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
\textbf{O}(N) non-linear $\sigma$-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 ($|\hat{\mu}| = 1$, $\mu = 1 \ldots d$)

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

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 $S^N = \text{contributions } q_i, \quad \sum_i q_i = Q \in \mathbb{Z}$ \quad (Berg/Lüscher '81)
Cluster algorithm:

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

(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

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

where \([\vec{e}'] = \text{conf. after flipping this cluster}\]
Cluster charge can be assigned locally, \textit{i.e.} indep. of the orientation of all other clusters, for constraint angles

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

\textit{E.g.} 2d triangular lattice with \( \delta = \frac{2\pi}{3} \) \hspace{1cm} (\text{W.B/Pochinsky/Wiese '95})

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

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

\[ \frac{1}{4} \left( \frac{1}{\uparrow\uparrow} + \frac{0}{\uparrow\downarrow} + \frac{0}{\downarrow\uparrow} + \frac{1}{\downarrow\downarrow} \right) = 1/2 \]

Statistics amplified by factor \( 2^{\text{number of neutral clusters}} \)
Quantum rotor: 1d O(2) model

Peculiarities: no constraint angle required; \( Q_{\text{cluster}} \in \{0, \pm 1/2\} \)

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

Converges to a stable continuum limit, in units of \( \xi \)

Meron size integral reproduces top. susceptibility \( \chi_t \xi = 1/2\pi^2 \)
Universality (even 1d): $S_{\text{standard}}, S_{\text{Manton}}, S_{\text{constraint}}$ 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 $\langle \text{frequency per conf.} \rangle \approx 8 \exp(-\text{size}/\xi)$
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 \( \Delta \varphi_{x,y} = (\varphi_y - \varphi_x) \mod 2\pi \in (-\pi, \pi] \)

Vortex number at plaquette \( x \)

\[
v_x = \frac{1}{2\pi} \left( \Delta \varphi_{x,x+\hat{1}} + \Delta \varphi_{x+\hat{1},x+\hat{1}+\hat{2}} + \Delta \varphi_{x+\hat{1}+\hat{2},x+\hat{2}} + \Delta \varphi_{x+\hat{2},x} \right) \in \{ +1, 0, -1 \}
\]

Periodic b.c. \( \rightarrow \) total vorticity \( N_V - N_{AV} = 0 \) for each conf.
Essential phase transition \((\text{order } \infty)\)

\[ S_{\text{standard}} : \quad \beta_c = 1.1199 \quad \text{(Hasenbusch '05)} \]
\[ S'_{\text{constraint}} : \quad \delta_c = 1.775(1) \quad \text{(WB/Bögli/Niedermayer/Pepe/Rejón-Barrera/Wiese '13)} \]

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 \(128 \times 128\) lattice at low, moderate, high \(\delta\)
• 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 $D = 1.85(1)$, except for tiny clusters; abundant 1-site clusters fill $V_{\text{continuum}}$
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 ($\xi_2$: second moment correlation length, $\xi_2 \lesssim \xi$).

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

$D = 1.93(1) \ldots 1.88(1)$, might converge to 2 for decreasing $\delta$ (large clusters fill $V$)
Vorticity of one cluster, defined similarly to top. charge,

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

\( \beta \)-dependence of \( \langle V_{\text{cluster}}^2 \rangle \) for \( S_{\text{standard}} \) and single-cluster algorithm

Left: histograms for lattice sizes \( L = 150 \ldots 1000 \), normalized by maximal value, with Gaussian interpolations
Right: thermodyn. extrapolation of \( \beta_{\text{max}} \); 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 $|\text{cluster vorticity}| \Rightarrow$ 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: $\text{SU}(2)_L \otimes \text{SU}(2)_R \rightarrow \text{SU}(2)_{L=R}$ isomorphic to $\text{O}(4) \rightarrow \text{O}(3)$

High-T $\rightarrow$ dim. reduction, top. sectors; $Q$ corresponds to baryon number
(Skyrme '61, Adkins/Nappi/Witten '83, Zahed/Brown '86, Rajagopal/Wilczek 1993)

$\mu_B \sim i\theta$, no sign problem, conjecture about the QCD phase diagram

Estimated Critical Endpoint: $(T, \mu_B)_{\text{CEP}} \simeq (140(5) \text{ MeV}, 168(16) \text{ MeV})$
(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 $S_{\text{standard}}$ at $\mu_B = 0$ and study cluster-size scaling for all clusters.

Critical coupling: $\beta_c = 0.93590$ (Oevers '96)
Symmetric phase: $\beta < \beta_c$, cluster-size scale $\xi^D$

3d O(4) model on $L^3$ lattices, standard action, massive phase

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: $\beta$ not fine-tuned, $\xi$ short
Phase of spontaneous symmetry breaking: $\beta > \beta_c$, 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 $\approx 1$ 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 $\beta$

Right: both phases, dependence on physical size $L/\xi$, 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

\[ M_{\text{rms}} := \frac{1}{V} \sqrt{\langle \vec{M}^2 \rangle}, \quad \vec{M} = \sum_x \vec{e}_x \]

At critical coupling, in volume \( V = L^d \), theory predicts

\[ M_{\text{rms}}|_{\beta_c} \propto L^{1-d/2-\eta/2} = L^{-\beta/\nu} \]

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

Engels/Fromme/Seniuch '03: \( \beta = 0.380, \nu = 0.7377 \Rightarrow \beta/\nu \simeq 0.515 \)
Left: 2-parameter fit $L = 16 \ldots 32$: $\beta/\nu = 0.514(1)$, consistent

Link to fractal dimension $D$ of cluster-size scaling:

$$D = d - \beta/\nu \simeq 2.485 \quad \text{works!}$$

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

For $N > 1$ not compelling, but still plausible, and numerically well in business
Systematic evaluation of optimal value for $D$:

$\chi^2$ for matching data from 5 volumes, $L = 16 \ldots 32$

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 $S_{\text{standard}}$

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

\[ \langle \vec{e}_x \cdot \vec{e}_y \rangle \propto |x - y|^{-\eta}; \quad \eta = \frac{1}{2\pi \beta} + \mathcal{O}(1/\beta^2) \] (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 $\rightarrow$ talk by J. Pinto-Barros

• Supposed to refine BKT mechanism in 2d XY model

• Improved estimator for magnetization relates $D$ to critical exponents