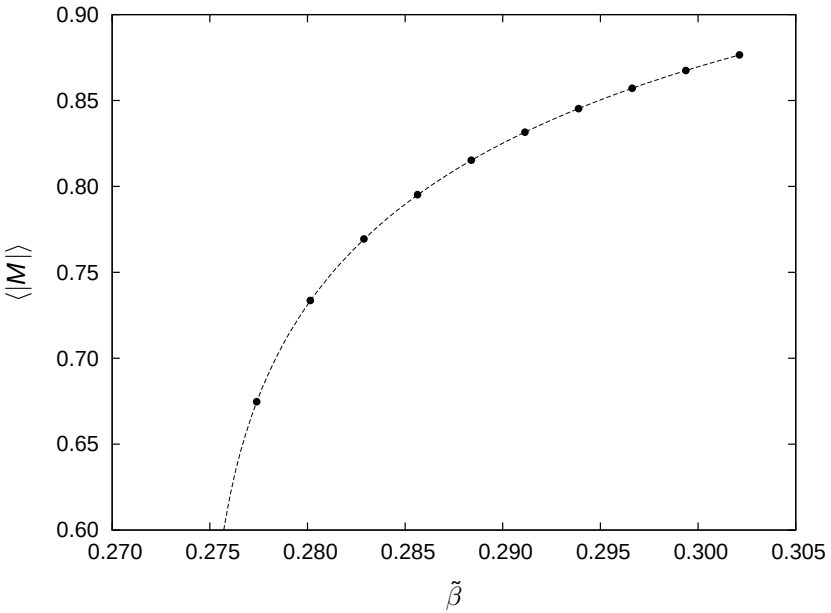
honeycomb lattice $\longleftarrow$ duality $\longrightarrow$ triangular (hexagonal) lattice

$$K = tanh\beta = e^{-2\tilde{\beta}}$$

β on honeycomb lattice ($K_c = 1/\sqrt{3}$)
$\tilde{\beta}$ on triangular (hexagonal) lattice ($\tilde{\beta}_c = \frac{1}{4}\ln 3$)

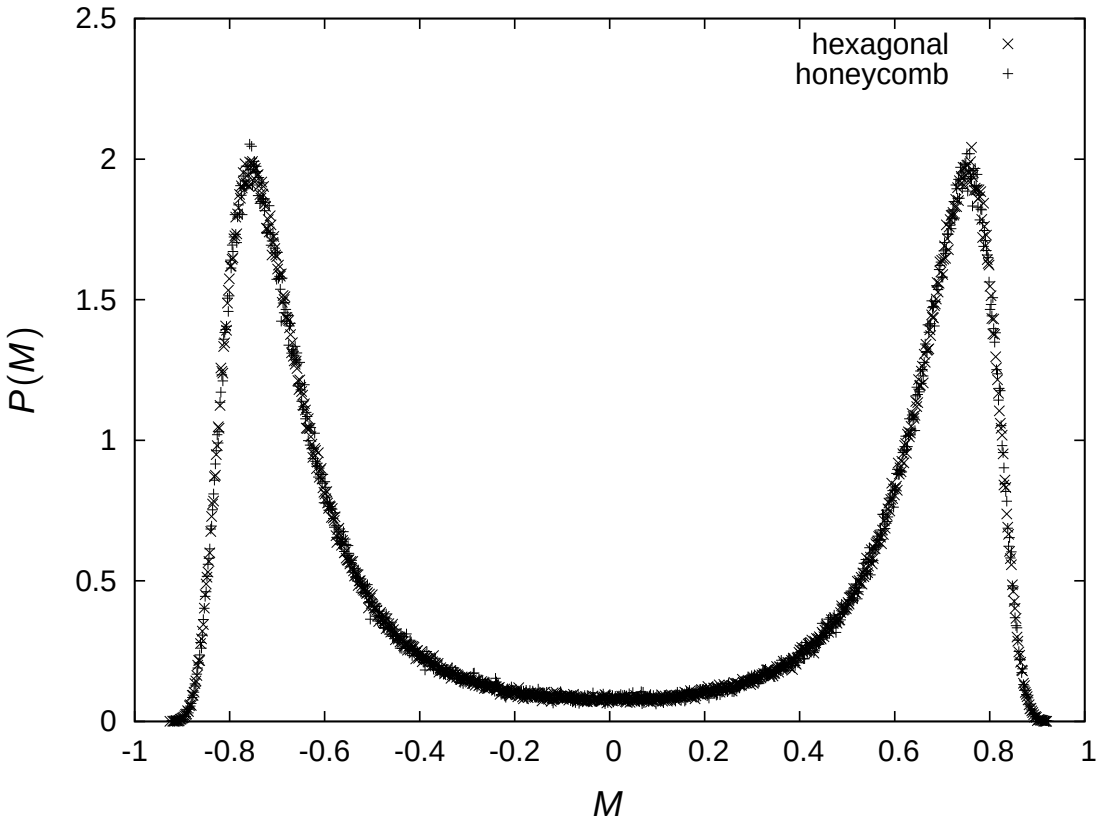
high temperature T $\longleftarrow$ duality $\longrightarrow$ low temperature $\tilde{T}$

Magnetization on triangular lattice as function of inverse temperature $\tilde{\beta}$ ("cold") from worm update on dual honeycomb lattice at $K = \tanh\beta$ ("hot"):



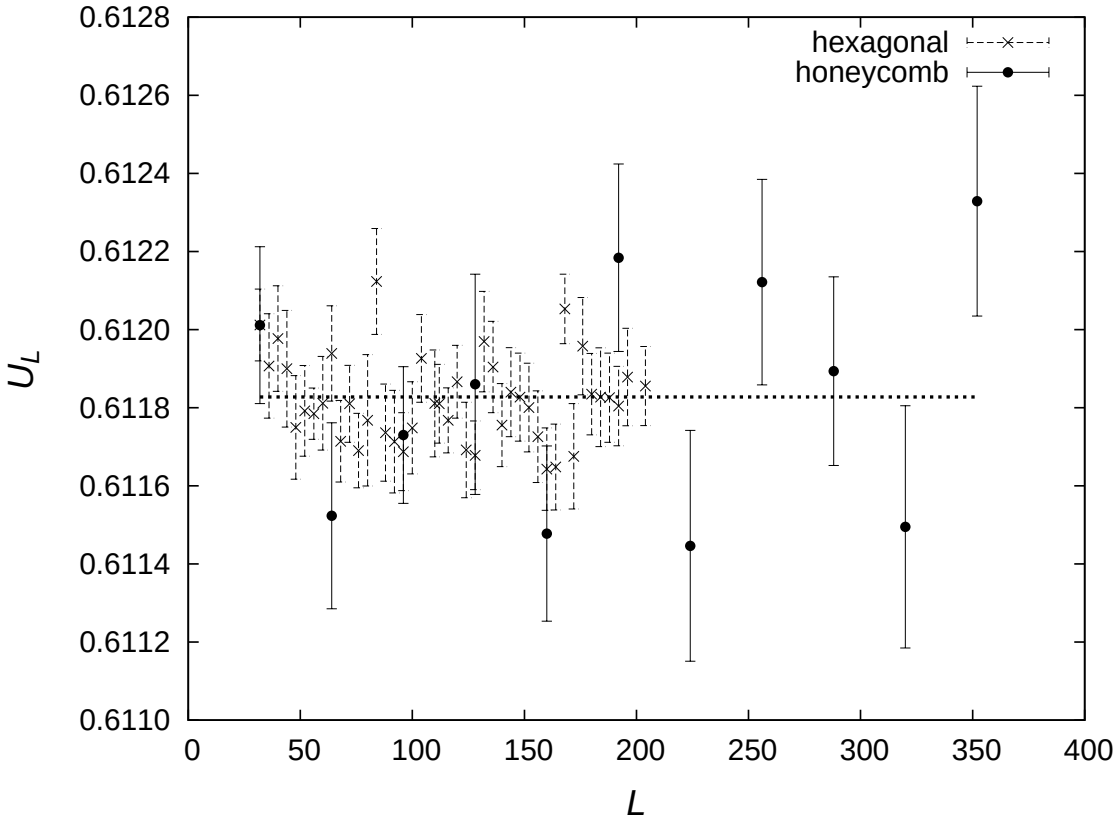
Dashed line: Exact result due to Potts, $M(\tilde{\beta}) = \left\{1 - 16\exp(-12\tilde{\beta})/[1 + 3\exp(-4\tilde{\beta})][1 - \exp(-4\tilde{\beta})]^3\right\}^{1/8}$

Magnetization distribution at criticality for $L = 32$



"hexagonal": Swendsen-Wang cluster update
"honeycomb": worms + duality

Finite-size scaling of Binder parameter $U_L = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2}$ at criticality



"hexagonal": Swendsen-Wang cluster update
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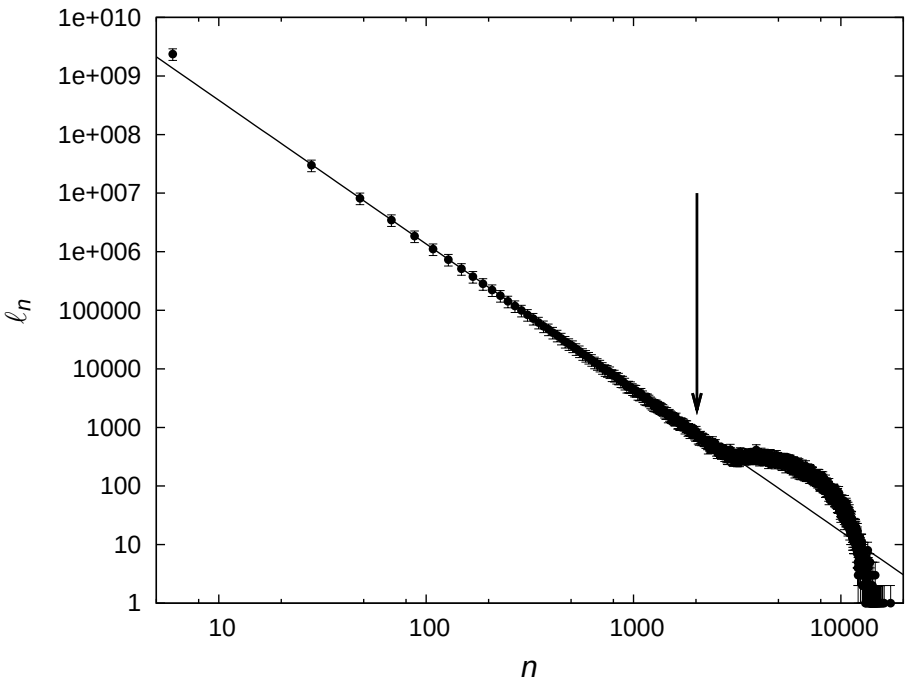
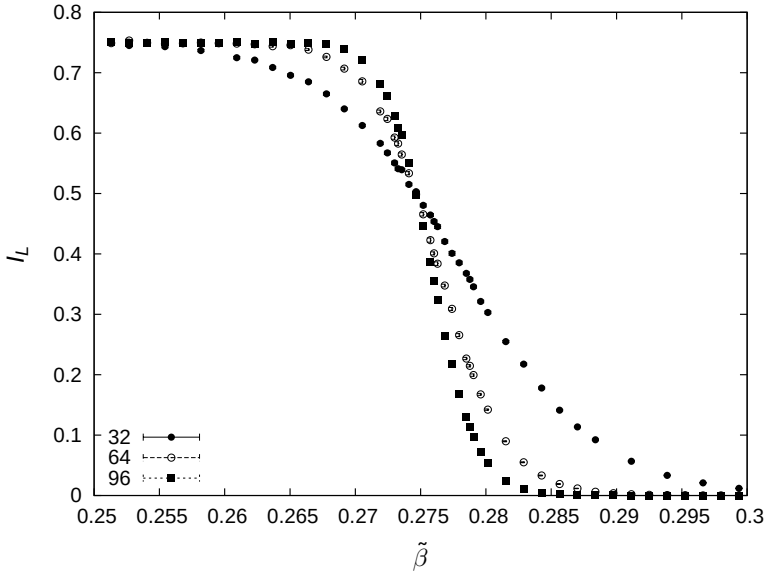
Results

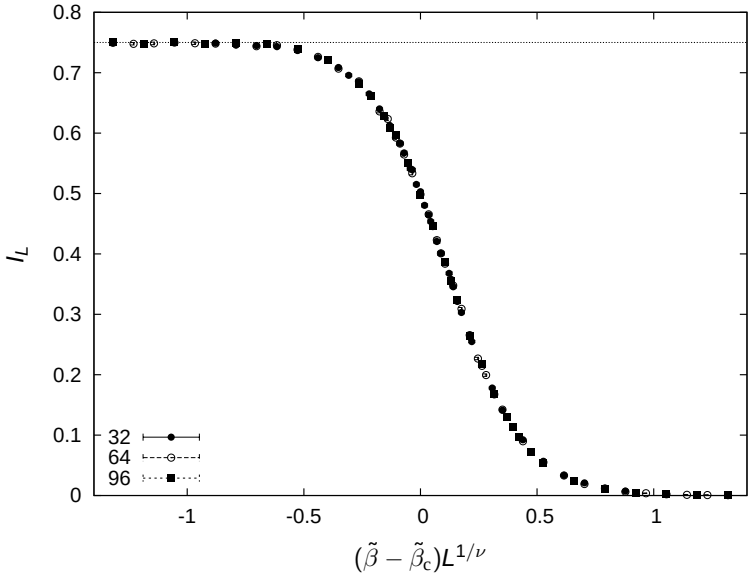
Loop distribution ℓ_n at criticality as function of loop length n



Honeycomb lattice with $L = 352$; straight line: $\ell_n \propto n^{-2/D-1}$ with $D = 11/8$ (bump for $n > 2000$: winding loops).

Binary variable: 0 – even winding numbers (unique magnetization transcription); 1 – odd winding numbers. Average $I_L(\tilde{\beta})$ ($L = 32, 64, 96$):

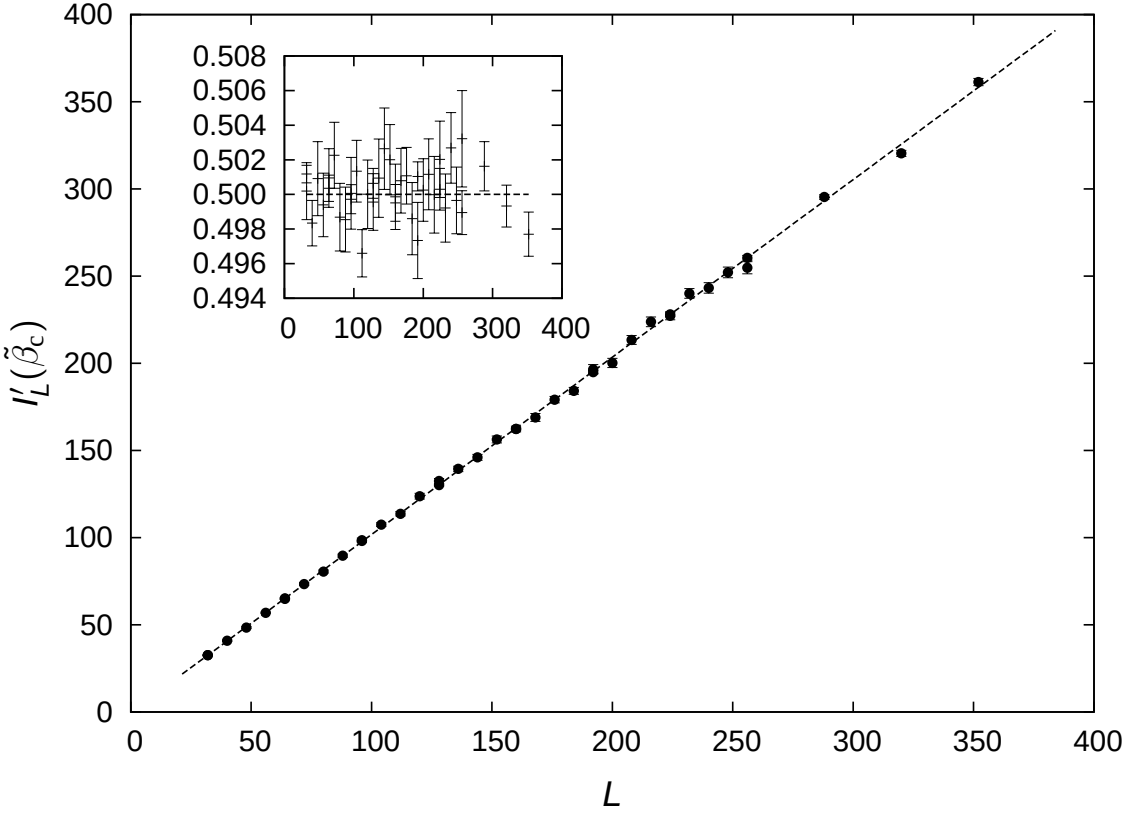




$I_L(\tilde{\beta}_c) = 0.50024(21)$

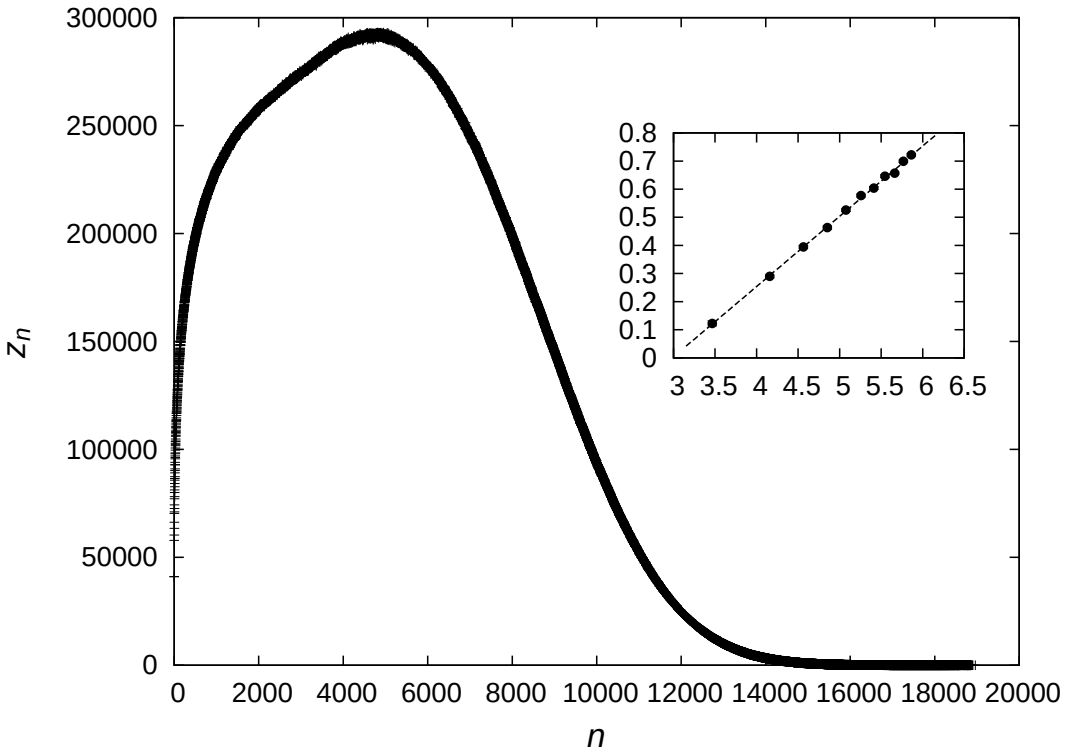
$\nu = 1$, straight line at $3/4$
"odd"/# "even" configs

Derivative of $I_L(\tilde{\beta})$ at criticality



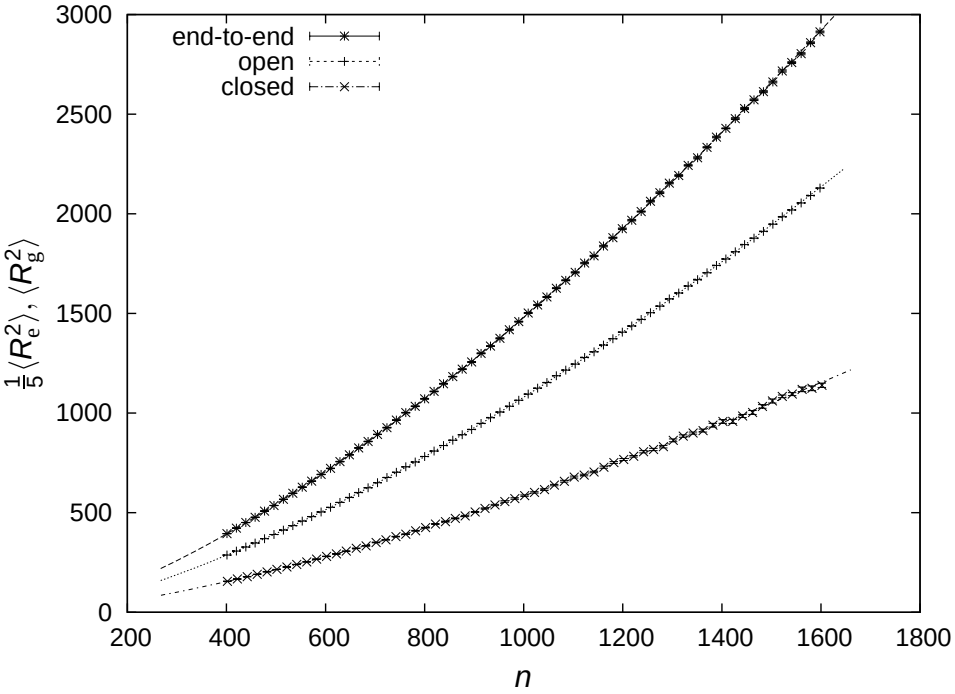
2-parameter fit: $1/\nu = 1.0001(15)$ (χ^2/dof$= 1.01$)
Inset: $I_L(\tilde{\beta}_c) = 0.50024(21)$.

Distribution z_n of open chains at criticality ($L = 352$).
Inset: Log-log plot of $L^2/\sum_n z_n = L^2/\chi \propto L^{2-\gamma/\nu} = L^\eta$ vs L



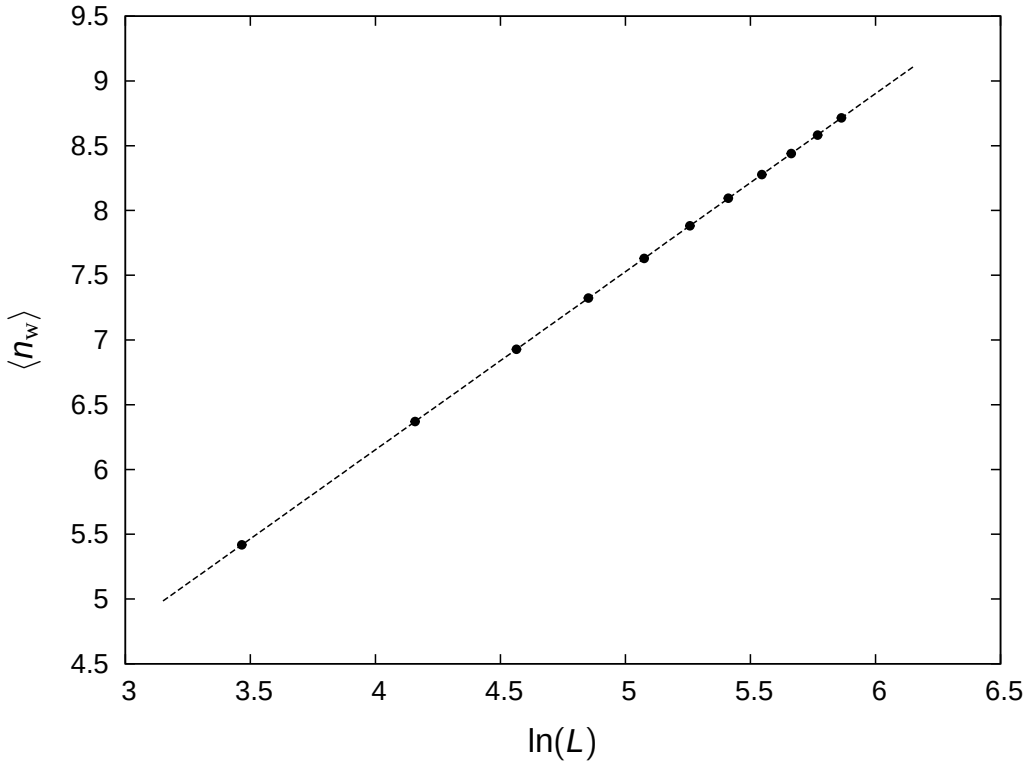
Inset: 2-parameter fit: $\eta = 0.2498(26) \approx 1/4$ (χ^2/dof$= 1.87$)

Average squared end-to-end distance (of chains) and radius of gyration of chains and loops $\propto n^{2/D}$, $D = 11/8 = 1.375$ ($L = 352$)



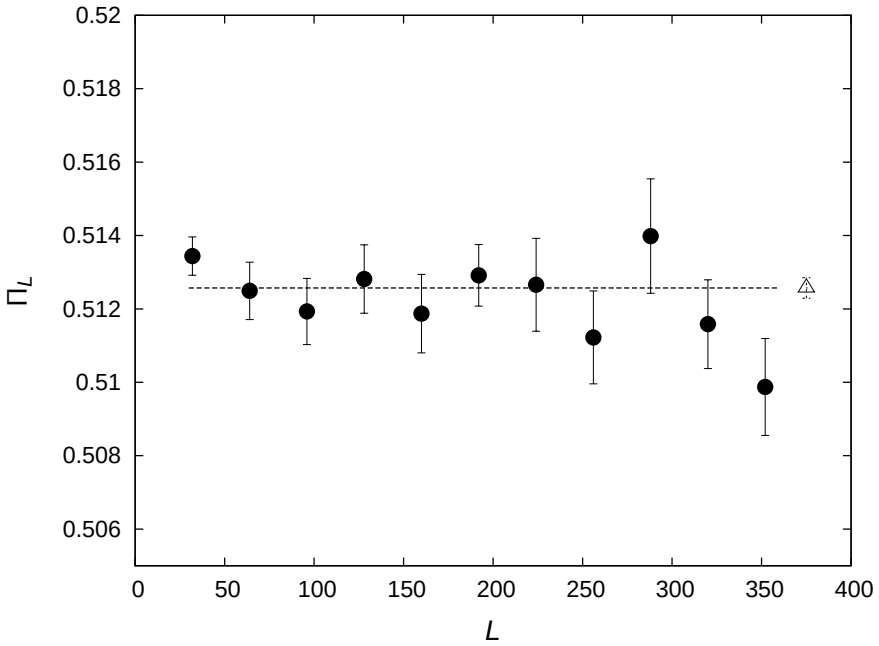
$\langle R_e^2\rangle$: $D = 1.3755(31) = 1.0004(23) D_{\text{exact}}$
$\langle R_g^2\rangle_{\text{chains}}$: $D = 1.3789(55) = 1.0028(40) D_{\text{exact}}$

Average length of winding loops on a honeycomb lattice of linear extent L, $\langle n_w \rangle \propto L^D$



2-parameter fit: $D = 1.37504(32) = 1.00003(24) D_{\text{exact}}$
(χ^2/dof$= 1.13$)

Probability Π_L that one or more loops wind the honeycomb lattice of linear size L at the critical point



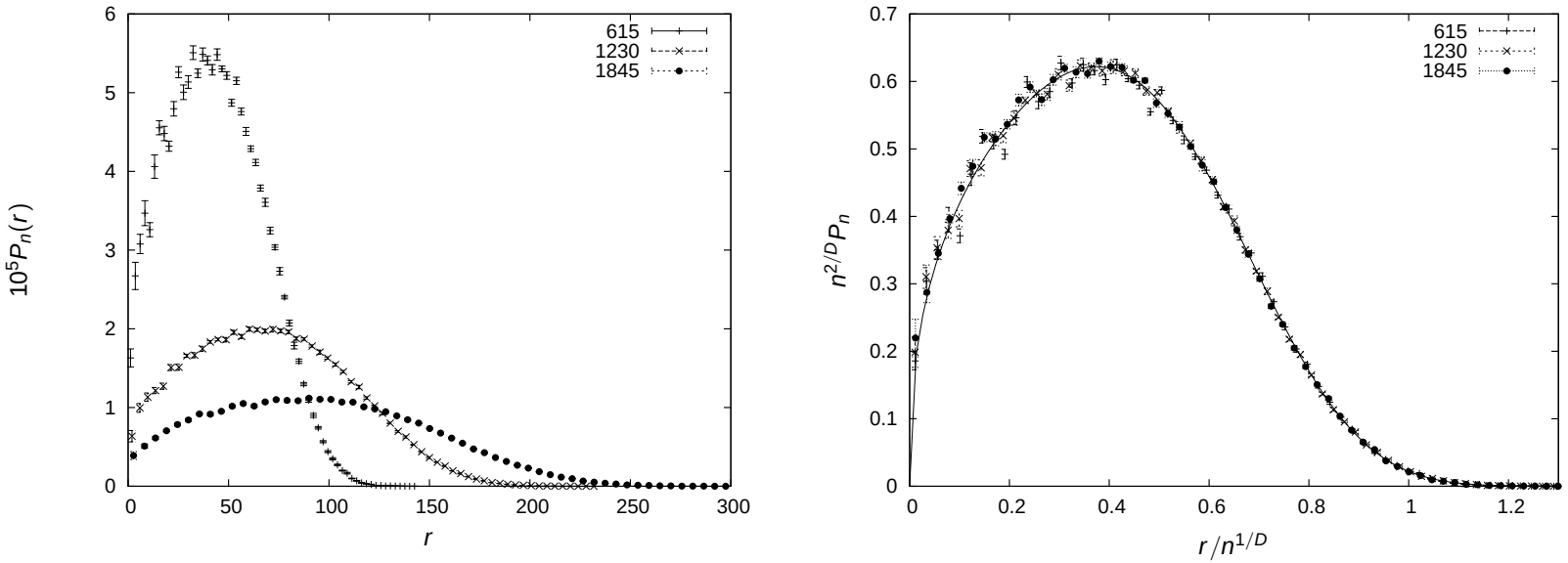
P_w for $L = 160$:

$P_0 = 0.48802(74)$
$P_1 = 0.49960(73)$
$P_2 = 0.01236(14)$
$P_3 = 0.0000299(64)$
$P_4 = 0$

$P_0 + P_2 + P_4 + \ldots$
$= 0.50038$

Average: $\Pi_L = 0.51257(27) > 0.5$ (χ^2/dof$= 1.08$)

Scaling behaviour of the distribution function $P_n(r)$ of the end-to-end distance r ($n = 615, 1230, 1845$, $L = 352$)



Perfect scaling collapse with $D = 11/8$. Scaling function is $\propto t^{\vartheta} \exp(-bt^{\delta})$; $t = r/n^{1/D}$, $\vartheta = 3/8$, $\delta = (1 - 1/D)^{-1} = 11/3$

Summary

- Worm update perfect tool for loop-gas approach to fluctuating fields on a lattice
- Concepts developed for self-avoiding walks ($N = 0$) generalized to Ising ($N = 1$) loops
- Extend study in future work to other numbers of colors N

Collaboration with **Thomas Neuhaus** (FZ Jülich) and **Adriaan Schakel** (then Leipzig, now Recife (Brazil))

WJ, T. Neuhaus & A.M.J. Schakel, Nucl. Phys. B **829** [FS] (2010) 573

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THANK YOU !

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