Solving the Sign Problem in a Toy Model

I. Physics and Results

Quantum spin chains, Haldane's conjecture

Mapping on the 2d $O(3)$ model with a θ-term

Mass gap, limit $\theta \rightarrow \pi$

II. Algorithm and its Interpretation

Cluster algorithm and Improved Estimator

A stochastic formulation of merons

Phase transition due to meron condensation

[W.B., A. Pochinsky and U.-J. Wiese, Phys. Rev. Lett. 75, p. 4524]

Anti-ferromagnetic quantum spin chain

1d, discrete, *e.g.* Heisenberg Hamiltonian $\mathcal{H} = J \sum_{<ij>} \vec{S}_i \vec{S}_j$

$< i, j >$: nearest neighbours, $J > 0$: anti-ferromagnet

Quantum spins: $[S^a, S^b] = \mathrm{i}\, \epsilon^{abc} S^c$, $\vec{S}^2 = s(s+1)$

Ground state not obvious ($\neq$ Néel state)

1931 : Bethe identifies ground state for $s = 1/2$

1950's - 60's : Spin wave theory (Anderson, Kubo . . .) predicts gap-less "quasi long range order": power decay of correlations (no Goldstone bosons)

1961 : Lieb-Schultz-Mattis Theorem: proves zero gap for $s = 1/2$

1983 : Haldane Conjecture: $s = \begin{cases} \text{half-integer} & : \quad \text{gap-less} \\ \text{integer} & : \quad \text{finite gap} \end{cases}$

Surprise for $s \in \mathbb{N}$: contradiction to Bethe ansatz ?

Numerics: confirms gap for $s = 1$ (Botet, Julien . . . 83-85)

Diagonalisation up to $L = 22$, extrapolation $\longrightarrow \Delta_1 = 0.4105\ J$

and $s = 2$ Simulation up to $L = 350 \longrightarrow \Delta_2 \simeq 0.085\ J$ (Jolicoeur/Schollwöck '95)

Large s : $\Delta_s \sim s^2 e^{-\pi s} \quad \Rightarrow \quad \Delta_2 \approx 0.07\ J$

Experiment: $CsNiCl_3$: quasi 1d anti-ferromagnet, $s = 1$: $Ni^{2+}Cl^{-}Ni^{2+}Cl^{-}$

$J \simeq 33$ K. Scatter polarised neutrons, multi-peak structure $\longrightarrow \Delta_1 \simeq 0.4\ J$

Analytic Proof:

- All half-integer s are gap-less (Affleck, Lieb '86)
- Gap for $s = 1$ (Affleck, Kennedy, Lieb, Tasaki '87)

Spin chain:

- Gap for s integer : $s = 1$ analytic, $s = 2$ numerical, $s > 2$ plausibility
- Gap-less for s half-integer : proved analytically

Mapping based on large s or low energy assumptions onto

2d $O(3)$ Model with $\theta = 2\pi s$ 2π periodic $\Rightarrow$ restriction to $\theta \in [0, 2\pi)$

- $\theta = 0$: gap well established
- $\theta = \pi$: (heuristic) meron picture suggests gap zero

Uncertain part flips

Simulation by Bhanot/Dashen/Seiberg/Levine ('84) not conclusive

$\Rightarrow$ New simulations with powerful cluster algorithm
Identify phase diagram, better insight into meron picture

2d $O(3)$ non-linear σ-model

Euclidean action:

$$S[\vec{e}] = \int d^2x \left[\frac{1}{2g}\partial_\mu \vec{e}\,\partial_\mu \vec{e} - \frac{\theta}{8\pi}\mathrm{i}\,\epsilon_{\mu\nu}\vec{e}(\partial_\mu \vec{e}\,\partial_\nu \vec{e})\right] = S_0[\vec{e}] - \mathrm{i}\,\theta Q[\vec{e}]$$

$S_0 \in \mathbb{R}_+$, $\vec{e}^{\,2}(x) \equiv 1$

counts how many times $\vec{e}$ covers S^2 $=$ topological charge $Q \in \mathbb{Z}$

2π periodic θ

s integer: $\theta = 0$: gap confirmed
s half-integer: $\theta = \pi$: gap-less ?

As in QCD : θ has no effect on classical solution and perturbation theory, must be explored non-perturbatively, but: *simulation has sign problem*

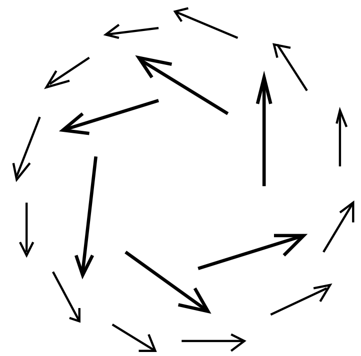
Heuristic picture of the mass gap at $\theta = 0$ (J. Affleck)

Introduce a potential $\frac{m^2}{2g} e_z^2 \;\Rightarrow\; \vec{e}$ prefers (e_x, e_y)-plane $(m \to \infty$: XY model)

Polar coordinates: φ : angle **in** (e_x, e_y)-plane
α : angle **out of** (e_x, e_y)-plane, $e_z = \sin\alpha \approx \alpha$

$$\mathcal{L}(\varphi, \alpha) \approx \frac{1}{2g}\Big[(\partial_\mu \varphi)^2 + (\partial_\mu \alpha)^2 + m^2 \alpha^2\Big]$$

(e_x, e_y)-plane could contain vortices, which destroy long-range order



$$q = \frac{1}{4\pi} \oint \vec{\nabla}\varphi(x)\, d\vec{s} = \pm\frac{1}{2} \quad \begin{cases} \text{meron} = \text{“half-instanton“} \\ \text{anti-meron} \end{cases}$$

r : radius from core, $|\vec{\nabla}\varphi| \propto 1/r$

Vortex action : $\int d^2x\, (\vec{\nabla}\varphi)^2 = 2\pi \ln L/a$ (L: size, a “lattice constant”)

$L \to \infty$ excludes a single vortex, but a region with zero vorticity

$$\frac{1}{2\pi} \oint_{\partial\,\text{region}} \vec{\nabla}\varphi\, d\vec{s} = 0$$

has an IR finite action, *e.g.* a meron–anti-meron pair

$m \to 0$:

$\vec{e}$ leaves preferred plane,
UV divergence at $r = 0$ can be avoided by $\alpha = \pm\pi/2$ in the core.

Condensation of vortex–anti-vortex pairs diffuses long range order
$\Rightarrow$ causes mass gap !

Now add θ-term : attaches factor $\exp(\pm i\theta/2)$ for $q = \pm 1/2$

Path integral over dilute vortex gas plus fluctuation $\Rightarrow$ identification with sine-Gordon model

$$\mathcal{L}[\tilde{\varphi}] = \frac{1}{2g}(\vec{\nabla}\tilde{\varphi})^2 - \text{const.}\cos\frac{\theta}{2}\ \cos\frac{2\pi\tilde{\varphi}}{g}$$

with $\partial_\mu \varphi = \epsilon_{\mu\nu}\partial_\nu \tilde{\varphi}$

Action due to meron–anti-meron pair picks up factor $\cos\frac{\theta}{2}$, suppressed as θ is switched on

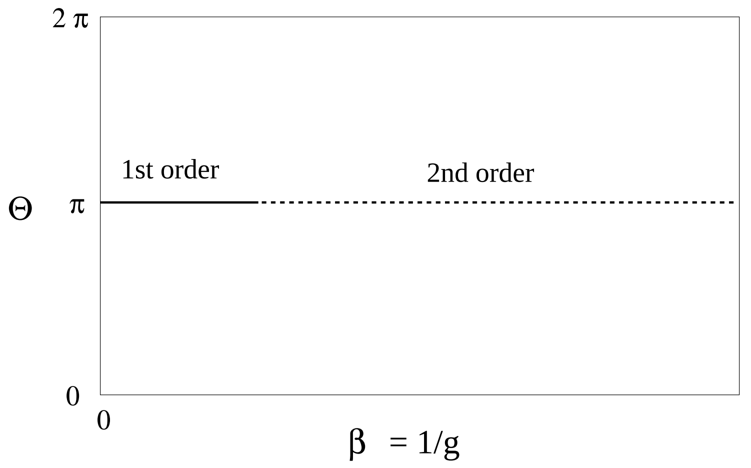
$\theta = \pi$: **vortices completely neutralised, "bound in pairs"** $\Rightarrow$ **mass gap vanishes**

$\Rightarrow$ $O(3)$ model gap-less at $\theta = \pi$ (?)

Uncertainties:

- $m \to 0$ at the end interchanges limits
- some multiple vortices do not cancel at $\theta = \pi$

Expected phase diagram



Phase transitions at $\theta = \pi$:

$1^{\rm st}$ order : at strong coupling for large $O(N \to \infty)$ (Seiberg '84), expected generally

$2^{\rm nd}$ order : moderate and weak coupling, based on mapping on WZNW model

Our lattice action truncates relative angles of neighbouring spins at $2\pi/3$

$\Rightarrow$ our restricted β_r corresponds to a standard $\beta > \beta_r$, even $\beta_r = 0$ in $2^{\rm nd}$ order regime

No scaling for $\beta \to \infty$, *i.e.* no sensible continuum limit

top. susceptibility diverges due to short-ranged "dislocations" with small action

BUT: for $\theta \to \pi$ at finite β (not too small) a critical point is expected

Map on $k = 1$ WZNW model predicts critical behaviour as $|\theta - \pi| \longrightarrow 0$

Gap introduces mass scale

$$\mu(\theta) = \frac{|\theta - \pi|^{2/3}}{|\ln(|\theta - \pi|)|^{1/2}}$$

(marginal operators provide log. correction)

Translates into powers of L with Fisher's parameter $z = \mu L$

Topological and magnetic susceptibility:

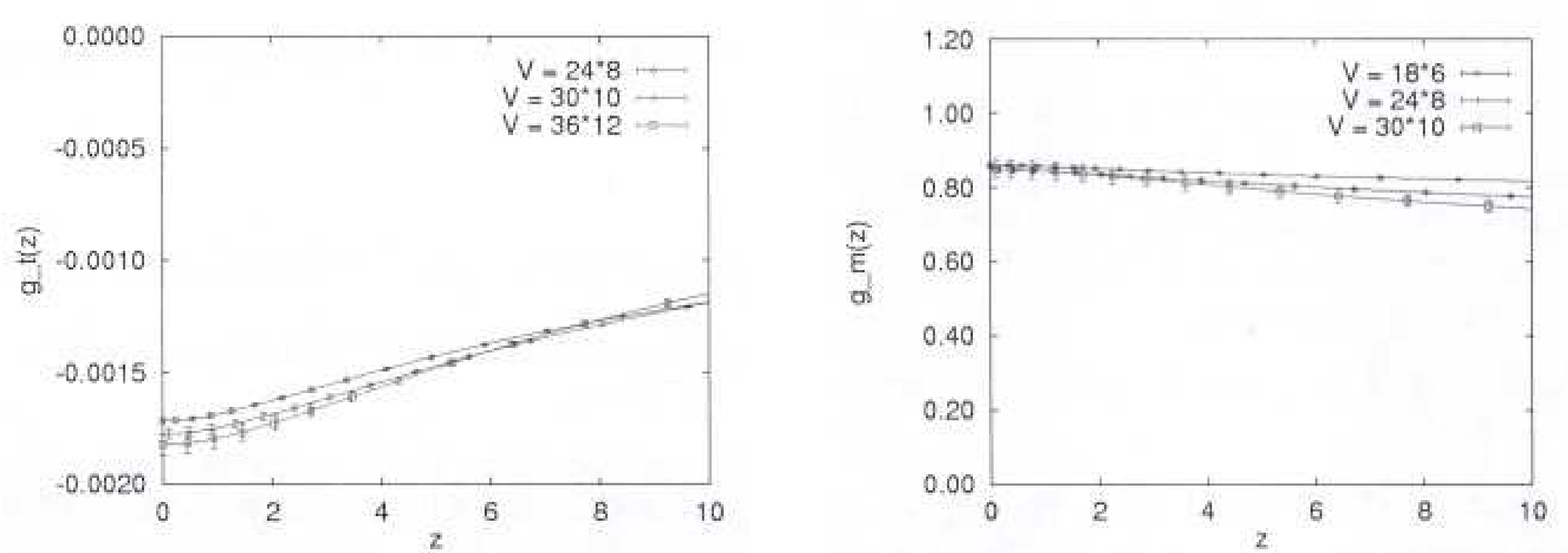
$$\chi_t := \frac{1}{V}(\langle Q^2\rangle - \langle Q\rangle^2)_\theta \simeq \frac{L}{\sqrt{\ln L}}\, g_t(z)$$

$$\chi_m := \frac{1}{V}(\langle \vec{M}^2\rangle - \langle \vec{M}\rangle^2)_\theta \simeq L\sqrt{\ln L}\, g_m(z) \qquad (\vec{M}[\vec{e}] = \int d^2x\, \vec{e}(x)\ )$$

Leading order: $\chi \propto L$ for 2^{nd} order phase transition ($\chi \propto L^2$ for 1^{st} order)

Close to phase transition (small μ, large L) :
$g_t(z)$ and $g_t(z)$ should be **universal functions**.

Confirmed for our plots, no fitting of any free parameters



Finite size scaling of 2$^{\rm nd}$ order phase transition, further improved by log. corrections

II. Algorithm and its Interpretation

Same problem as in QCD with a θ, or with chemical potential $\leftrightarrow$ finite baryon density
Complex Boltzmann factor $\exp(-S_0 + \mathrm{i}\theta Q) \neq$ probability, direct Monte Carlo fails.

Procedure: Simulation at $\theta = 0$, then attach phase factor.

Correct, but a lot of cancellation
requires *much* more statistics: $\propto \exp(\mathrm{const.}\, V)$ for stable errors, "sign problem"

Include phase factor: need very precise top. charge distribution $p(Q) =: \bar{p}(Q)/Z(0)$

$$\bar{p}(Q) = \int D\vec{e}\; \delta_{Q,Q[\vec{e}]}\, e^{-S_0[\vec{e}]} \quad \Rightarrow \quad Z(\theta) = \sum_Q \bar{p}(Q) e^{\mathrm{i}\,\theta Q}$$

$$\text{Observable at fixed } Q,\ \theta = 0\ :\ \langle \mathcal{O} \rangle_Q \quad = \quad \frac{1}{\bar{p}(Q)} \int D\vec{e}\; \delta_{Q,Q[\vec{e}]}\, \mathcal{O}[\vec{e}]\, e^{-S_0[\vec{e}]}$$

$$\Rightarrow \quad \langle \mathcal{O} \rangle_\theta \quad = \quad \frac{1}{Z(\theta)} \sum_Q \bar{p}(Q)\, \langle \mathcal{O} \rangle_Q\, e^{\mathrm{i}\,\theta Q}$$

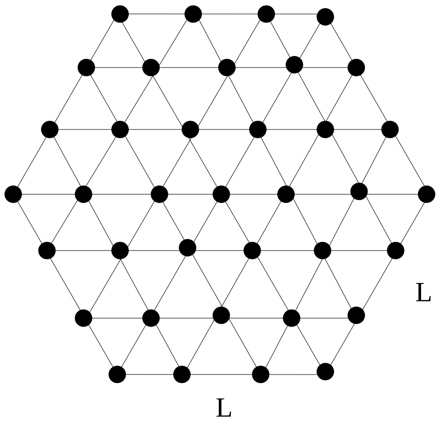
Triangular lattice in a hexagon with periodic b.c., $3L^2$ sites x with spins $\vec{e}_x$, $|\vec{e}_x| = 1$

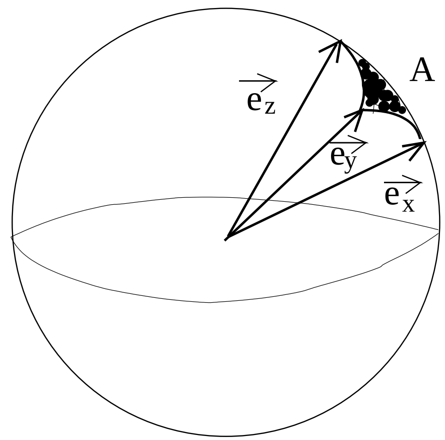
Top. charge of one (oriented) triangle:

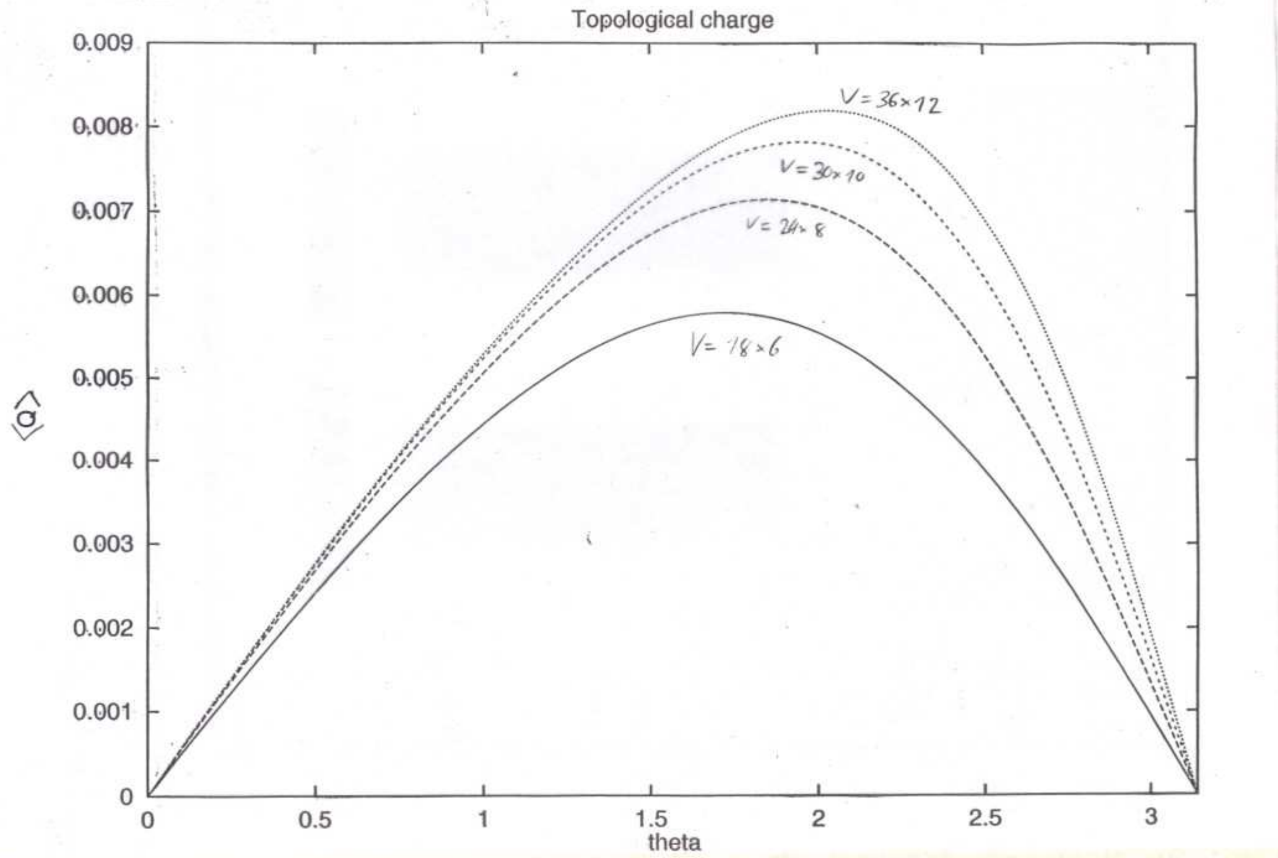
$$q(\vec{e}_x, \vec{e}_y, \vec{e}_z) = \frac{1}{4\pi} A(\vec{e}_x, \vec{e}_y, \vec{e}_z) \qquad (A \ : \ \text{minimal spherical angle})$$

$$\Rightarrow \quad Q = \sum_{<xyz>} q(\vec{e}_x, \vec{e}_y, \vec{e}_z) \in \mathbb{Z} \qquad (\text{virtue of geom. definition})$$

Total charge Q counts how many times sum of spherical triangles wraps around S^2





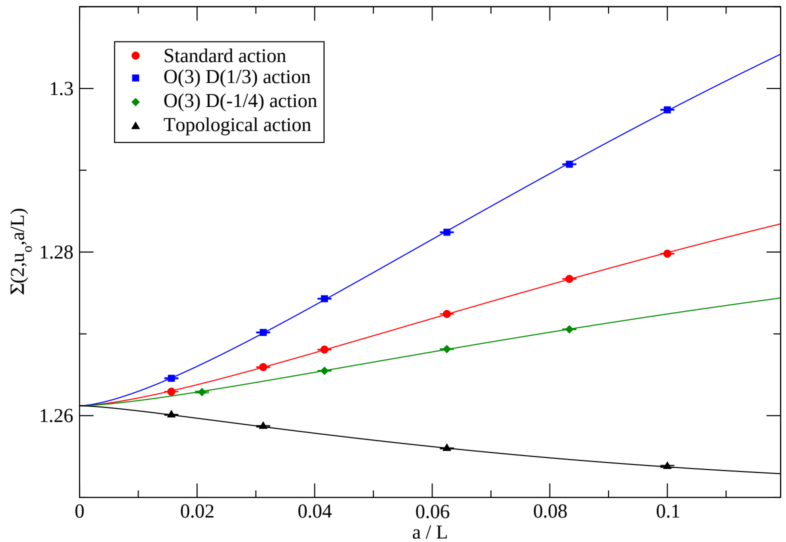


Topological charge $\langle Q \rangle$ as a function of θ, in volumes $18 \times 6 \; \ldots \; 36 \times 12$

Lattice action at $\theta = 0$:

$$S_0[\vec{e}] = \sum_{<xy>} s(\vec{e}_x, \vec{e}_y) \ , \qquad s(\vec{e}_x, \vec{e}_y) = \begin{cases} \frac{1}{g}(1 - \vec{e}_x \vec{e}_y) & \vec{e}_x \vec{e}_y > -\frac{1}{2} \\ \infty & \text{otherwise} \end{cases}$$

$i.e.$ angle between nearest neighbours $< 2\pi/3$ [Reason: Improved Estimator, see below]
Unusual, but in *universality class of the non-linear σ-model.* (same dim's and sym.)



Test with step scaling function: $\beta = 0$, vary constraint angle (W.B./Gerber/Pepe/Wiese '10)

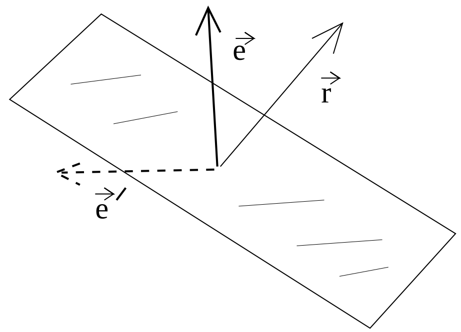
Multi-Cluster Algorithm (U. Wolff '89)

1) Choose random direction $\vec{r}$ $(|\vec{r}| = 1)$.
"Flipping" a spin $\vec{e}_x$ means $\vec{e}_x \longrightarrow \vec{e}_x{}' - 2(\vec{r} \cdot \vec{e}_x)\vec{r}$ (use plane vertical to $\vec{r}$ as a mirror)

2) Connect neighbouring spins $\vec{e}_x$, $\vec{e}_y$ by a bond with probability

$$p = \begin{cases} 0 & \text{flip reduces relative angle} \\ 1 - \exp[s(\vec{e}_x, \vec{e}_y) - s(\vec{e}_x{}', \vec{e}_y)] & \text{otherwise} \end{cases}$$

Bonds define the clusters. *Entire clusters* can be *flipped independently,* detailed balance holds thanks to prescription for cluster formation. Flip each cluster with probability $1/2$, return to 1). Suppresses auto-correlation and critical slowing down. [$O(3)$ symmetry is guaranteed by new $\vec{r}$ each time.]



Flip one cluster: total charge $Q \longrightarrow Q'$

Def.: top. charge of this cluster $q := \frac{1}{2}(Q - Q') \in$ { integer or half-integer }

Constraint on relative angles: bond is always set if flip would increase angle beyond $2\pi/3$

Angles at cluster boundaries are moderate (not too large or small)

Adjacent cluster don't feel flips much

Consequence: Charge of one cluster is independent of the orientation of all other clusters!
We can assign a top. charge locally to each cluster.

Example for $V = 36 \times 12, \ \beta_r = 0$:

$\|q\| = 0$	most clusters	$\langle$ size $\rangle = 1.5$ sites
$1/2$	4 %	10 sites
1	0.1 %	32 sites
> 1	very rare	

This property enables an Improved Estimator for $p(Q)$ and for $\langle \vec{M}^{\,2} \rangle$,

which fix $\chi_t(Q)$ and $\chi_m(Q)$.

- $p(Q)$

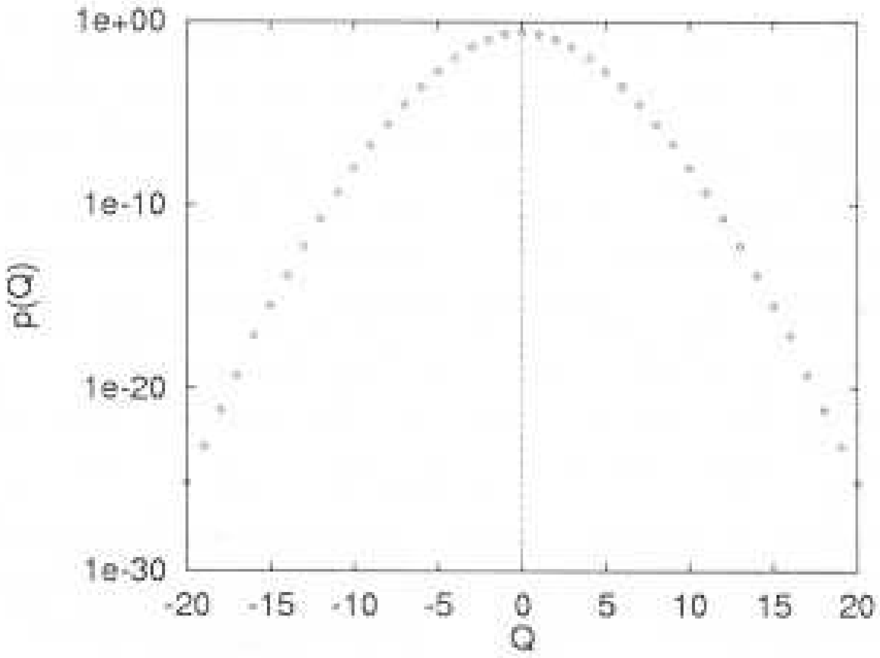
A conf. with N clusters is related to 2^N other conf's by cluster flips.
Once we know each cluster charge, the total charges Q for all these 2^N conf's can be summed by simple combinatorics.

Typically $N = O(100) \quad \Rightarrow$ tremendous gain in statistics.

- $\langle \vec{M}^{\,2} \rangle$

We have to keep Q fixed in order to measure $\langle \vec{M}^{\,2} \rangle_Q$, but we can still flip (virtually) all *neutral* clusters.

Almost the same, huge improvement factor



E.g. in $V = 36 \times 12$ we can measure the variation $p(Q)$ over 25 orders of magnitude, hopeless without Improved Estimator.

Interpretation

Cluster formulation: not only super-efficient algorithm, also suggests a top. picture

Clusters as physical objects, crucial degrees of freedom

Clusters with $q = \pm 1/2$: (anti-)merons **Def. beyond semi-classical approx.**

$\theta = 0$: Clusters independent $\rightarrow$ ideal meron gas $\longrightarrow$ mass gap

Include $e^{i\theta Q} \underbrace{\rightarrow}_{\theta=\pi} (-1)^Q$

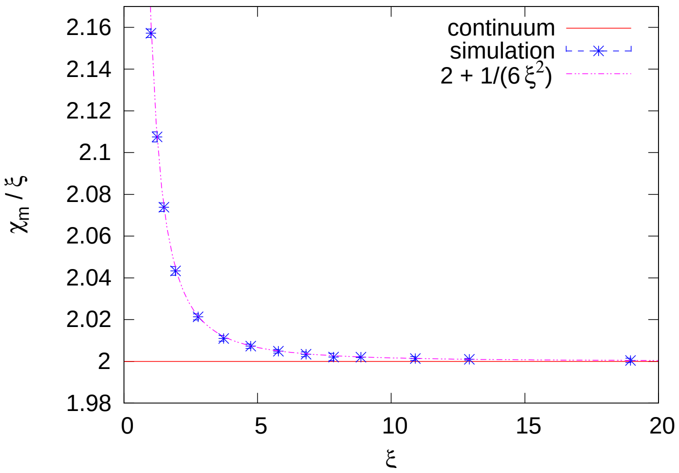
If conf. contains clusters of half-integer charge (must be even number) :
flipping one of these cluster changes Q : even $\leftrightarrow$ odd
$\Rightarrow$ Conf's in this ensemble cancel in $Z(\theta = \pi)$
Ensembles provide only positive contributions, overcomes sign problem

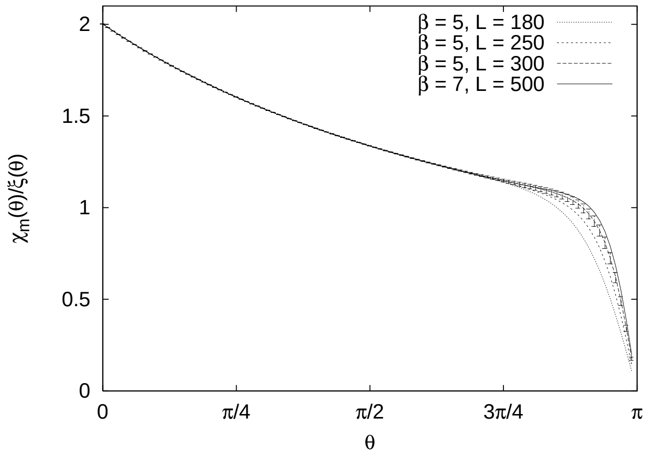
Merons are "bound in pairs", can no longer disorder the system, mass gap $\Rightarrow 0$

Precise formulation of Affleck's non-perturbative picture, no $O(3)$ sym. breaking

Final remarks:

- Result agrees with alternative approach by Alles/Papa '08 with imaginary θ
- Meron cluster algorithm also applied to 1d O(2) model, no angular constraint needed





Left: χ_m at $\theta = 0$. Right: $\chi_m(\theta)/\xi(\theta)$, reliable up to $\theta \lesssim \pi$ (Boyer/W.B. '07)

- 3d $O(4)$ model should be tractable in this way
- Successful application to purely fermionic systems (Chandrasekharan et al. '03)
- Could top. interpretation of the clusters give us a hint for an efficient cluster algorithm in lattice gauge theory ? *Could* be the key to the QCD phase diagram...