# Topological Lattice Actions

## I. Concept and Motivation

**Probing universality in an extreme case**

**Test-bed: non-linear $\sigma$-models**

## II. Quantum Mechanics $(d = 1)$

**Are there still facets of universality ?**

## III. 2d O(3) Model

**Step Scaling Function**

**Topology revisited**

## IV. 2d XY Model

**Is there a Berezinskiĭ-Kosterlitz-Thouless (BKT) phase transition when vortices cost zero energy ?**

**A vortex-free phase transition, to be explored**

*Based on :*

- W.B., U. Gerber, M. Pepe and U.-J. Wiese, JHEP 1012 (2010) 020.
- W.B., M. Bögli, F. Niedermayer, M. Pepe, F.G. Rejón-Barrera and U.-J. Wiese, JHEP 1303 (2013) 141.
- W.B., U. Gerber and F.G. Rejón-Barrera, J. Stat. Mech. 1312 (2013) P12009.

## I. Topological Lattice Actions: Concept and Motivation

Lattice studies usually start by discretising some continuum Lagrangian
$\Rightarrow$ UV regularisation. Prototype:

$$\mathcal{L}(\Phi(x), \partial_\mu \Phi(x)) \ \to \ \mathcal{L}_{\rm lat}(\Phi_x, \frac{1}{a}[\Phi_{x+a\hat{\mu}} - \Phi_x])$$

Standard lattice action, $a$: lattice spacing, $|\hat{\mu}| = 1$

(With gauge fields: link variables for covariant lattice derivatives)

Or: couplings beyond nearest neighbour sites.

Symanzik improvement: tune couplings to eliminate dominant lattice artifacts (analytically on tree level, numerically on non-perturbative level).

**Universality :** Continuum limits of dim'less ratio of observables coincide.

Different lattice formulations of some model belong to the **same universality class,** determined by **space-time dimension** and **symmetries of the order parameter.**

Condition: **locality**, *i.e.* couplings should decay at least exponentially, *e.g.* $c_{xy}\Phi_x\Phi_y$ with $|c_{xy}| \leq c_0 \exp(-c_1|x-y|)$ ... "and of course the classical continuum limit should work," *e.g.* $\frac{1}{a}[\Phi_{x+a\hat{\mu}} - \Phi_x] \overset{a\to 0}{\Longrightarrow} \partial_\mu\Phi(x)$

Often assumed as another condition, "goes without saying", **does it ?**

**Here we discuss counter-examples: lattice actions without any $c_{xy}$, no classical limit. Let's probe how far universality reaches !**

**Surprise: Quantum continuum limit is still correct, and such "weird" lattice actions even provide practical benefits and new insights !**

We consider O($N$) models (non-linear $\sigma$-models). Field (or "classical spin")

$$\vec{e}_x = (e_x^{(1)}, \dots, e_x^{(N)}) \ , \quad |\vec{e}_x| = 1 \quad \forall x = na \ , \quad n \in \mathbb{Z}^d \ .$$

Cubic lattice in $d$-dimensional Euclidean space, with lattice spacing $a$, and periodic boundary conditions (b.c.).

Specifically:

If $N = d + 1$, *i.e.* $\vec{e}_x \in S^d$, the field configurations are divided into **topological sectors**. Each sector has a **top. charge** $Q \in \mathbb{Z}$ (as in 4d Yang-Mills gauge theories and QCD), since $\Pi_d[S^d] = \mathbb{Z}$

We deal with $d = 1, \ 2$,

and $N = 2$ (XY model, relevant for superfluids, superconductors, liquid crystals etc.)

or $N = 3$ (Heisenberg model, describes (anti-)ferromagnets, 2d: toy model for QCD)

Simplest topological lattice action : **Constraint Action**

Angle between any pair of nearest neighbour spins $< \delta$

$$S[\vec{e}] = \sum_{\langle x,y \rangle} s(\vec{e}_x, \vec{e}_y) \quad , \qquad s(\vec{e}_x, \vec{e}_y) = \begin{cases} 0 & \vec{e}_x \cdot \vec{e}_y > \cos\delta \\ +\infty & \text{otherwise} \end{cases}$$

Most small deformations of a configuration (here: within the allowed set) **do not cost any action**

$\Rightarrow$ **"topological lattice action"** (*no* discrete derivatives)

Continuum limit: $\delta \to 0$, such that correlation length $\xi \to \infty$

$\Leftrightarrow$ phase transition of order $\geq 2$

Moreover, for models with top. charges, $Q = \sum_{\langle x,y,\dots\rangle} q_{x,y,\dots}$
($q$: top. charge density), we introduce a "$Q$-suppressing action"

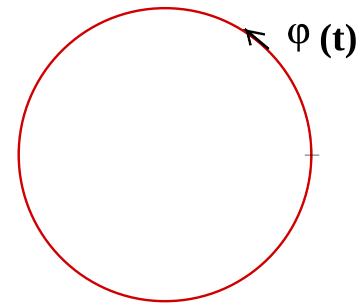
$$S[\vec{e}\,] = \lambda \sum_{\langle x,y,\dots\rangle} |q_{x,y,\dots}| \ , \qquad \lambda > 0 \ .$$

For 2d XY model: no top. sectors, but each plaquette has a vortex number, $v_\square \in \{0, \pm 1\}$, which can be suppressed analogously: $S[\vec{e}\,] = \lambda \sum_\square |v_\square|$ .

We consider constraint actions, topology (or vortex) suppressing actions, and combinations.

All are **topological lattice actions**:
$S[\vec{e}\,]$ is invariant under (most) small deformations of a configuration $[\vec{e}\,]$.

# II. 1d O(2) model : the rotator




Periodic b.c. $\varphi(\beta) = \varphi(0)$

## 1. Continuum:

$$S[\varphi] = \frac{I}{2}\int_0^\beta dt\ \dot{\varphi}(t)^2 \qquad (I\ :\ \text{moment of inertia})$$

energy spectrum $$E_n = \frac{1}{2I}n^2 \quad \Rightarrow \quad \xi \doteq \frac{1}{E_1 - E_0} = 2I\ , \quad \frac{E_2 - E_0}{E_1 - E_0} = 4$$

top. charge $$Q[\varphi] = \frac{1}{2\pi}\int_0^\beta dt\ \dot{\varphi}(t) \in \mathbb{Z} \quad (\text{winding number})$$

top. susceptibility $$\chi_{\mathrm{t}} = \frac{1}{\beta}\langle Q^2\rangle = \cdots = \frac{1}{4\pi^2 I}\ , \quad \chi_{\mathrm{t}}\,\xi = \frac{1}{2\pi^2}$$

## 2. Constraint Lattice Action

$$\varphi_t \ , \quad \Delta\varphi_t := (\varphi_{t+a} - \varphi_t) \bmod 2\pi \in (-\pi, \pi] \ , \quad |\Delta\varphi_t| < \delta \ \ \forall t$$

$$\text{Geometric def. of top. charge :} \quad Q[\varphi] = \frac{1}{2\pi} \sum_t \Delta\varphi_t \in \mathbb{Z}$$

Scaling quantities: (lengthy but straightforward calculation)

$$\frac{E_2 - E_0}{E_1 - E_0} = 4\Big(1 + \frac{3a}{5\xi} + \dots\Big) \ , \quad \chi_{\rm t}\, \xi = \frac{1}{2\pi^2}\Big(1 - \frac{a}{5\xi} + \dots\Big) \ .$$

Correct continuum limit, up to $\mathcal{O}(a)$ artifacts
(for usual lattice actions: $\mathcal{O}(a^2)$ artifacts)

Continuum formulation: $S[\varphi] \geq \frac{2\pi^2 I}{\beta} Q[\varphi]^2$ (minimum at fixed $Q$ for $\varphi(t) = \varphi(0) + \frac{2\pi Q}{\beta}\, t$, "instanton", but no localisation in Euclidean time).
Violated by Constraint Action $\Rightarrow$ not crucial for continuum limit.

## 3. $Q$-Suppressing Action

$$S[\varphi] = \lambda \sum_t |\Delta\varphi_t| = \lambda \sum_t |\text{ top. charge density }| \qquad (\lambda > 0)$$

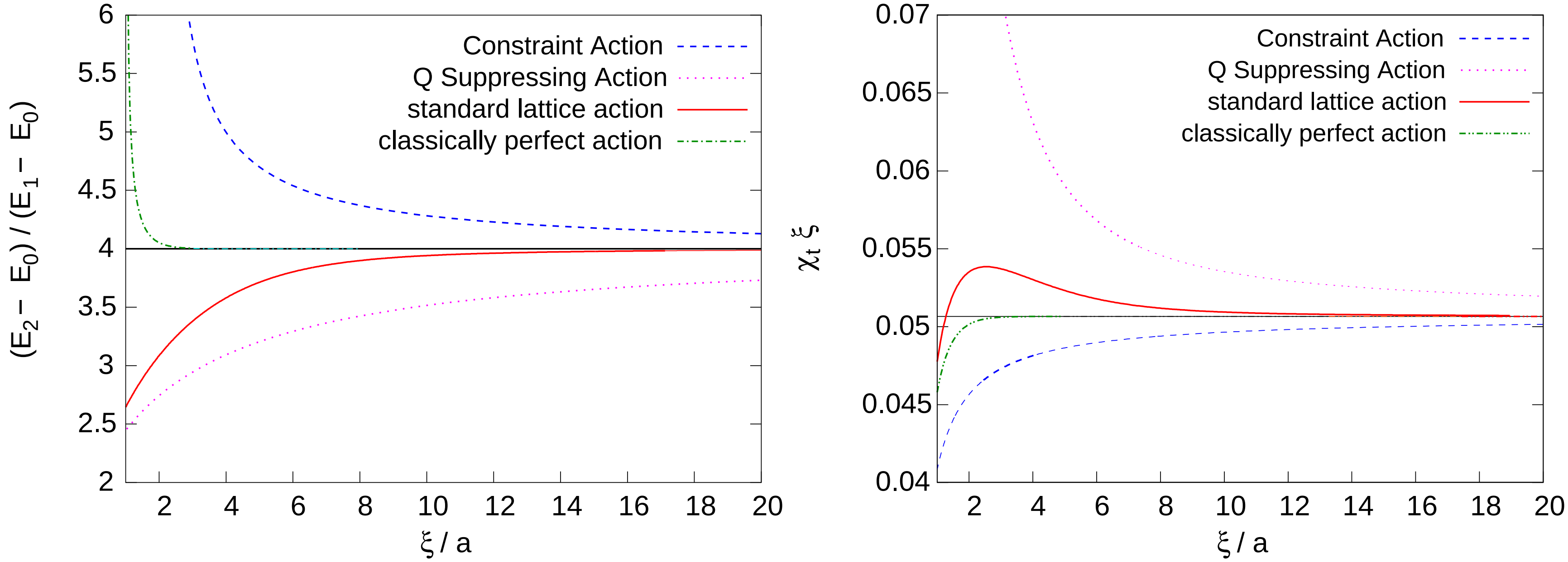
Again correct scaling, up to $\mathcal{O}(a)$ artifacts:

$$\frac{E_2 - E_0}{E_1 - E_0} = 4\Big(1 - \frac{3a}{2\xi} + \dots\Big) \ , \quad \chi_{\rm t}\ \xi = \frac{1}{2\pi^2}\Big(1 + \frac{a}{2\xi} + \dots\Big)$$

4. Same features also for 1d O(3) model :

$$\text{Continuum :} \quad E_n \ = \ \frac{n(n+1)}{2I} \quad \to \quad \frac{E_2 - E_0}{E_1 - E_0} = 3$$

$$\text{Constraint Lattice Action :} \qquad \frac{E_2 - E_0}{E_1 - E_0} = 3\Big(1 + \frac{a}{3\xi} + \dots\Big)$$




Linear lattice artifacts are unusual for these models, but main observation:

**Correct continuum limit !**

Although universality is only assumed in field theory, $i.e.\ d \geq 2$ (?)

["classically perfect action": improved by means of Renormalisation Group techniques, (W.B./Brower/Chandrasekharan/Wiese '97)]

## III. The 2d O(3) Model

$\vec{e}(x) \in S^2$ with periodic b.c., topological sectors
asymptotically free, dyn. generated mass gap $\sim$ QCD

1. Continuum

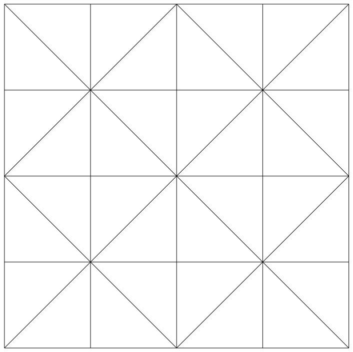
$$S[\vec{e}] = \frac{1}{2g^2} \int d^2x \; \partial_\mu \vec{e} \cdot \partial_\mu \vec{e} \; , \quad Q[\vec{e}] = \frac{1}{8\pi} \int d^2x \; \epsilon_{\mu\nu} \, \vec{e} \cdot (\partial_\mu \vec{e} \times \partial_\nu \vec{e}) \in \mathbb{Z}$$

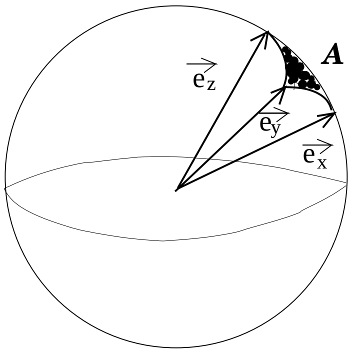
Schwarz inequality: $S[\vec{e}] \geq \frac{4\pi}{g^2} \, |Q[\vec{e}]|$

2. Lattice: Geometric def. of $Q$ (Berg/Lüscher '81)

$$Q[\vec{e}] = \sum_{\langle x,y,z \rangle} A_{x,y,z}$$

$\langle x, y, z \rangle$ triangle decomposition of a plaquette






$A_{x,y,z}$ : (minimal) oriented solid angle spanned by $\vec{e}_x,\ \vec{e}_y,\ \vec{e}_z$

Lattice actions:

$$\text{Standard} \quad S[\vec{e}] \;=\; -\frac{1}{g^2}\sum_{x,\mu}\vec{e}_x\cdot\vec{e}_{x+a\hat{\mu}}$$

$$\text{Constraint} \quad S[\vec{e}] \;=\; \sum_{x,\mu} s(\vec{e}_x,\vec{e}_{x+a\hat{\mu}})\ ,\ s(\vec{e}_x,\vec{e}_{x+a\hat{\mu}}) = \begin{cases} 0 & \vec{e}_x\cdot\vec{e}_{x+a\hat{\mu}} > \cos( \\ +\infty & \text{otherwise}\end{cases}$$

$$Q\text{-Suppressing} \quad S[\vec{e}] \;=\; \lambda\sum_{\langle x,y,z\rangle}|A_{x,y,z}|$$

Consider on an $L \times L$ lattice the ratio $u_0 = L/\xi(L)$ , and
Step-2 **Step Scaling Function (SSF)** $\sigma(2, u_0)$ (Lüscher/Weisz/Wolff '91)

$$\sigma(2, u_0) = 2L/\xi(2L)$$

Continuum values known analytically, $e.g.$ (Balog/Niedermayer/Weisz '09)

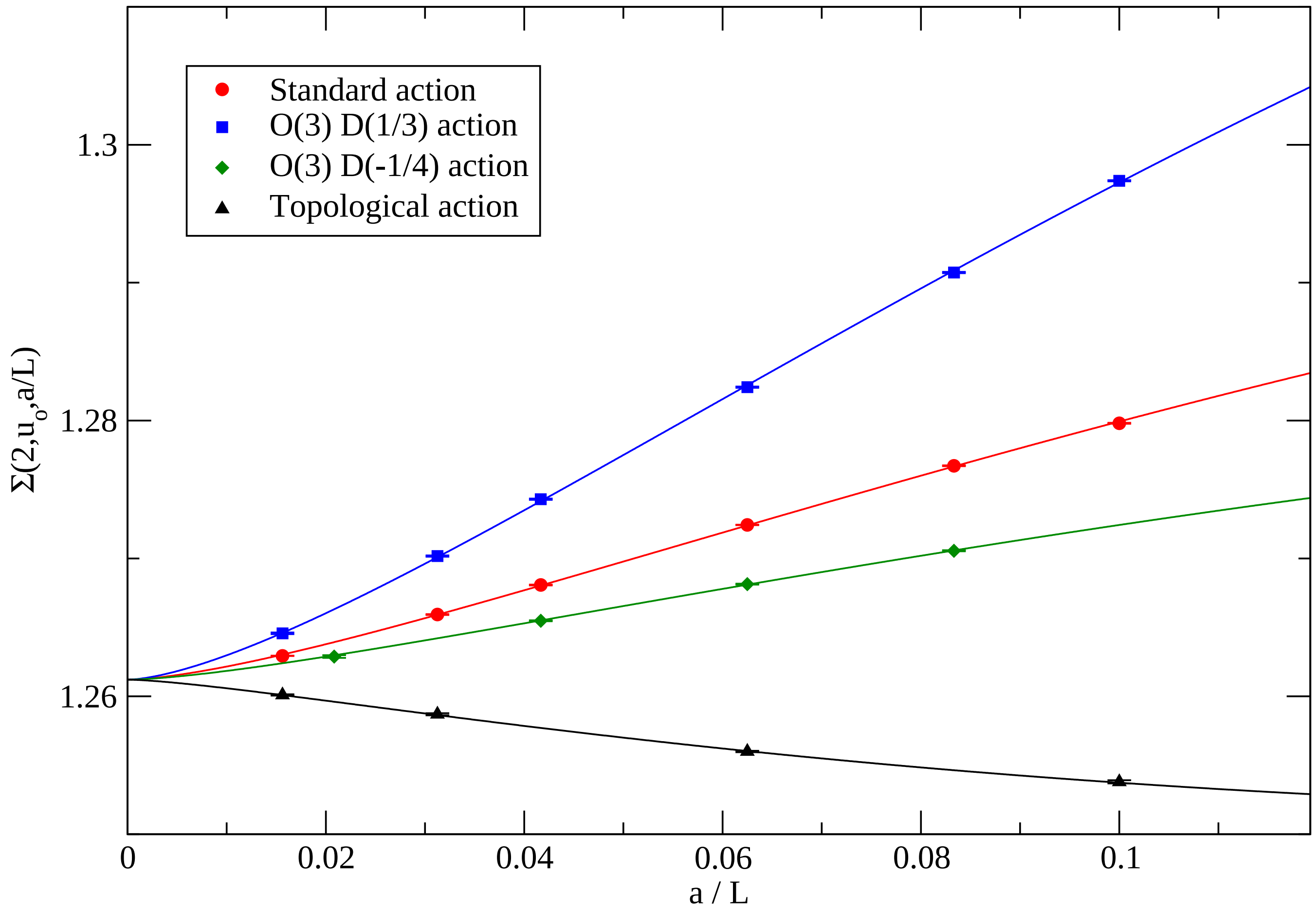
$$\sigma(2, u_0 = 1.0595) = 1.26121$$

Must be reproduced in continuum extrapolation of simulation results with any lattice action in the right universality class.

[ Take some $L$; tune $g$ for desired $u_0$-value. Double $L$ and determine $\xi(2L)$

by measuring $\langle \vec{e}_x \cdot \vec{e}_{x+r} \rangle \propto \exp(-|r|/\xi)$ ]

High precision thanks to **cluster algorithm** !




Extrapolation: $\Sigma(2, u_0, a/L) = \sigma(2, u_0) + \frac{a^2}{L^2}\Big(c_1 \ln^3 \frac{a}{L} + c_2 \ln^2 \frac{a}{L} + \dots\Big)$

Here **Constraint Action** follows **same** form of **artifacts**, in agreement with Symanzik's theory; **scales better** than Standard and "Improved" Actions

(data from Balog/Niedermayer/Weisz '10)

## $Q$ Suppressing Action

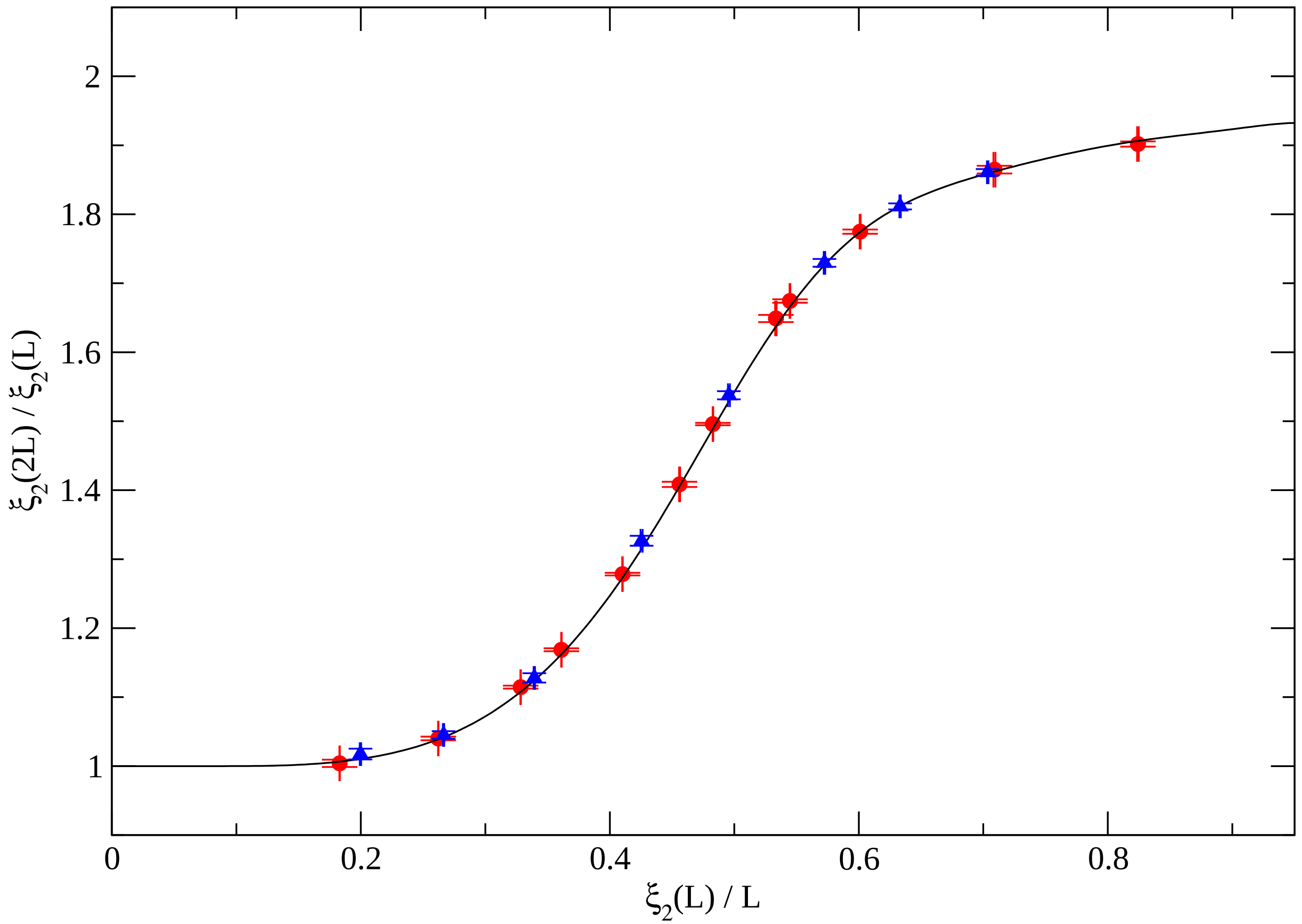
$$S[\vec{e}] = \lambda \sum_{\langle x,y,z \rangle} |A_{x,y,z}| \geq \lambda \left| \sum_{\langle x,y,z \rangle} A_{x,y,z} \right| = 4\pi\lambda \, |Q[\vec{e}]|$$

Metropolis simulation (cluster algorithm does not apply)

$\rightarrow$ use "$2^{\mathrm{nd}}$ moment correlation length" $\xi_2 \cong \xi$ (easier to measure)

$$\lim_{L\to\infty} \xi/\xi_2 = 1.0007(1)$$ (Campostrini/Pelisetto/Rossi/Vicari '97)

"Universal curve" $\xi_2(2L)/\xi_2(L)$ (as a function of $\xi_2(L)/L$ )
was identified for the Standard Action (Caracciolo/Pelissetto/Rossi/Vicari '95)




Both topological actions (Constraint Action, $Q$-suppressing action) follow the *universal curve* $\Rightarrow$ in same universality class as **Standard Action**.

Topological susceptibility : $\chi_{\rm t} = \frac{1}{V}\,\langle Q^2 \rangle$

"Scaling term" $\chi_{\rm t}\ \xi^2$ diverges in cont. limit

(small "dislocations" are not sufficiently suppressed)

Semi-classical consideration: $\chi_{\rm t}\ \xi^2 \propto (\xi/a)^p, \quad p \simeq 0.9$ (Lüscher '82)

Study with "classically perfect action" which eliminates dislocations $\to$ log divergences (Blatter/Burkhalter/Hasenfratz/Niedermayer '96)

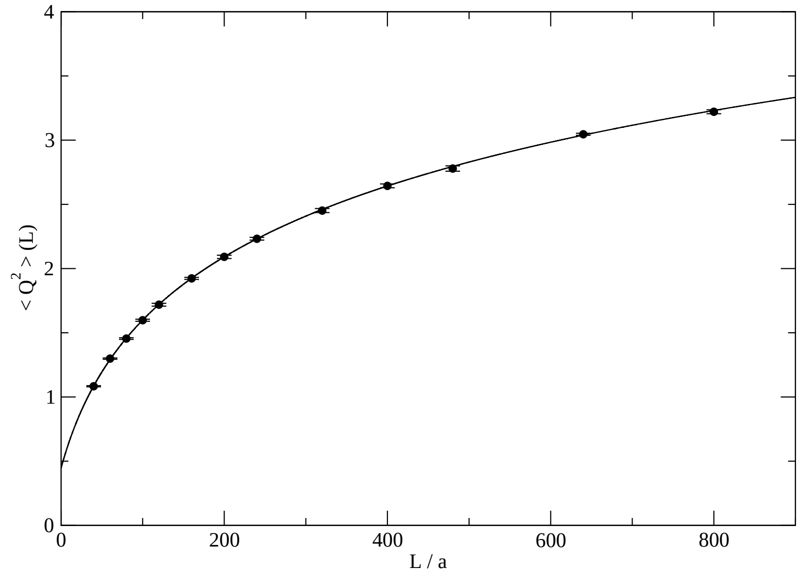
How about top. actions ?

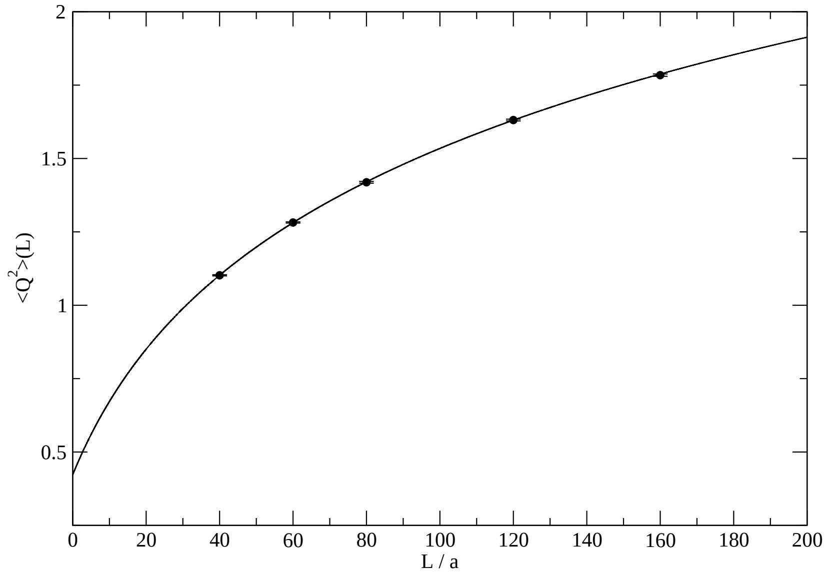
*E.g.* Constraint Action does not suppress dislocations at all . . .

We fix $L/\xi_2 = 4$ and consider

$$16\ \chi_{\rm t}\,\xi_2^2 = 16\ \frac{\langle Q^2 \rangle}{L^2}\ \Big(\frac{L}{4}\Big)^2 = \langle Q^2 \rangle$$

as a function of $L/a = 4\,\xi_2/a$ :






Divergence in the cont. limit is **only logarithmic**, both for Constraint Action (left, dislocations **not** suppressed) and $Q$-Suppressing Action (right).

Therefore the 2d O(3) model is sometimes considered "ill", *but* top. charge density correlation $\langle q(0)q(x)\rangle\,\xi^4$ has finite cont. limit at any $x \neq 0$.

Divergence of $\xi^2\,\chi_{\rm t} = \xi^2\,\sum_x \langle q_0\, q_x\rangle$ *solely* due to $x = 0$.

## Conclusion for the 2d $\mathrm{O}(3)$ model with top. lattice actions

No classical limit, no perturbative expansion,
in part: violation of Schwarz ineq., but correct quantum cont. limit !

Lattice formulations do not need to start from classical cont. theory and discretise, universality includes more on the quantum level.

Symanzik's theory (cont. theory plus all possible lattice terms) captures artifacts in field theory (*not* in $d = 1$).

"Tree level impaired", but excellent scaling at $\lambda = 0$ — can be further improved by combining standard coupling and constraint (Bögli et al. '12)

$\chi_{\mathrm{t}}\, \xi^2$ diverges just logarithmically, even if dislocations cost zero action.

- Analogue in lattice gauge theory: (smooth) constraint on plaquette value

4d U(1): **Akerlund/de Forcrand '15**

4d SU(3): Fukaya et al. '06, W.B. et al. '06, Banerjee et al. '16

## IV. The 2d XY Model

$$\vec{e}_x = (\cos\varphi_x, \sin\varphi_x) \in S^1$$

$$\Delta\varphi_{x,x+a\hat{\mu}} := (\varphi_{x+a\hat{\mu}} - \varphi_x) \bmod 2\pi \; \in (-\pi, \pi]$$

Standard action: (Berezinskii '70, '71, Kosterlitz/Thouless '73, BKT)

$$S[\vec{e}] = \beta \sum_{x,\mu} (1 - \vec{e}_x \cdot \vec{e}_{x+a\hat{\mu}}) = \beta \sum_{x,\mu} (1 - \cos\Delta\varphi_{x,x+a\hat{\mu}})$$

BKT transition : essential phase transition (order $\infty$)

$$\xi(T \gtrsim T_c) \propto \exp\left(\frac{\text{const.}}{\sqrt{T - T_\text{c}}}\right) \;, \quad aT_\text{c} = a/\beta_\text{c} \simeq 1.1199(1)$$

(Hasenbusch '05)

No global top. charge, but each plaquette $\square$ (corners $x_1, \dots, x_4$) has a **vortex number:** (with periodic b.c.: sum $= 0$, Stokes' Theorem)

$$v_\square = \frac{1}{2\pi}(\Delta\varphi_{x_1,x_2} + \Delta\varphi_{x_2,x_3} + \Delta\varphi_{x_3,x_4} + \Delta\varphi_{x_4,x_1}) \in \{0, \pm 1\} \ , \ \sum_\square v_\square = 0$$

**BKT transition:** $(T = 1/\beta$ : temperature)

- $T > T_{\mathrm{c}}$ : isolated vortices condense, disorder the system, massive
- $T < T_{\mathrm{c}}$ : bound vortex–anti-vortex pairs, long-range correlation, massless

KT estimated $T_{\mathrm{c}}$ from energy cost for isolated vortices (see below).

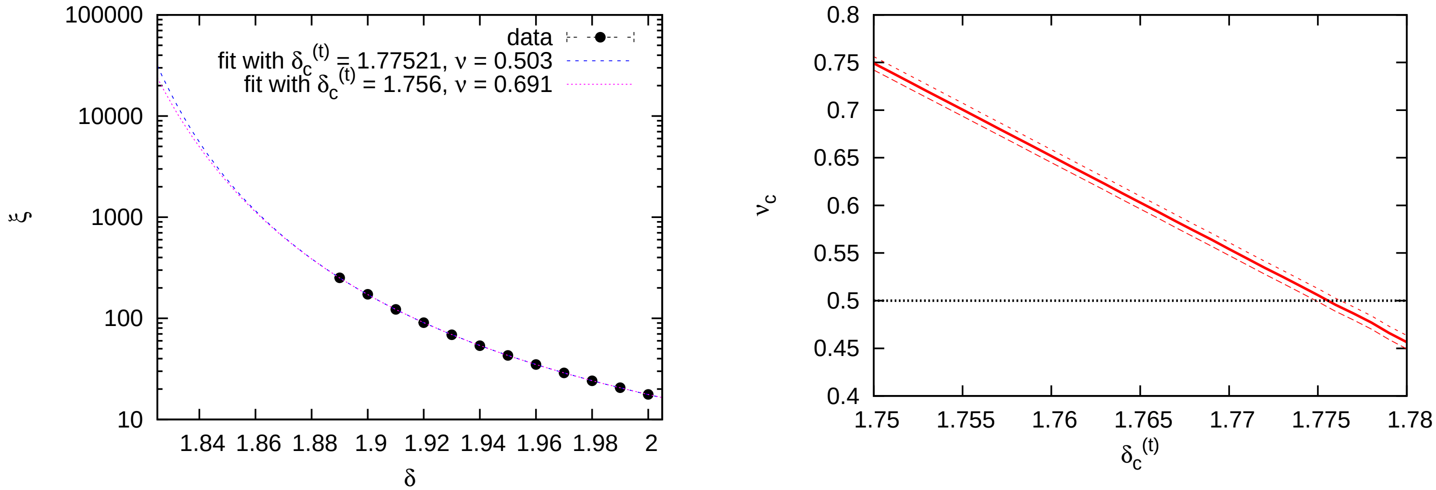
**Topological lattice actions:**

- Constraint Action : $|\Delta\varphi_{x,x+a\hat{\mu}}| < \delta \qquad \forall x, \mu$
- Vortex Suppressing Action : $S[\vec{e}] = \lambda \sum_\square |v_\square|$

$E.g.$ Constraint Action ($\lambda = 0$):

Fit to ansatz $\xi \propto \exp\left(\mathrm{const.}/(\delta - \delta_{\mathrm{c}}^{(\mathrm{t})})^{\nu}\right)$

$\delta_{\mathrm{c}}^{(\mathrm{t})}$: trial value for the critical $\delta$, $\nu$: essential critical exponent



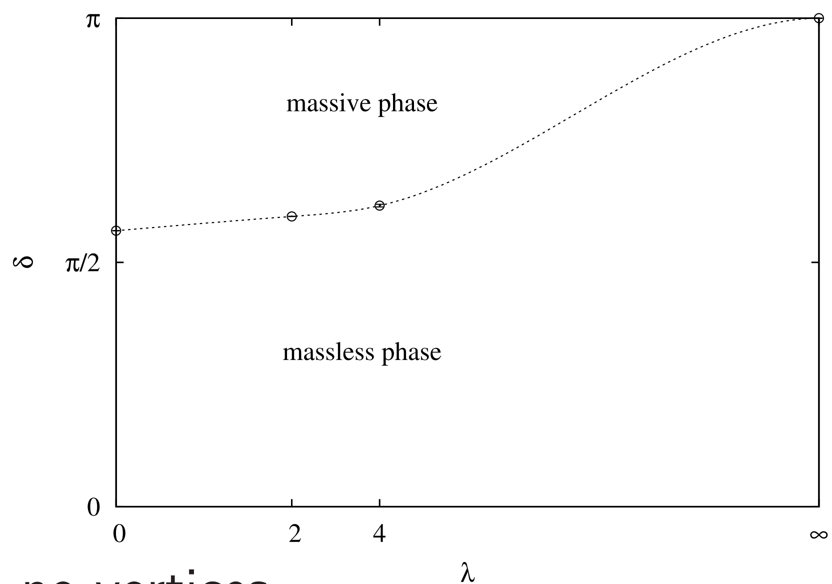

Left: exponential fit works over a range of $\delta_{\mathrm{c}}^{(\mathrm{t})}$, including 1.756
(obtained from spin wave theory applied to $\xi_2$ and Binder cumulant $U_4$).

However, the $\nu = 0.5$ singles out the optimal value $\delta_{\mathrm{c}} = 1.775(1)$

A new type of cluster algorithm still applies at $\lambda > 0$. At fixed $\lambda$ :
$\delta_c(\lambda = 0) = 1.775(1)\,,\ \delta_c(\lambda = 2) = 1.867(1)\,,\ \delta_c(\lambda = 4) = 1.936(1)$

$$\xi(\delta \gtrsim \delta_c) \propto \exp\left(\frac{\text{const.}}{\sqrt{\delta - \delta_c}}\right)$$

Transition of the BKT type, although at $\lambda = 0$ isolated (anti-)vortices cost zero energy !?!?

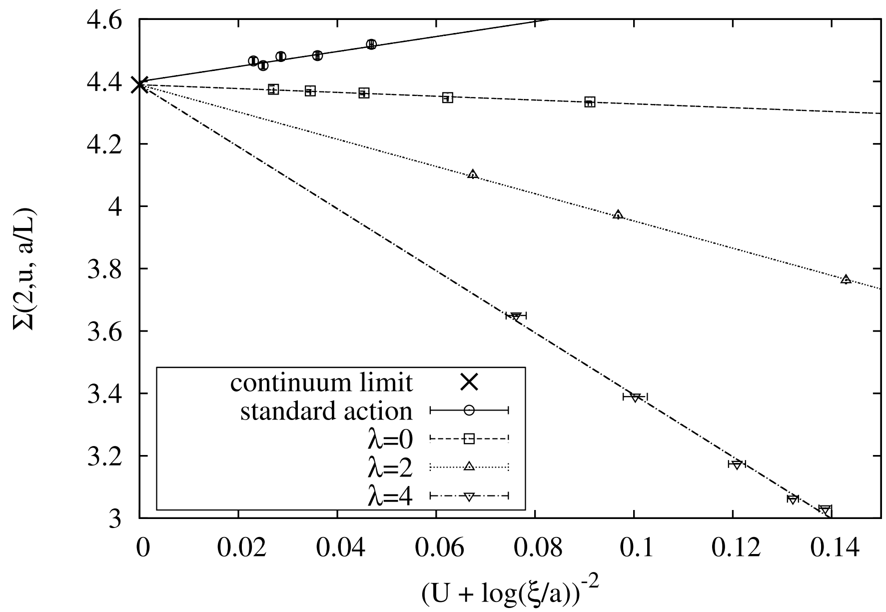



$\delta < \pi/2$ or $\lambda = +\infty$ : no vortices

Tests of BKT universality in 1. massive, 2. massless phase :

1. **Step-2 SSF:** Continuum: $\sigma(2, u := 2L/\xi = 3.0038) = 4.3895$

Standard action, cont. extrapolation: $4.40(2)$ (Balog/Knechtli/Korzec/Wolff '03)




$\Sigma(2, u, a/L) = \sigma(2, u) + \frac{c}{[\ln(\xi/a)+U]^2} + \mathcal{O}(\ln^{-4}(\xi/a))$ following Balog et al.

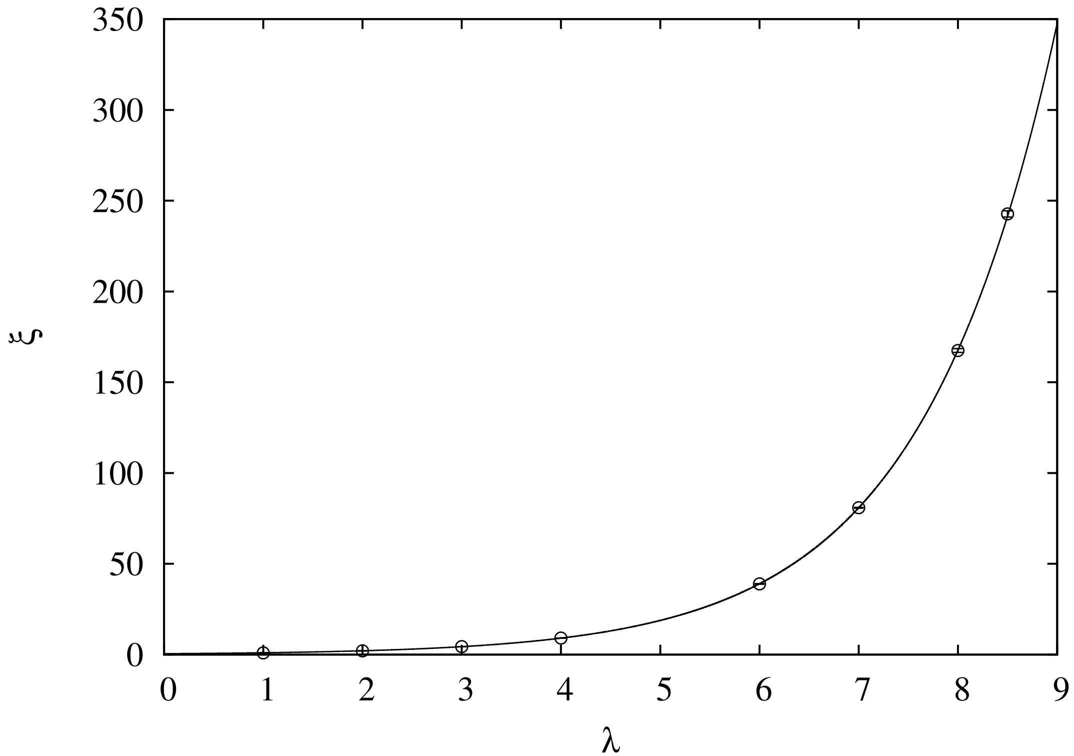
Top. lattice actions are consistent. Excellent scaling for Constraint Action!

$c \simeq 2.6$ was claimed to be universal, but $c < 0$ for top. actions

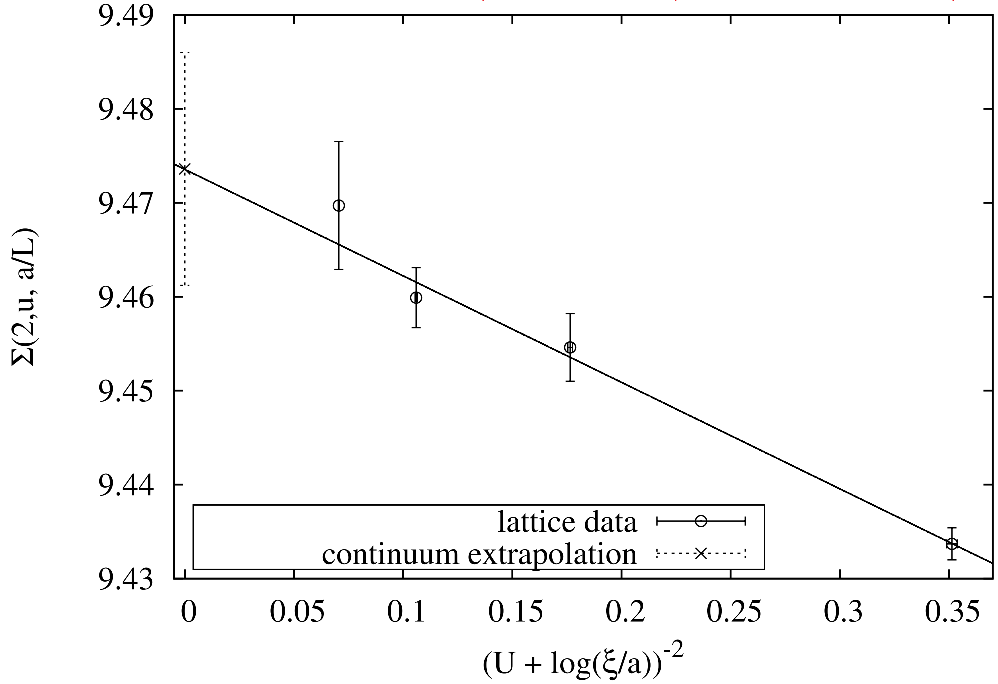
$\delta = \pi$ : Pure Vortex Suppressing Action, upper axis in phase diagram:

good fit with ansatz (originally not expected)

$$\xi(\lambda) = c_0 \exp(c_1 \lambda) \quad \Rightarrow \quad \lambda_c = +\infty$$



Step-2 SSF has extrapolation $\sigma(2, u = 6)_{\mathrm{fit}} = 9.474(12)$




BKT value: $\sigma(2, u = 6)_{\mathrm{BKT}} = 11.53$ (Balog '12)

NO BKT transition, consistent with vortex picture

(vortex–anti-vortex pair formation drives BKT transition, here absent).

**New transition, overlooked in (tremendous) literature on this model.**

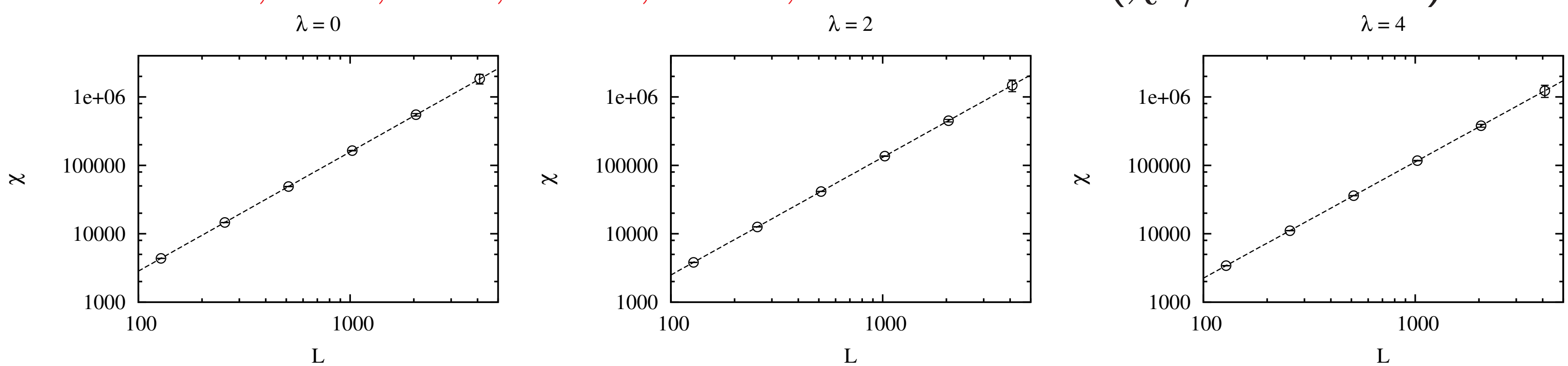
## 2. Magnetic susceptibility in massless phase (near transition)

$$\chi_{\rm m} \quad = \quad \frac{1}{V}\left\langle\left(\sum_x \vec{e}_x\right)^2\right\rangle \propto L^{2-\eta}(\ln L)^{-2r}\left(a_1 + a_2\frac{\ln(\ln L)}{\ln L}\right)$$

$$\eta_{\rm c} = 1/4\ , \quad r_{\rm c} = -1/16 \qquad (\text{Kosterlitz '74})$$

Fits with free parameters $a_1$, $a_2$ work very well, *e.g.* for

$L = 128,\ 256,\ 512,\ 1024,\ 2048,\ 4096$ $\qquad$ ($\chi^2$/d.o.f. $< 1$)




For Standard Action: similar results by Hasenbusch '05 ($L$ up to 2048).

Direct determination of $\eta_{\rm c}$, $r_{\rm c}$ difficult due to $\ln L$ effects.

**Related actions in the 2d XY literature:**

- **Step Action :** $s_{x,x+a\hat{\mu}} = \begin{cases} 0 & \Delta\varphi_{x,\mu} < \pi/2 \\ S_0 & \text{otherwise} \end{cases}$

  BKT transition at critical $S_0$

  (Kenna/Irving '95, Olsson/Holme '01, Minnhagen/Kim '03)

  $S_0 \to \infty$ : Constraint Action at $\delta = \pi/2$, no vortices

- **Extended XY Model** (Domany/Schick/Swendsen '84)

$$S[\varphi] = \beta \sum_{x,\mu} \Big[ 1 - \cos^{2q}(\Delta\varphi_{x,\mu}/2) \Big]$$

$q = 1 \sim$ Standard Action; increasing $q$: stronger vortex suppression.

$q \gtrsim 8$ BKT replaced by $1^{\mathrm{st}}$ order transition, still driven by vortices

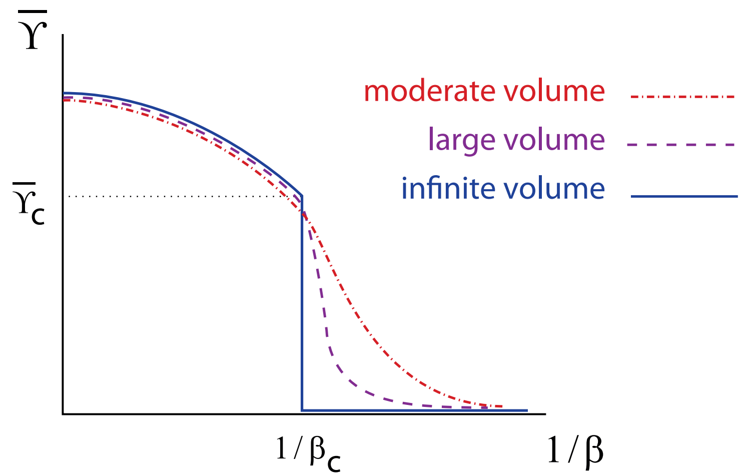
(analytic: van Enter/Shlosman '02; numerical: *e.g.* Ota/Ota '06, Shinha/Roy '10)

**Not observed in our phase diagram, but new transition at $\lambda \to \infty$**

3. Helicity modulus: $\Upsilon := \frac{\partial^2}{\partial\alpha^2} F(\alpha)|_{\alpha=0}$, $F = -\frac{1}{\beta}\ln Z$ (free energy)

$\alpha$: twist angle in boundary conditions (in one direction)

To capture formulations without $\beta$: dim'less helicity modulus $\bar{\Upsilon} := \beta\Upsilon$.



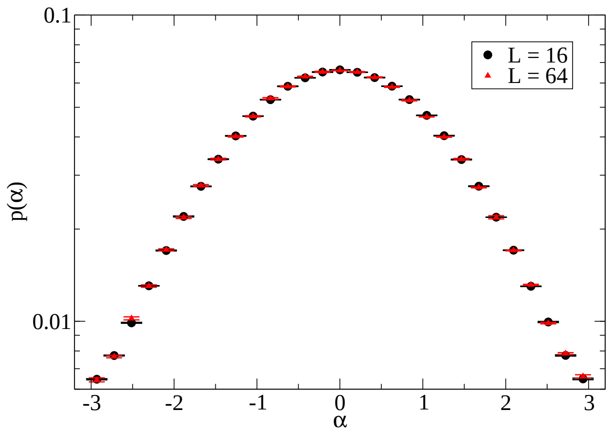

Gap predicted as [Nelson/Kosterlitz '77, Prokof'ev/Svistunov '00]

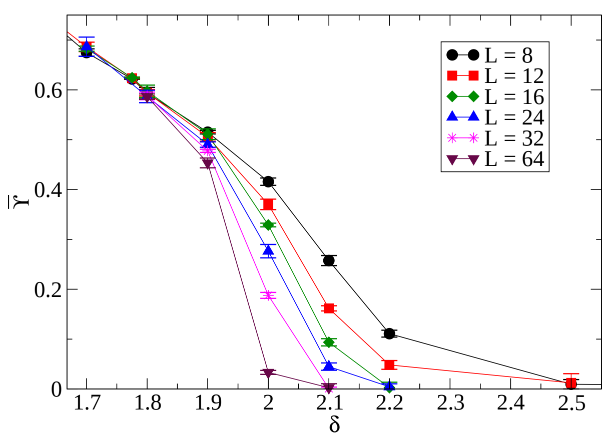
$$\bar{\Upsilon}_{\mathrm{c,theory}} = \frac{2}{\pi}\left(1 - 16e^{-4\pi}\right) \simeq 0.6365$$

Constraint action: actually $F(\alpha \approx 0) \equiv 0$
$\Rightarrow$ simulate with dynamical $\alpha$ and refer to its probability density $p(\alpha)$:

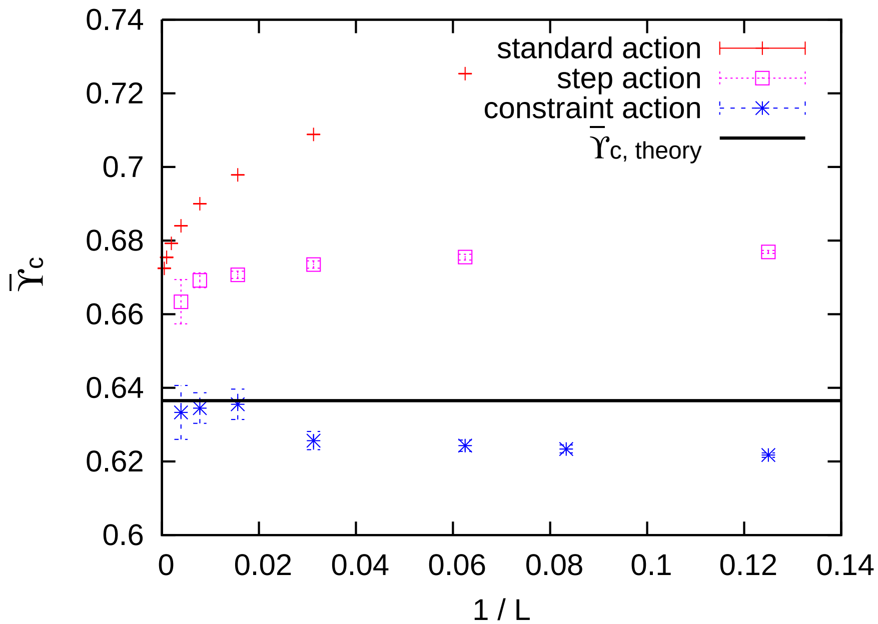
$$\bar{\Upsilon} = -\frac{\partial^2}{\partial \alpha^2} p(\alpha)|_{\alpha=0}$$

Curvature of the histogram in its maximum at $\alpha = 0$ ($e.g.$ at $\delta_c$)




Results compatible with expected behaviour
at $L = \infty$: sudden drop of $\bar{\Upsilon}$ as $\delta$ exceeds $\delta_c$.




- standard action $\bar{\Upsilon}(L = 2048) = 0.67826(7)$ (Hasenbusch '05)
- step action: $\bar{\Upsilon}(L = 256) = 0.663(6)$ (Olsson/Holme '01)

- constraint action at $\delta_{\rm c}$: $\bar{\Upsilon}(L = 8) = 0.622(1)$ , $\bar{\Upsilon}(L = 64) = 0.636(4)$

**Incredibly small finite size effects!** $(\bar{\Upsilon}_{\rm c,theory} \simeq 0.6365)$

**Compelling numerical evidence for a BKT transition**

# Driving force of the BKT transition: Vortex (un-)binding mechanism

## Nobel Prize Committee (2016):

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4 OCTOBER 2016

Scientific Background on the Nobel Prize in Physics 2016

TOPOLOGICAL PHASE TRANSITIONS AND
TOPOLOGICAL PHASES OF MATTER

compiled by the Class for Physics of the Royal Swedish Academy of Sciences



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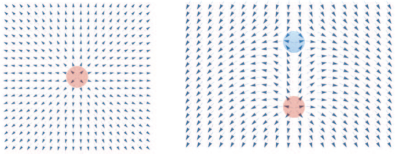


Figure 3: *To the left a single vortex configuration, and to the right a vortex-antivortex pair. The angle $\theta$ is shown as the direction of the arrows, and the cores of the vortex and antivortex are shaded in red and blue respectively. Note how the arrows rotate as you follow a contour around a vortex.*

by the Hamiltonian,

$$H_{XY} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \qquad (3)$$

where $\langle ij \rangle$ again denotes nearest neighbours and the angular variables, $0 \leq \theta_i < 2\pi$ can denote either the direction of an XY-spin or the phase of a superfluid. We shall discuss this model in some detail below.

Although the GL and BCS theories were very successful in describing many aspects of superconductors, as were the theories developed by Lev Landau (Nobel Prize 1962), Nikolay Bogoliubov, Richard Feynman and others for the Bose superfluids, not everything fit neatly into the Landau paradigm of order parameters and spontaneous symmetry breaking. Problems occur in low-dimensional systems, such as thin films or thin wires. Here, the thermal fluctuations become much more important and often prevent ordering even at zero temperature [39]. The exact result of interest here is due to Wegner, who showed that there cannot be any spontaneous symmetry breaking in the XY-model at finite temperature [53].

So far we have discussed phenomena that can be understood using classical concepts, at least as long as one accepts that superfluids are characterised by a complex phase. There are however important macroscopic phenomena that cannot be explained without using quantum mechanics. To find the ground state of a quantum many-body problem is usually very difficult, but there are some important examples where solutions to simplified problems give deep physical insights. Electromagnetic response in crystalline materials is an



a critical exponent which is characteristic of a *universality class*, which can encompass many different systems that all behave in a similar way close to the phase transition.

To see what happens in two dimensions, we take the continuum limit of the Hamiltonian Eq. (3), to get

$$H_{XY} = \frac{J}{2} \int d^2r \, (\vec{\nabla}\theta(\vec{r}))^2 \,. \qquad (4)$$

A simplification is to extend the range of the angular variable to $-\infty < \theta < \infty$ to get a free field Hamiltonian and thus Gaussian fluctuations, and a direct calculation using a short distance cutoff $a$ gives

$$\langle e^{i(\theta(\vec{r})-\theta(\vec{0}))} \rangle \sim \left(\frac{a}{r}\right)^{\frac{k_B T}{2\pi J}} \,. \qquad (5)$$

This is a power law even at high temperatures, where an exponential fall-off would be expected. Kosterlitz and Thouless [35, 36] resolved the apparent paradox by showing that there is indeed a finite temperature phase transition, but of a new and unexpected nature where the vortex configurations play an essential role.

The glitch in the argument leading to Eq. (5) is that the periodic, or U(1), nature of $\theta$ cannot be ignored, since that amounts to neglecting vortex configurations. A vortex like the one in Fig. 3 is characterised by a non zero value of the vorticity,

$$v = \frac{1}{2\pi} \oint_C d\vec{r} \cdot \vec{\nabla}\theta(\vec{r}) \qquad (6)$$

where $C$ is any curve enclosing the centre position of the vortex. The integral measures the total rotation of the spin vector along the curve, so after dividing with $2\pi$, $v$ is simply the number of full turns it makes when circling the vortex. From this, we also understand that there can also be antivortices, where the spin rotates in the opposite direction as seen in the right panel in Fig.3. For a rotationally symmetrical vortex with $v = \pm 1$ it follows from Eq. (6) that $|\vec{\nabla}\theta(\vec{r})| = 1/r$, so the energy cost for a single vortex becomes,

$$E_v = \frac{J}{2} \int d^2r \left(\frac{1}{r}\right)^2 = J\pi \ln \frac{L}{a} \qquad (7)$$

where $L$ is the size of the system, and $a$ a short distance cutoff that can be thought of as the size of the vortex core. So for a large system, the energy cost

Continuum: vorticity $v = \frac{1}{2\pi} \oint d\vec{x} \cdot \vec{\nabla}\theta(\vec{x})$

For $|\vec{\nabla}\theta(\vec{x})| = 1/|\vec{x}| \equiv 1/r$, energy cost of one vortex V (or anti-vortex A)

$$E_v = \text{const.} \int d^2x\, r^{-2} \propto \ln L/a$$

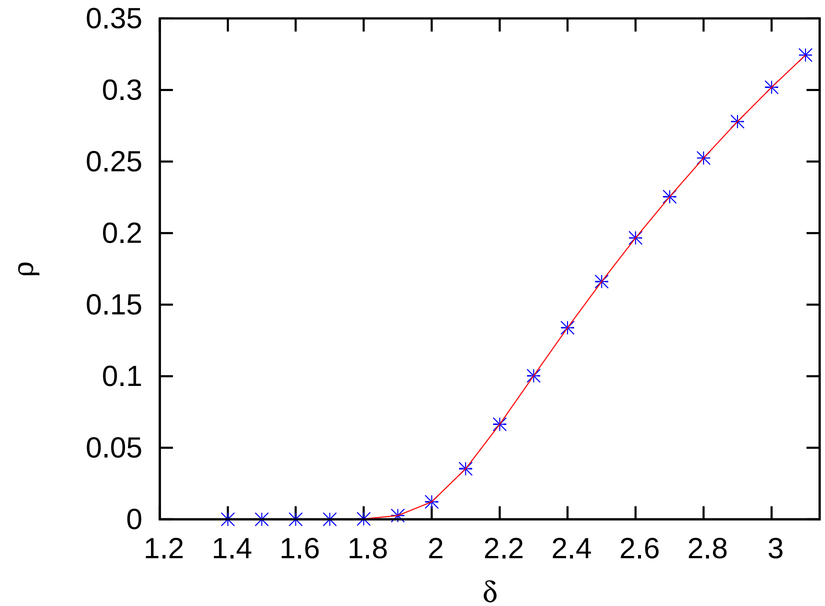
$L$ size (physical units), $a$: short distance cutoff

But: energy required for **V-A pair** only $\propto \ln r/a$ ($r$: separating distance)
$\Rightarrow$ V-A attracting force $\propto 1/r$

Free energy of single vortex composed of potential energy and entropy term

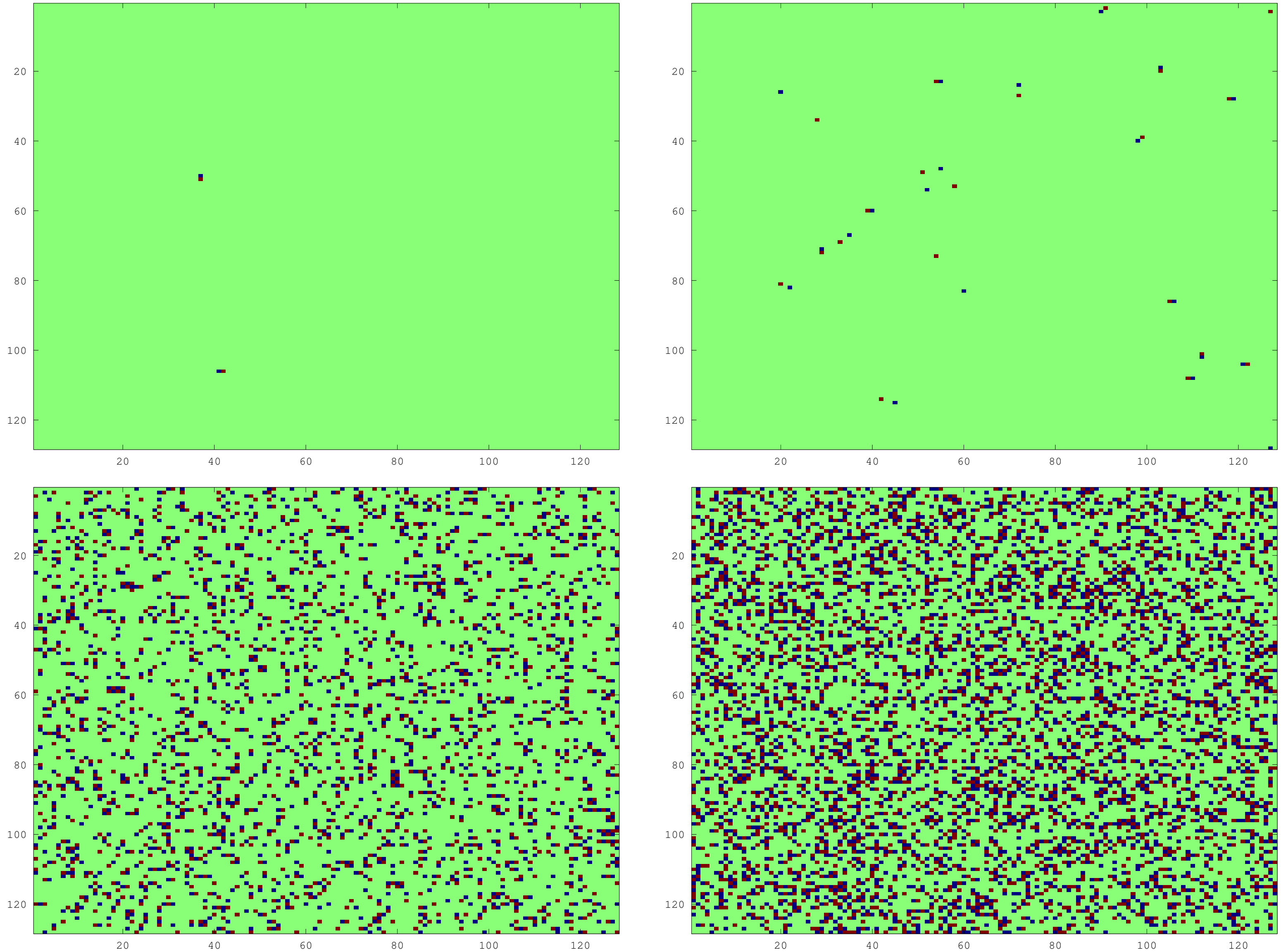
$$F = E - TS = \pi \ln(L/a) - T \ln(L^2/a^2) \quad \longrightarrow \quad T_{\rm c} = \pi/2$$

V-A (un-)binding also for BKT transition with constraint action ???
Supposed to be general mechanism, but $E \equiv 0 \Rightarrow$ above explanation fails.



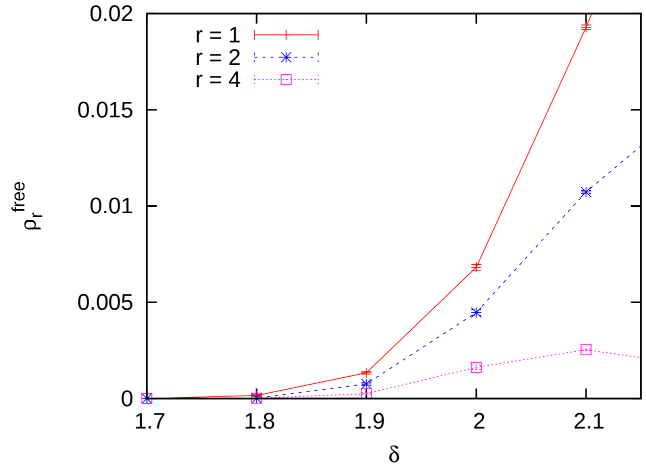

First observation: the **density** $\rho$ **of vortices plus anti-vortices** (V plus A) takes off around $\delta_c \simeq 1.775$ (the pseudo-critical value at finite $L$ is somewhat larger; data here and below at $L = 128$).

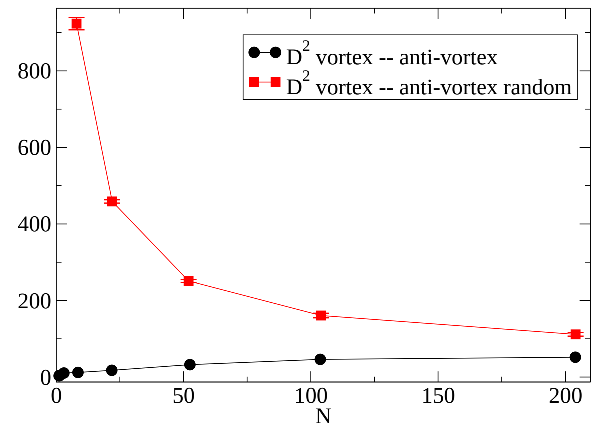
Question: is there any trend for a V-A pair formation at low $\delta$ ?




Vortex and Anti-Vortex distributions for typical configurations on a $128 \times 128$ lattice, at $\delta = 1.8,\ 1.9,\ 2.5$ and $3.1$.

Left: the **density of "free vortices"**, *i.e.* vortices without any anti-vortex (or vice versa) within distance $r$

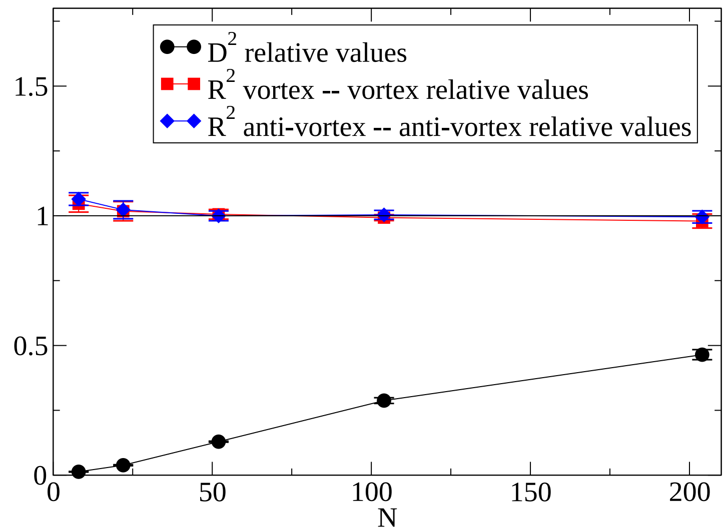



Right: for a conf. with $N$ vortices (and $N$ anti-vortices), we define $D^2 = \frac{1}{N}\sum_{i=1}^{N} d^2_{\mathrm{VA},i}$, with $d_{\mathrm{VA},i}$ = distance V-A, for pairing with minimal $D^2$ (identified by simulated annealing). $\delta = 1.9$ leads to $N \approx 50$.

Comparison to $D^2$ for random distributed V, A

Pair formation extreme at small $N \Leftrightarrow$ small $\delta$; fades away for increasing $\delta$.




Define analogously $R^2_{\rm VV} = \frac{2}{N} \sum_{i=1}^{N/2} d^2_{{\rm VV},i}$ , $\quad R^2_{\rm AA} = \frac{2}{N} \sum_{i=1}^{N/2} d^2_{{\rm AA},i}$

Normalise $D^2$, $R^2$ by dividing by value for random distributed V and A.

**(Un-)binding of V-A pairs is still observed at BKT transition !**
**Picture is correct, and reaches beyond standard argument with energy cost $\Rightarrow$ That argument is incomplete**

## Conclusion about the 2d XY Model

$\delta$-constraint and $0 \le \lambda < \infty$ :

Phase transition at $\delta_c(\lambda)$ with BKT behaviour

SSF: correct value in continuum extrapolation, at $\lambda = 0$: excellent scaling.

$\chi_m \to \eta_c,\ r_c$ : large $L$ extrapolation *compatible* with BKT prediction.

$\underline{\lambda = 0:}$ First clear confirmation of $\bar{\Upsilon}_c$ predicted at a BKT transition.

Vortex–Anti-Vortex (V-A) pair (un-)binding mechanism applies, even without any energy requirement for "free vortices".

Famous Kosterlitz-Thouless mechanism is valid, predictions correct, but standard argument to be reconsidered.

$\underline{\lambda \to \infty}$ (without $\delta$-constraint):
no vortices; new phase transition and universality class, not of BKT type.

Appendix A: **Predictions by Spin Wave Theory (SWT)**

(Connected) correlation function: (lattice units)

$$G(x-y) \doteq \langle \vec{e}_x \cdot \vec{e}_y \rangle \quad , \qquad \tilde{G}(p) = \frac{1}{V} \sum_x G(x) \exp(ipx)$$

2nd moment correlation length $\xi_2$ ($\simeq \xi$, but easier to measure) is obtained from magnetic susceptibility $\chi_{\rm m} = \tilde{G}(0) = \frac{1}{V}\langle \vec{M}^2 \rangle$ ($\vec{M} = \sum_x \vec{e}_x$) and $\phi \doteq \tilde{G}(2\pi/L, 0)$. Related: Binder cumulant $U_4$

$$\xi_2 \doteq \left( \frac{\chi_{\rm m} - \phi}{4\phi \sin^2(\pi/L)} \right)^{1/2} \quad , \quad U_4 = \frac{\langle (\vec{M}^2)^2 \rangle}{(V\chi_{\rm m})^2}$$

SWT predicts at large $L$: $\xi_2/L = 1.018\ldots$, $U_4 = 0.751\ldots$ plus log corrections (universality predictions for them fail again).

Fit : $\delta_{\rm c,sw} = 1.756(2) < \delta_{\rm c} = 1.775(1) \;\Rightarrow$ SWT prediction not accurate

## Appendix B: **Topological charge density correlation**

The 2d O(3) model is sometimes considered “ill”, at least regarding top. aspects, since $\chi_\mathrm{t}\,\xi^2$ diverges in the continuum limit.

However, the **correlation of top. charge density,** $\langle q(0)q(x)\rangle\,\xi^4$, with

$$q(x) = \frac{1}{8\pi}\,\epsilon_{\mu\nu}\,\vec{e}\cdot(\partial_\mu\vec{e}\times\partial_\nu\vec{e})$$

*does* have a finite cont. limit, at any $x \neq 0$.

Divergence with $\chi_\mathrm{t} = \sum_x \langle q_0\, q_x\rangle$ solely due to $x = 0$.

At $x = 0$: cancellation of power divergences, log. divergence persists.

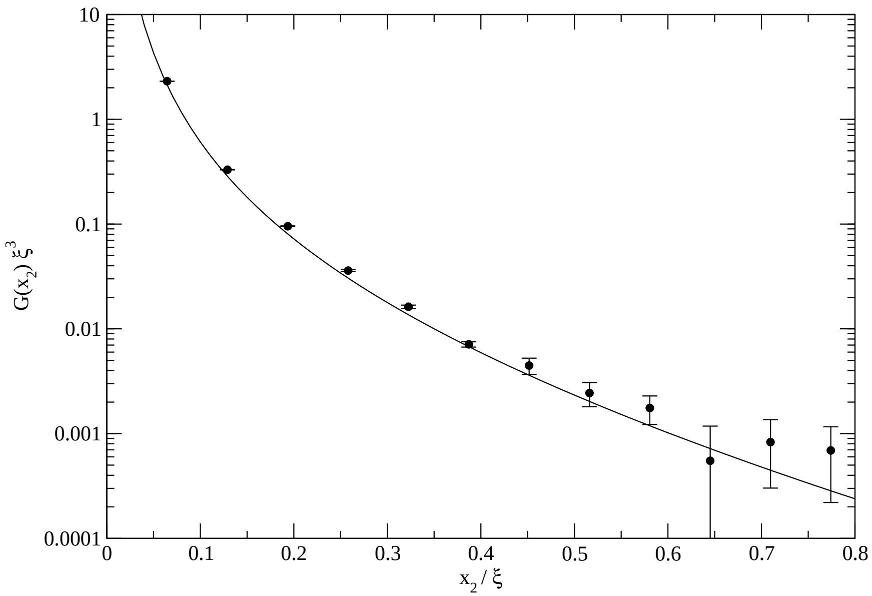
Cancellation of $|x|^{-d}$ divergences also in QCD with chiral quarks, $q$ defined with Ginsparg-Wilson Dirac operator (Giusti/Rossi/Testa '04, Lüscher '04)

Point-to-time-slice correlator: $(x = (x_1, x_2))$

$$G(x_2) = \int_0^L dx_1 \; \langle q(0) q(x) \rangle$$

**Constraint Action**

$G(x_2)\,\xi^3$ vs. $x_2/\xi$




Data are continuum extrapolated. Curve predicted by Balog/Niedermaier '97