Cluster-size scaling in O(N)-models

W.B. (UNAM, Mexico), Stephan Caspar, Manes Hornung,
João Pinto Barros, Uwe-Jens Wiese (Univ. of Bern, Switzerland)

Spin clusters as physical objects, with fractal dimension D

- Quantum rotor, $D = 1$; merons: clusters with topological charge $1/2$
- 2d XY model, $D < 2$; cluster vorticity may refine the interpretation of the Berezinskii-Kosterlitz-Thouless phase transition
- 3d O(4) model, $D < 3$ related to critical exponents, effective theory for high-T 2-flavor QCD, $Q \sim$ baryon number
- 2d Heisenberg model: talk by J. Pinto Barros

Clusters as physical carriers of topological charge and vorticity, beyond semi-classical approximations

O(N) non-linear σ-models on the lattice

Classical spins $\vec{e}_x \in S^N$ at sites $x \in \mathbb{Z}^d$, periodic boundary conditions

Lattice actions to be considered ($|\hat{\mu}| = 1,\ \mu = 1 \dots d$)

$$
\begin{aligned}
S_{\rm standard}[\vec{e}] &= \beta \sum_{x,\,\mu} (1 - \vec{e}_x \cdot \vec{e}_{x+\hat{\mu}}) \\
S_{\rm Manton}[\vec{e}] &= \tfrac{1}{2}\,\beta\,\varphi_{x,\mu}^2\ , \qquad \varphi_{x,\mu} = \arccos(\vec{e}_x \cdot \vec{e}_{x+\hat{\mu}}) \in (-\pi, \pi] \\
S_{\rm constraint}[\vec{e}] &= \begin{cases} 0 & \text{if } |\varphi_{x,\mu}| < \delta \quad \forall x,\ \mu \\ +\infty & \text{otherwise} \end{cases}
\end{aligned}
$$

For $d = N - 1$: top. charge $Q[\vec{e}] \in \mathbb{Z}$

Geometric definition: split unit hypercube into pieces with N spins (*e.g.* $d = 2$: divide plaquettes into triangles). Oriented volume of minimal surface spanned on S^N = contributions q_i, $\sum_i q_i = Q \in \mathbb{Z}$ (Berg/Lüscher '81)

Cluster algorithm:

(1) Choose random direction $\vec{r} \in S^N$. **Spin flip**: $\vec{e}_x \to \vec{e}_x{}' := e_x - 2(\vec{e}_x \cdot \vec{r})\,\vec{r}$

(2) Set a **bond** between any $\vec{e}_x$ and $\vec{e}_{x+\hat{\mu}}$, with probability

$$p = \begin{cases} 0 & \Delta s \leq 0 \\ 1 - e^{-\Delta s} & \Delta s > 0 \end{cases}$$

where $S = \sum_{x,\,\mu} s_{x,\mu}$ and $\Delta s = s'_{x,\mu} - s_{x,\mu}$

(3) Sets of spins connected by bonds $:=$ **clusters**
entire clusters can be flipped collectively, in agreement with detailed balance

- **Multi-cluster** (Swendsen-Wang):
  divide the whole lattice into clusters, flip each one with $p = \frac{1}{2}$

- **Single-cluster** (Wolff): build one cluster starting from a random seed, flip it

Back to (1)

Superior to local update algorithms:
suppresses auto-correlation and critical slowing down

Enables sometimes "improved estimator": implicit sum over contributions to some observable from all cluster orientations, drastic gain in statistics

So far considered an algorithmic tool, now also physical interpretation

For topological models: top. charge of one cluster

$$Q_{\rm cluster} := \frac{1}{2}(Q[\vec{e}\,] - Q[\vec{e}\,']) \in \{0,\ \pm\frac{1}{2},\ \pm 1,\ \pm\frac{3}{2},\ \pm 2\ \dots\}$$

where $[\vec{e}\,'] =$ conf. after flipping this cluster

Cluster charge can be assigned locally, $i.e.$ indep. of the orientation of all other clusters, for constraint angles

$$\delta \leq \frac{2\pi}{\#\ \text{spins in one unit cell},\ e.g.\ \text{hypercube}}$$

$E.g.$ 2d triangular lattice with $\delta = 2\pi/3$ (W.B/Pochinsky/Wiese '95)

Clusters with $Q_{\text{cluster}} = 1/2\ \ (-1/2)$: merons (anti-merons)

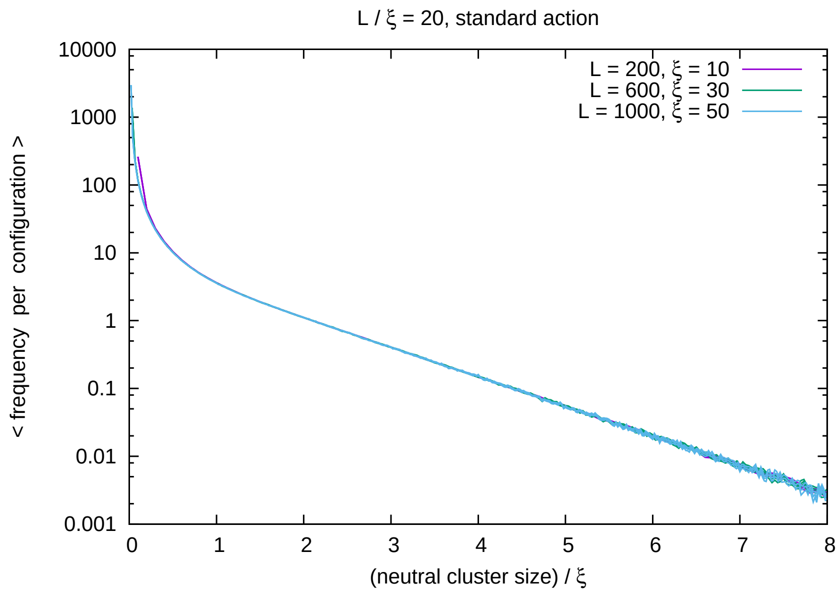
Improved estimator for $\langle Q^2 \rangle$: a meron–anti-meron pair contributes

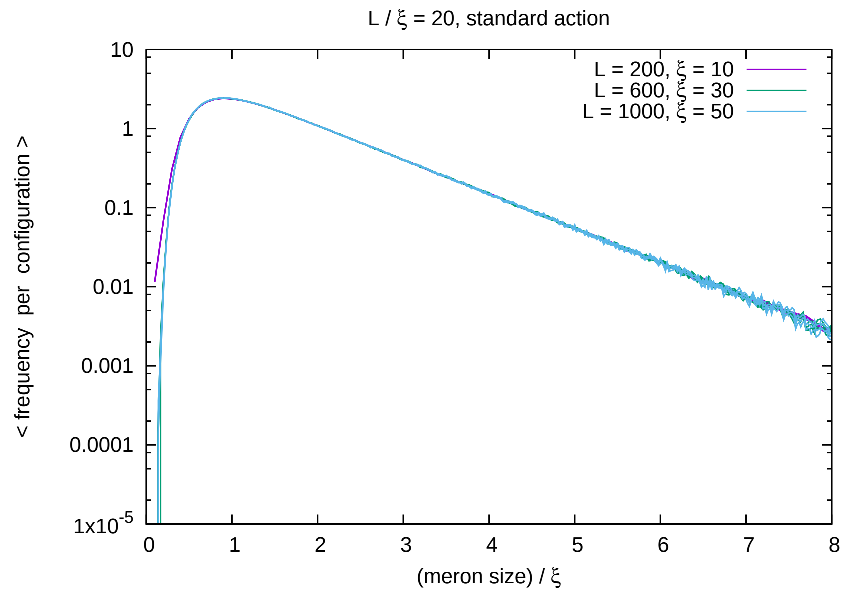
$$\frac{1}{4}(\underbrace{1}_{\uparrow\uparrow} + \underbrace{0}_{\uparrow\downarrow} + \underbrace{0}_{\downarrow\uparrow} + \underbrace{1}_{\downarrow\downarrow}) = 1/2$$

Statistics amplified by factor $2^{\text{number of neutral clusters}}$

Quantum rotor: 1d O(2) model

Peculiarities: no constraint angle required; $Q_{\rm cluster} \in \{0, \pm 1/2\}$



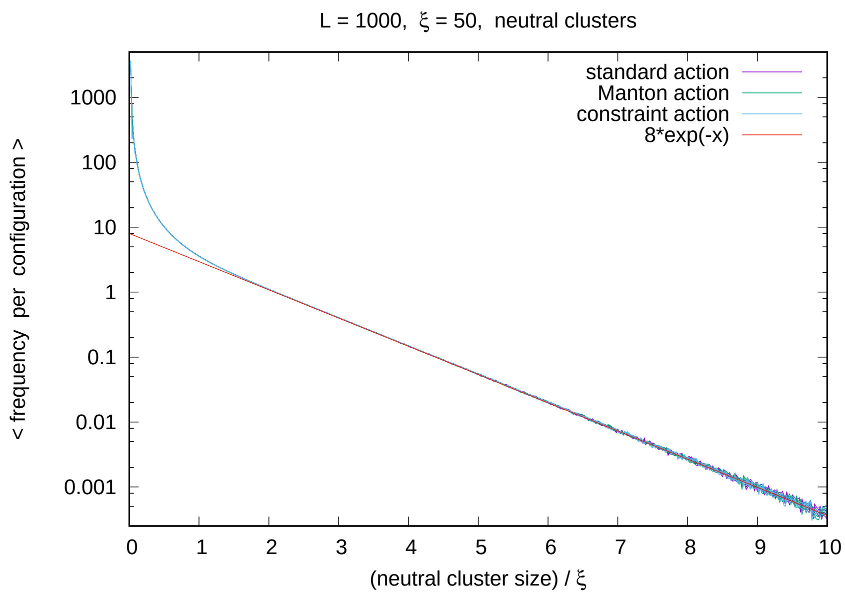


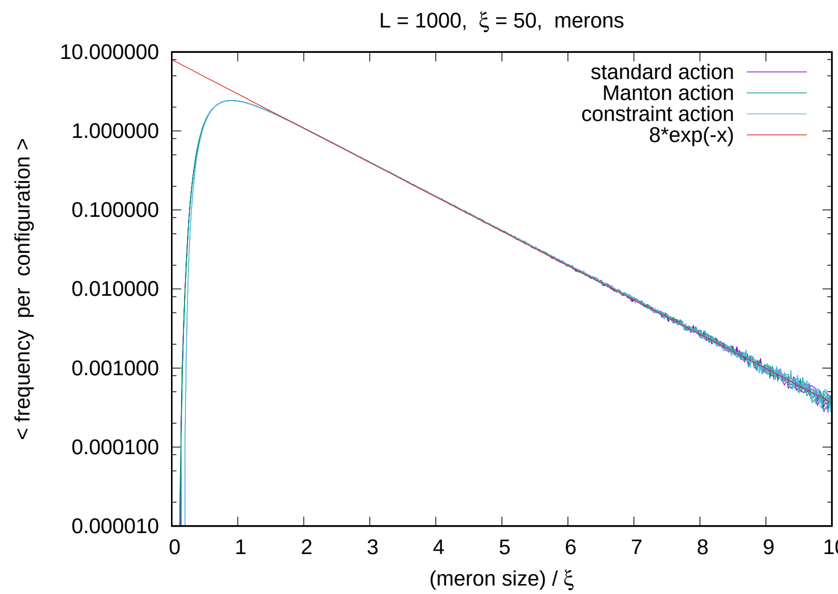
Histograms for the size distribution of clusters with $Q = 0$ (left) and $|Q| = 1/2$ (right), for $S_{\rm standard}$, physical size $L/\xi = 20$, correlation length $\xi = 10,\ 30,\ 50$

Converges to a stable continuum limit, in units of ξ

Meron size integral reproduces top. susceptibility $\chi_{\rm t}\,\xi = 1/2\pi^2$

Universality (even 1d): S_{standard}, S_{Manton}, $S_{\text{constraint}}$ at $L = 1000$, $\xi = 50$





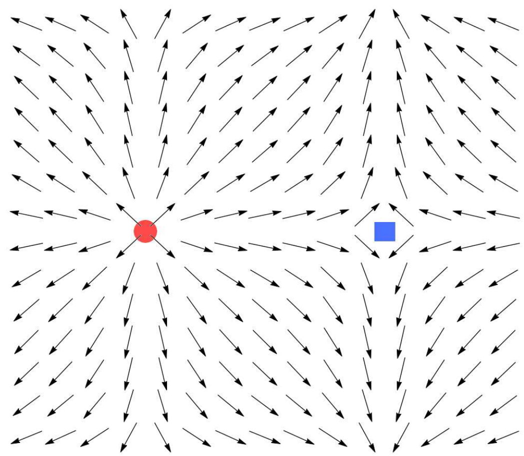
For all three lattice actions, the size distributions of neutral clusters and of merons coincide.

Small clusters (size $\leq \mathcal{O}(\xi)$) are mostly neutral.

For size $> \mathcal{O}(\xi)$ neutral clusters and merons (including anti-merons) are equally frequent, with $\langle$ frequency per conf. $\rangle \simeq 8\exp(-\text{size}/\xi)$

2d XY model or O(2) model

No global topology, but plaquettes may carry a vortex (V, ●) or an anti-vortex (AV, ■), *e.g.*



Minimal relative angle between two spins $\Delta\varphi_{x,y} = (\varphi_y - \varphi_x) \bmod 2\pi \in (-\pi, \pi]$

Vortex number at plaquette x

$$v_x = \frac{1}{2\pi}\Big(\Delta\varphi_{x,x+\hat{1}} + \Delta\varphi_{x+\hat{1},x+\hat{1}+\hat{2}} + \Delta\varphi_{x+\hat{1}+\hat{2},x+\hat{2}} + \Delta\varphi_{x+\hat{2},x}\Big) \in \{+1, 0, -1\}$$

Periodic b.c. $\longrightarrow$ total vorticity $N_{\rm V} - N_{\rm AV} = 0$ for each conf.

Essential phase transition (order ∞)

$S_{\rm standard}: \quad \beta_{\rm c} = 1.1199$ (Hasenbusch '05)

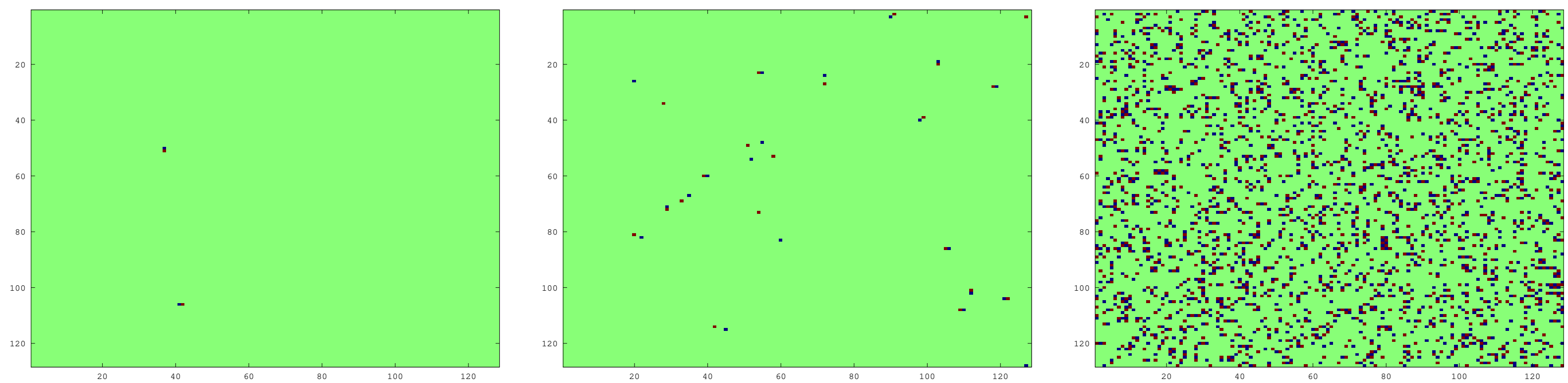
$S_{\rm constraint}: \quad \delta_{\rm c} = 1.775(1)$ (WB/Bögli/Niedermayer/Pepe/Rejón-Barrera/Wiese '13)

massless $\Leftrightarrow$ massive phase, but no spont. sym. breaking

Berezinskii-Kosterlitz-Thouless (BKT) mechanism:

$\xi = \infty$: pairs of near-by V–AV, invisible at large length scale

$\xi < \infty$: pairs break up, V and AV (quasi-)random distributed

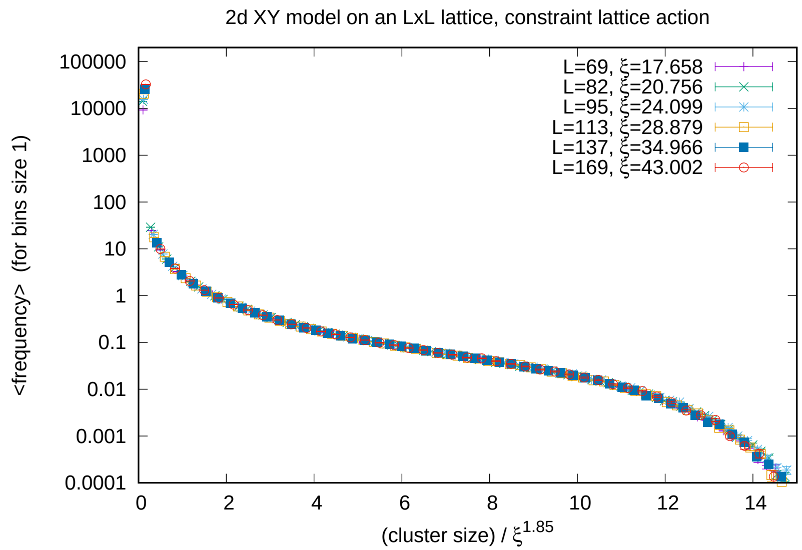


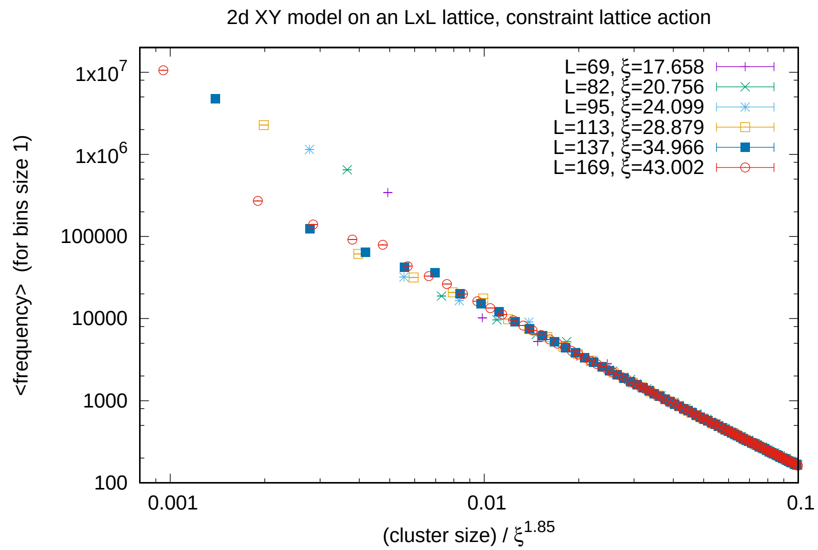
Typical confs on 128×128 lattice at low, moderate, high δ

• BKT mechanism: attractive V–AV force minimizes free energy $\mathcal{F}$, **but** effect still works with constraint action, where $\mathcal{F} \equiv 0$

Confirmed by "free" V or AV density (no counterpart within "short range"), or summed V–AV (distance)^2 for optimal pairing (WB/Gerber/Rejón-Barrera '13)

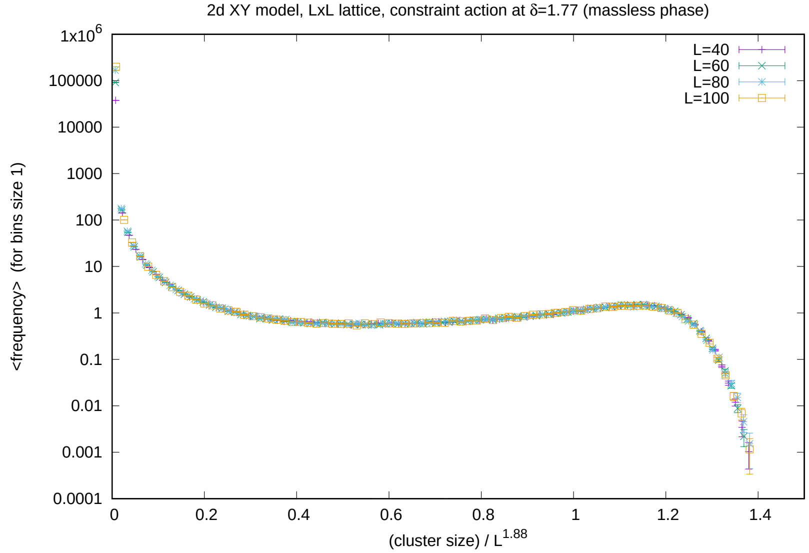
• Cluster-size scaling for *all* clusters in the *massive phase:*

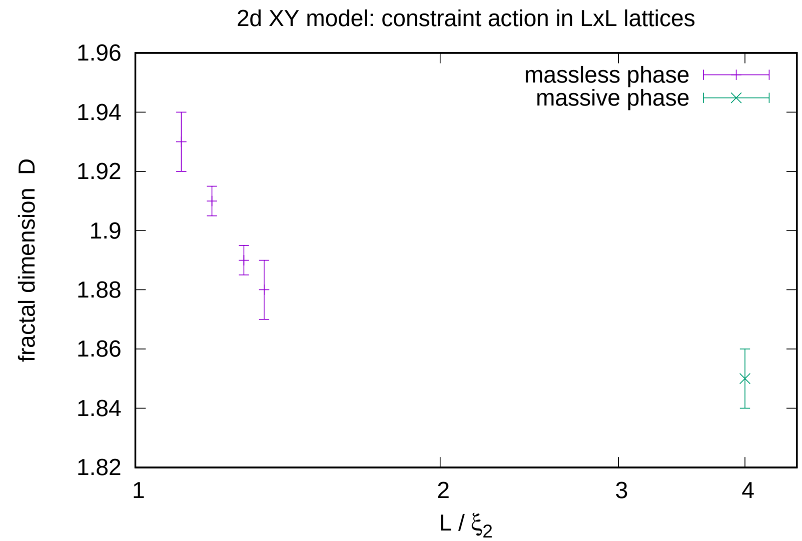




Tune $\delta > \delta_c$ such that $L/\xi = 3.93(1)$, $\xi \simeq 17.7 \ldots 43.0$. Cont. scaling for **fractal dimension $\mathbf{D = 1.85(1)}$**, except for tiny clusters; abundant 1-site clusters fill $V_{\rm continuum}$

Massless phase: cluster-size scaling in units of L^D





Left: example for $\delta = 1.77 < \delta_c$: for varying L, $L/\xi_2 = 1.34$ is $\simeq$ constant (ξ_2: second moment correlation length, $\xi_2 \lesssim \xi$).

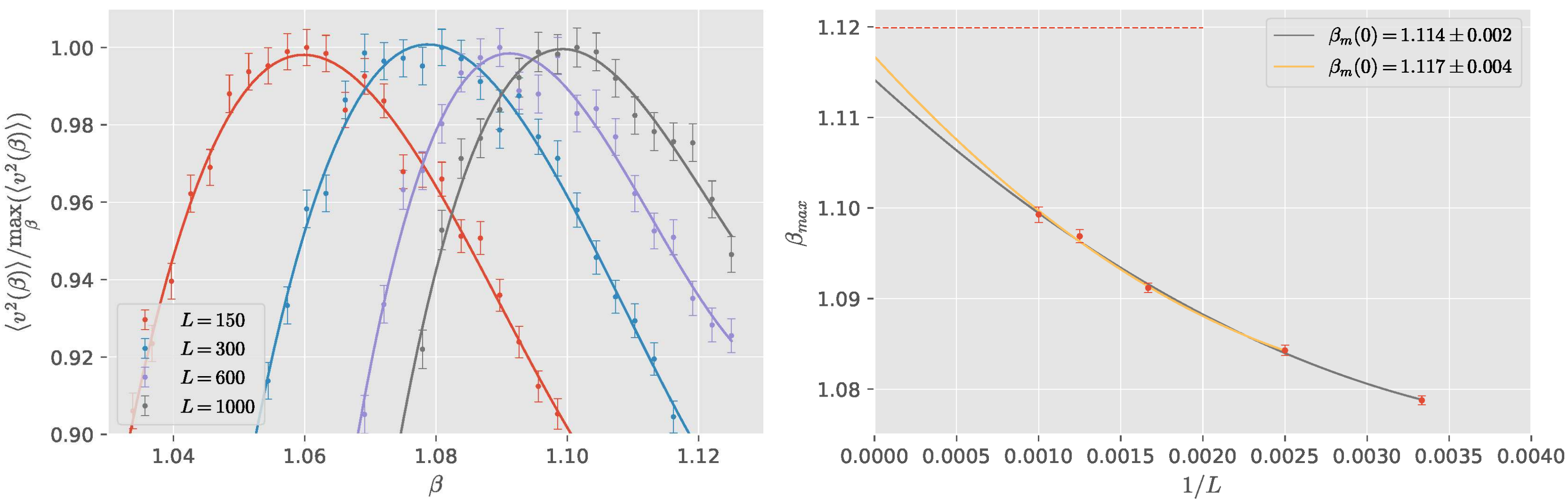
Right: fractal dimension D as a function of the quasi-physical size L/ξ_2: $\delta = 1.5,\ 1.6,\ 1.7,\ 1.77 < \delta_c = 1.775$ with $L/\xi_2 = 1.11 \dots 1.34$ (as a finite-size effect). Each $\delta \leq \delta_c$ represents a university class. $\langle$cluster size$\rangle = 3.39 \dots 2.87$

$D = 1.93(1) \dots 1.88(1)$, might converge to 2 for decreasing δ (large clusters fill V)

Vorticity of one cluster, defined similarly to top. charge,

$$V_{\text{cluster}} := \tfrac{1}{2}(N_{\text{V}}[\vec{e}] - N_{\text{V}}[\vec{e}\,']) \ , \quad [\vec{e}\,'] \ \text{conf. after cluster flip}$$

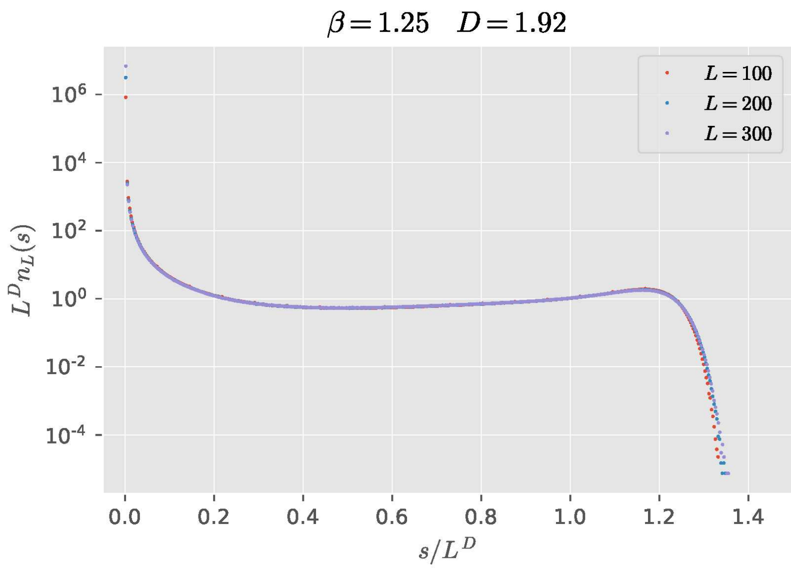
β-dependence of $\langle V^2_{\text{cluster}} \rangle$ for S_{standard} and single-cluster algorithm

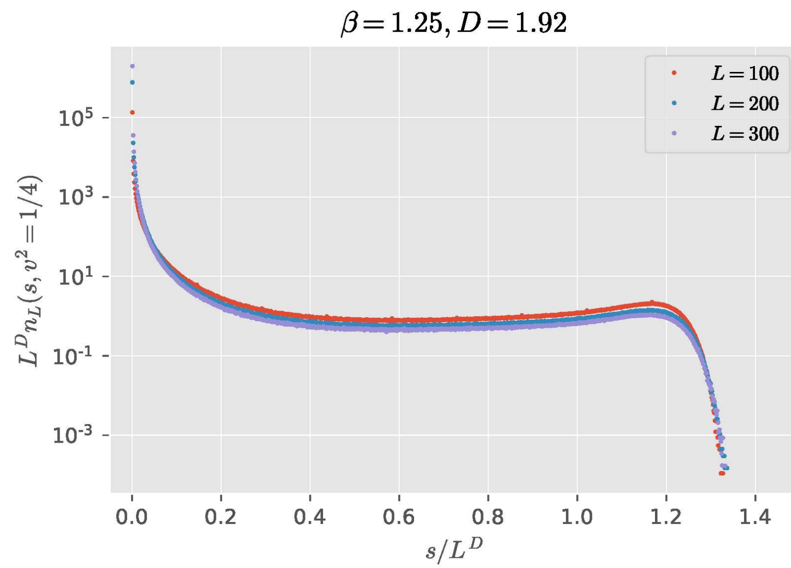


Left: histograms for lattice sizes $L = 150 \ldots 1000$, normalized by maximal value, with Gaussian interpolations

Right: thermodyn. extrapolation of β_{max}; with largest 4 sizes, compatible with $\beta_c \simeq 1.12$

Cluster-size histograms for $\beta = 1.25$ (massless): all clusters, and $|v| = 1/2$





If scaling is confirmed at fixed |cluster vorticity| $\Rightarrow$ clear-cut criterion which V and AV count for the BKT phase transition: those which induce a non-zero cluster vorticity.

With improved estimator: prospects for unambiguous stochastic formulation of the BKT mechanism, in terms of vorticity-carrying clusters

3d O(4) model

Low-energy effective theory for 2-flavor QCD in the chiral limit

SSB: $\mathrm{SU}(2)_L \otimes \mathrm{SU}(2)_R \to \mathrm{SU}(2)_{L=R}$ isomorphic to $\mathrm{O}(4) \to \mathrm{O}(3)$

High-T $\to$ dim. reduction, top. sectors; Q corresponds to baryon number

(Skyrme '61, Adkins/Nappi/Witten '83, Zahed/Brown '86, Rajagopal/Wilczek 1993)

$\mu_B \sim \mathrm{i}\theta$, no sign problem, conjecture about the QCD phase diagram
Estimated Critical Endpoint: $(T, \mu_B)_{\mathrm{CEP}} \simeq (140(5)\,\mathrm{MeV},\ 168(16)\,\mathrm{MeV})$

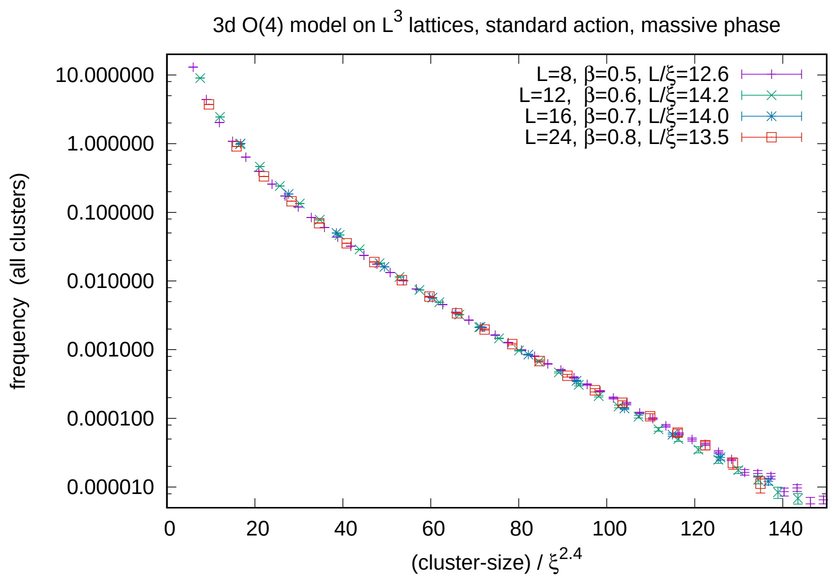
(Nava Blanco, MSc. thesis '19)

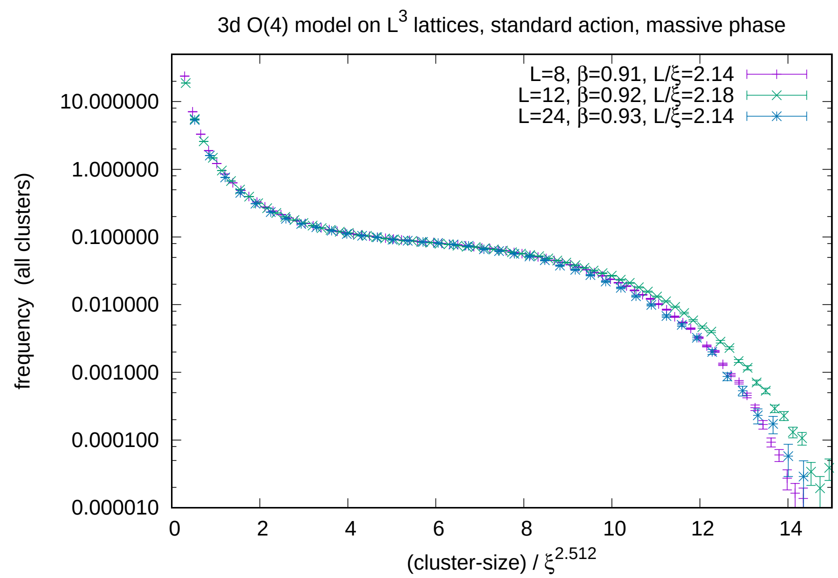
Meron concept (local assignment of top. cluster charges) requires here a very restrictive constraint, only very smooth confs.

- We use S_{standard} at $\mu_B = 0$ and study cluster-size scaling for *all* clusters.

Critical coupling: $\beta_{\mathrm{c}} = 0.93590$ (Oevers '96)

Symmetric phase: $\beta < \beta_c$, cluster-size scale ξ^D



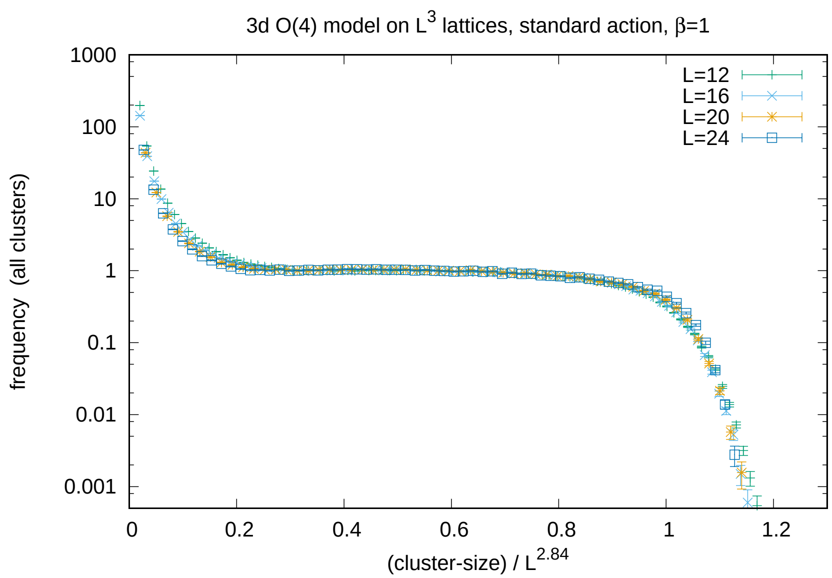


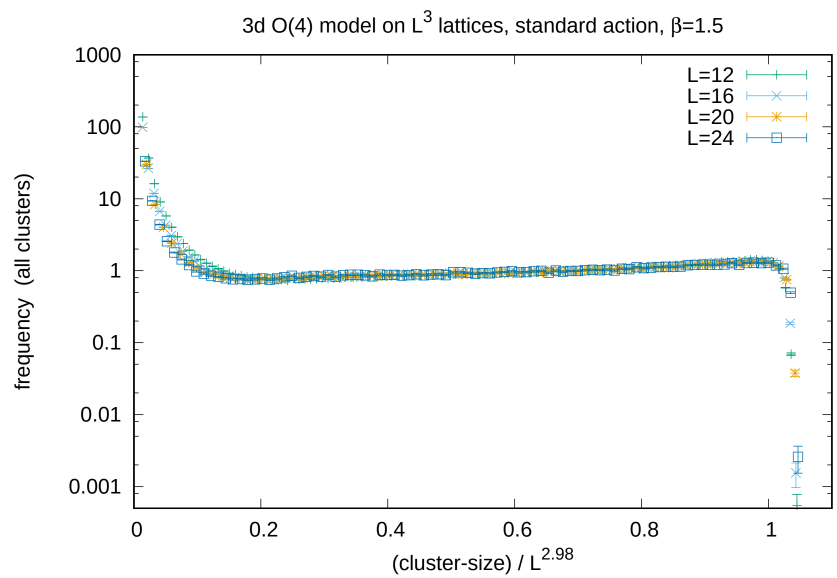
Left: $\beta = 0.5 \ldots 0.8$, $L/\xi \simeq 13.6$: $D \approx 2.4$

Right: $\beta = 0.91 \ldots 0.93$, $L/\xi \simeq 2.15$: $D \approx 2.5$

rough and preliminary: β not fine-tuned, ξ short

Phase of spontaneous symmetry breaking: $\beta > \beta_{\rm c}$, cluster-size scale L^D





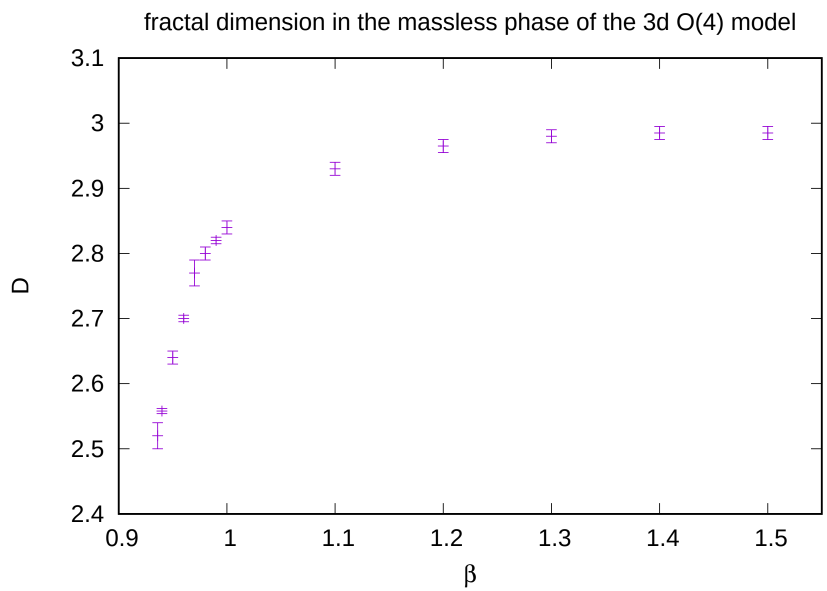
$$L = 12 \ldots 24$$

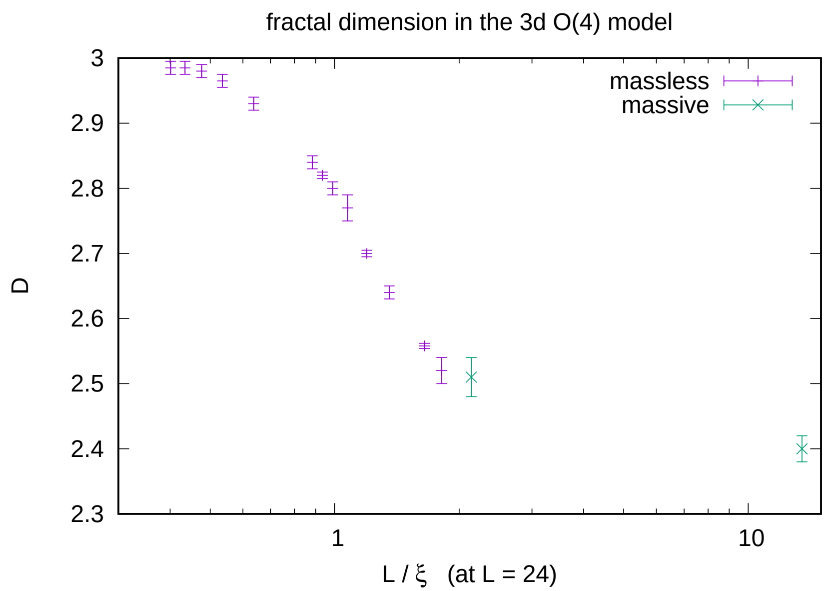
Left: $\beta = 1, \;\; D = 2.84(1)$ Right: $\beta = 1.5, \;\; D = 2.98(1)$

Long plateaux at ≈ 1 cluster /conf

Slight increase for $\beta = 1.5$: finite-size effect (clusters close across boundary)

Overview over fractal dimension D





Left: massless phase, dependence on β

Right: both phases, dependence on physical size L/ξ, kink

D seems to converge to $d = 3$ in the weak-coupling limit,
in analogy to the 2d XY model

Best motivated: finite-size scaling at the critical point

Magnetization

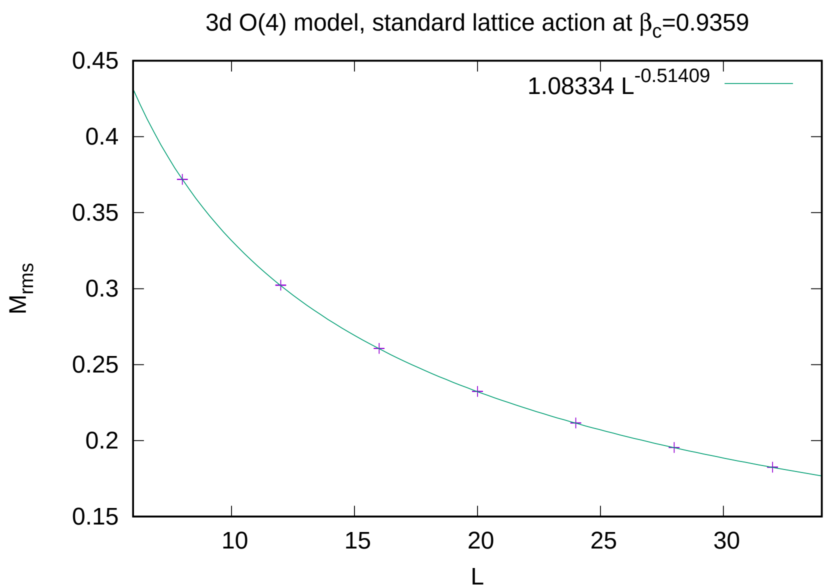
$$M_{\rm rms} := \frac{1}{V}\sqrt{\langle \vec{M}^{\,2}\rangle}\ , \qquad \vec{M} = \sum_x \vec{e}_x$$

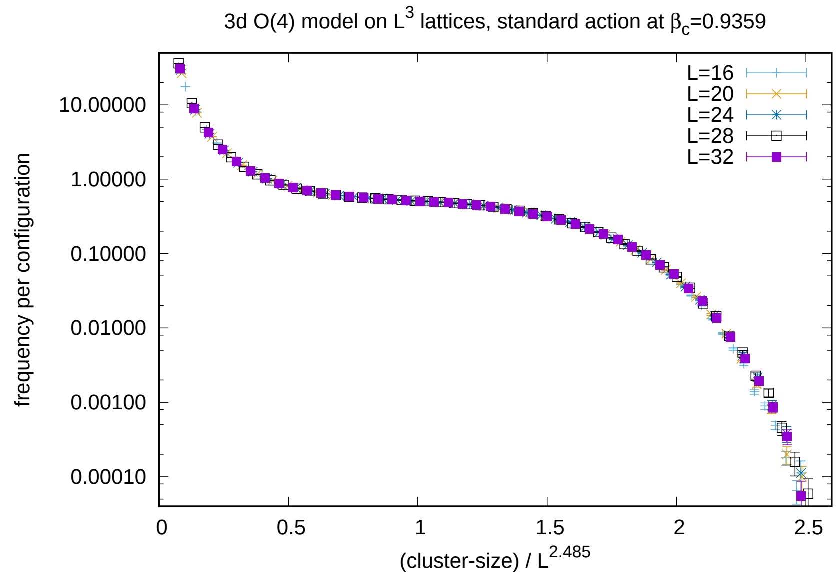
At critical coupling, in volume $V = L^d$, theory predicts

$$M_{\rm rms}|_{\beta_c} \propto L^{1-d/2-\eta/2} \stackrel{!}{=} L^{-\beta/\nu}$$

employing (hyper-)scaling–relations: $2-\eta = \gamma/2,\ \ d\nu = 2\beta + \gamma$

Engels/Fromme/Seniuch '03: $\beta = 0.380,\ \nu = 0.7377 \ \Rightarrow\ \underline{\beta/\nu \simeq 0.515}$





Left: 2-parameter fit $L = 16 \ldots 32$: $\beta/\nu = 0.514(1)$, consistent

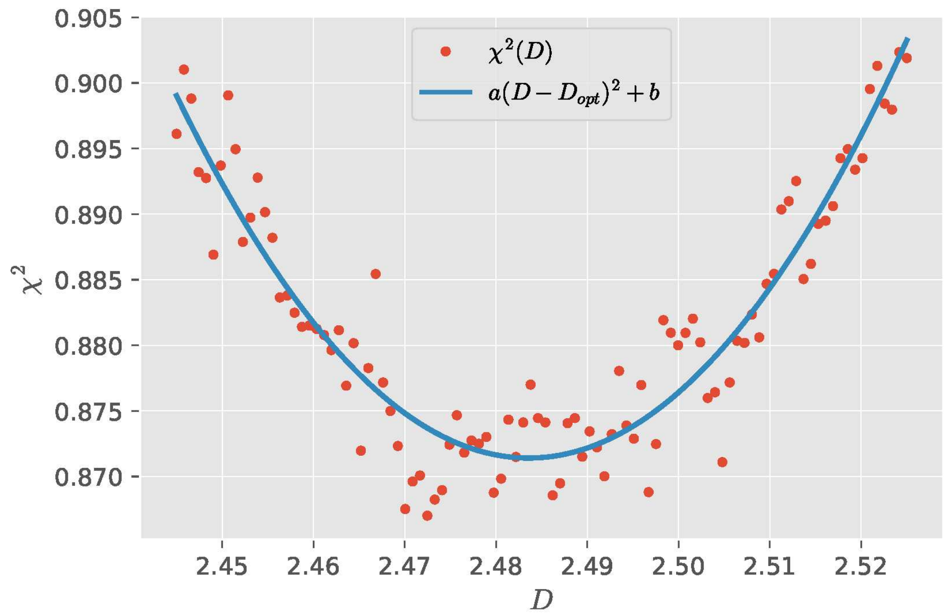
Link to fractal dimension D of cluster-size scaling:

$$D = d - \beta/\nu \simeq 2.485 \qquad \textbf{works!}$$

Ising model: improved estimator $\rightarrow$ cluster-size fixes $M_{\rm rms}$

For $N > 1$ not compelling, but still plausible, and numerically well in business

Systematic evaluation of optimal value for D :

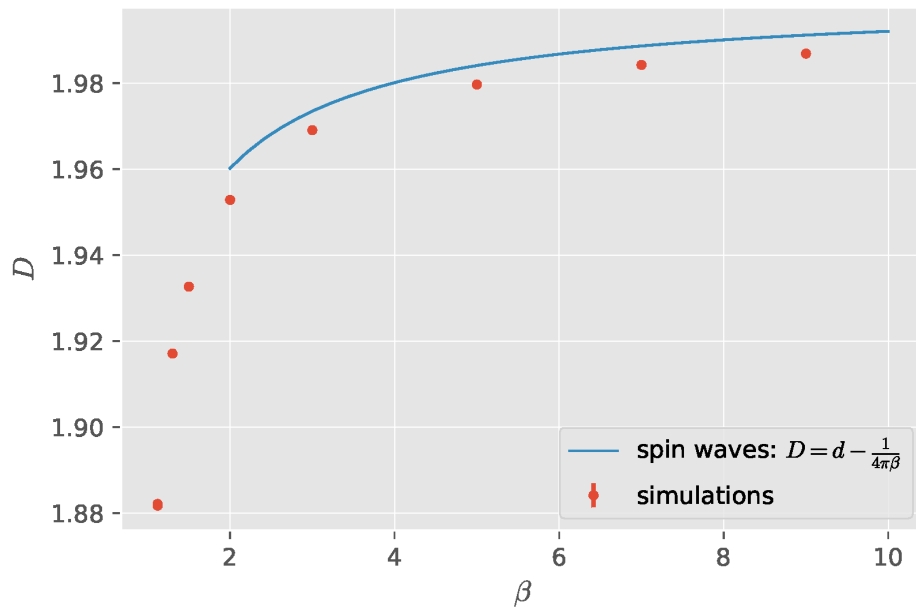


χ^2 for matching data from 5 volumes, $L = 16 \dots 32$

Parabolic interpolation takes minimum compatible with $D = 2.485$

Back to the 2d XY model:

Application of the same relation to critical line $D(\beta > \beta_c)$ for $S_{\rm standard}$



Spin wave weak-coupling expansion to $\mathcal{O}(1/\beta)$: $\quad \beta/\nu = \eta/2 \approx 1/4\pi\beta$

$$\langle \vec{e}_x \cdot \vec{e}_y \rangle \propto |x-y|^{-\eta}; \quad \eta = 1/2\pi\beta + \mathcal{O}(1/\beta^2)$$

(Berezinskii '70, Kosterlitz '74)

Conclusions

- Cluster-size continuum scaling observed in a set of O(N) models, clusters can be interpreted as physical objects
- In $d = 1$: scales with dimension $D = 1$. In $d > 1$ fractal scaling dimension $D \leq d$, space filled by non-scaling tiny clusters.
- Physical carriers of top. charge (merons and beyond), and of vorticity. Picture captures all confs. (not just semi-classical), explains top. susceptibility $\longrightarrow$ talk by J. Pinto-Barros
- Supposed to refine BKT mechanism in 2d XY model
- Improved estimator for magnetization relates D to critical exponents