Topological Lattice Actions

I. Motivation

Probing universality in an extreme case

Testbed: non-linear σ-models

II. Quantum Mechanical Models $(d = 1)$

Are there still facets of universality ?

III. 2d O(3) Model

Step Scaling Function

Topological susceptibility

IV. 2d XY Model (or O(2) Model)

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

A vortex-free phase transition, to be explored

Based on :

[1] W.B., U. Gerber, M. Pepe and U.-J. Wiese, JHEP 1012 (2010) 020.

[2] W.B., M. Bögli, F. Niedermayer, M. Pepe, F.G. Rejón-Barrera and U.-J. Wiese, JHEP 1303 (2013) 141.

[3] W.B., U. Gerber and F.G. Rejón-Barrera, arXiv:1307.0485 [hep-lat].

I. Topological Lattice Actions

Usually we discretize some continuum Lagrangian, $e.g.$

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

Universality : Different lattice formulations: **same universality class,** determined by *space-time dimension* and *symmetries of the order parameter.*

Conditions : locality, and of course correct classical continuum limit, $e.g.$ $\frac{1}{a}[\Phi_{x+a\hat{\mu}} - \Phi_x] \xrightarrow{a \to 0} \partial_\mu \Phi(x)$. "Goes without saying", *does it ?*

Counter-examples: lattice actions without any classical limit. Let's probe how far universality really reaches !

Surprise: Quantum continuum limit may still be correct, and such "absurd" lattice actions even provide practical benefits !

$O(N)$ lattice models:

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

We consider $d = 1, \ 2$,

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

or $N = 3$ (Heisenberg model, describes ferromagnets, 2d: asympt. freedom $\sim$ QCD).

For $N = d + 1$: *topological sectors.*

Simplest topological lattice action :

Constraint Action

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

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

Deformations of a configuration (within allowed set) do not cost any action
$\Rightarrow$ "topological lattice action" ($\neq$ lattice actions with discrete derivatives)

No classical limit, no perturbative expansion

Continuum limit: $\delta \to 0$

For models with top. charges, $Q = \sum_{\langle x,y,\dots \rangle} q_{x,y,\dots}$ (q: top. charge density)

Q Suppressing Action

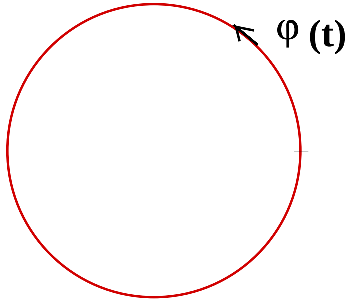
$$S[\vec{e}] = \lambda \sum_{\langle x,y,\dots \rangle} |q_{x,y,\dots}| \ , \qquad \lambda > 0 \ .$$

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

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

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

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



$$S[\phi] = \frac{I}{2}\int_0^\beta dt\ \dot{\varphi}(t)^2 \quad , \quad \text{periodic b.c.} \quad \varphi(\beta) = \varphi(0)$$

Scaling term	continuum	constraint action	Q suppressing action
$\frac{E_2-E_0}{E_1-E_0}$	4	$4\left(1+\frac{3}{5}\frac{a}{\xi}+\dots\right)$	$4\left(1-\frac{3}{2}\frac{a}{\xi}+\dots\right)$
$\chi_t\,\xi = \frac{\langle Q^2\rangle}{L(E_1-E_0)}$	$\frac{1}{2\pi^2}$	$\frac{1}{2\pi^2}\left(1-\frac{1}{5}\frac{a}{\xi}+\dots\right)$	$\frac{1}{2\pi^2}\left(1+\frac{1}{2}\frac{a}{\xi}+\dots\right)$

Linear lattice artifacts are unusual for scalar models, but:

Correct continuum limit !

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

III. The 2d O(3) Model

1. Continuum

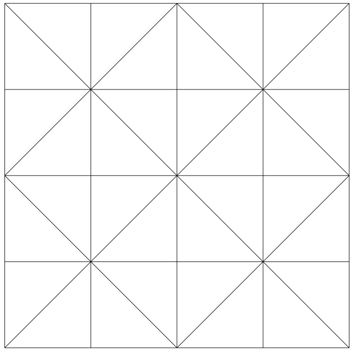
$$S[\vec{e}] = \frac{1}{2g^2} \int d^2x \; \partial_\mu \vec{e} \, \partial_\mu \vec{e} \,, \quad Q[\vec{e}] = \frac{1}{8\pi} \int d^2x \; \epsilon_{\mu\nu} \, \vec{e} \, (\partial_\mu \vec{e} \, \partial_\nu \vec{e}) \in \mathbb{Z}$$

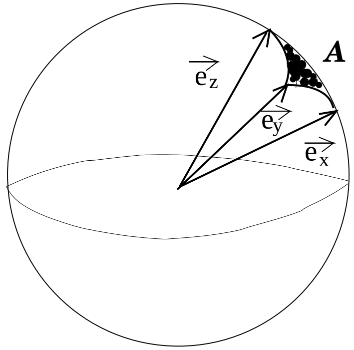
Schwarz inequality: $S[\vec{e}] \geq \frac{4\pi}{g^2} \, |Q[\vec{e}]|$

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

$$Q[\vec{e}] = \frac{1}{4\pi} \sum_{\langle x,y,z \rangle} A_{x,y,z}$$

$\langle x, y, z \rangle$ triangles, decomposition of square lattice





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

Lattice actions:

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

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

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

Consider $L \times L$ lattices, ratio $u = L/\xi(L)$, and
Step-2 **Step Scaling Function (SSF)** (Lüscher/Weisz/Wolff '91)

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

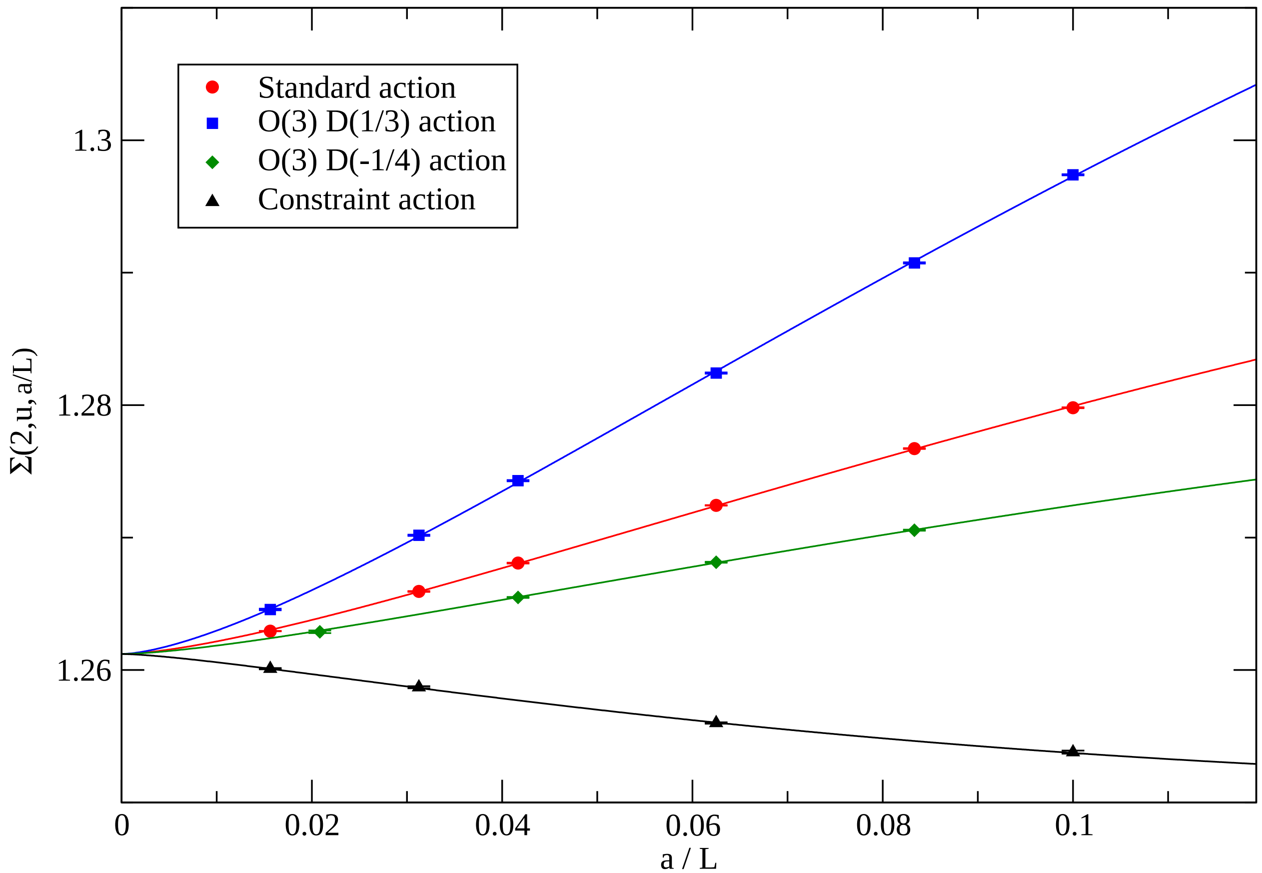
Continuum values are known,

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

(Balog/Niedermayer/Weisz '09)

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

High precision thanks to **cluster algorithm** !



Extrapolation: $\Sigma(2,u,a/L) = \sigma(2,u) + \frac{a^2}{L^2}\left(c_1 \ln^3 \frac{a}{L} + c_2 \ln^2 \frac{a}{L} + \ldots\right)$

Constraint Action: now **same** form of **artifacts**, following Symanzik's theory, and **scales better** than Standard and Improved Actions

(data from Balog/Niedermayer/Weisz '10)

Top. actions (constraint and Q suppressing [1]) : **correct cont. limit!**

Topological susceptibility : $\chi_t \doteq \frac{1}{V}\langle Q^2\rangle$

"Scaling term" $\chi_t\,\xi^2$ diverges in cont. limit

(small "dislocations" not sufficiently suppressed)

Semi-classical: $\chi_t\,\xi^2 \propto (\xi/a)^p, \quad p \simeq 0.9$ (Lüscher '82)

"Classically perfect action" eliminates dislocations $\rightarrow$ log divergences

(Blatter/Burkhalter/Hasenfratz/Niedermayer '96)

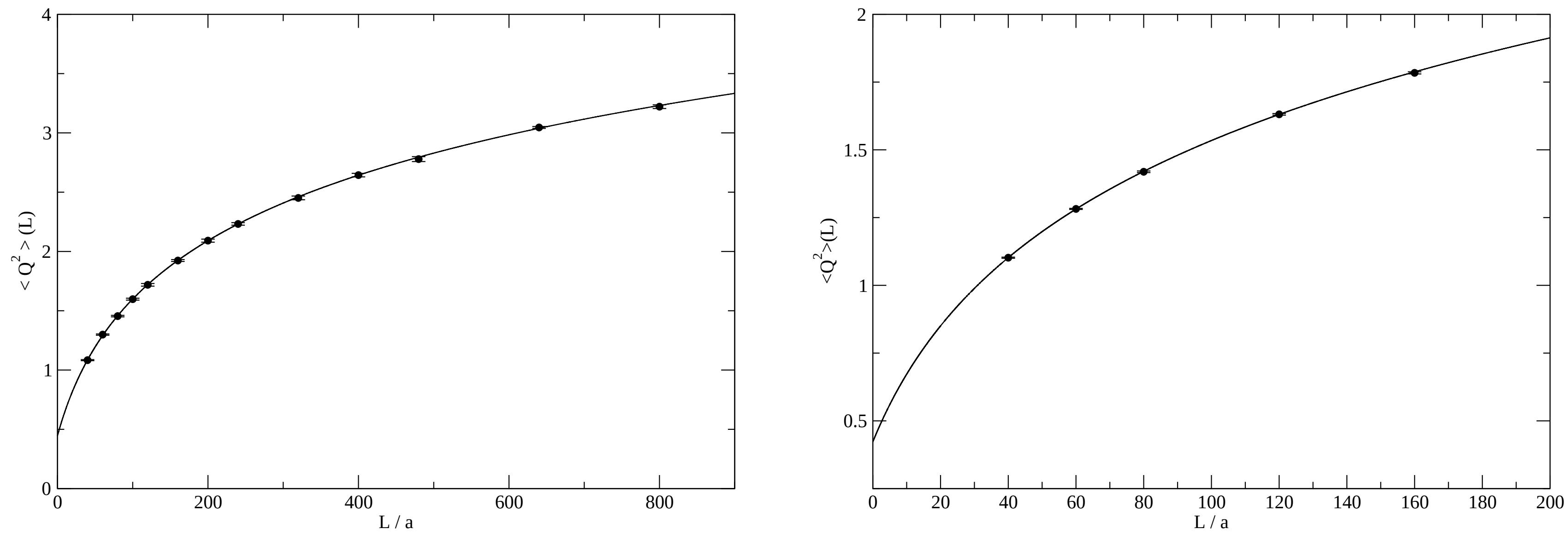
How about top. actions ?

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

We fix $L/\xi_2 = 4$ and consider (ξ_2 : 2^{nd} moment correlation length)

$$16\;\chi_t\,\xi_2^2 = 16\,\frac{\langle Q^2\rangle}{L^2}\left(\frac{L}{4}\right)^2 = \langle Q^2\rangle$$

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 correlation $\langle q(x) q(y) \rangle$ at $x \neq y$ is finite [1].

Conclusion for the 2d $O(3)$ model

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

On quantum level, universality is powerful!

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

"Tree level impaired", but very good scaling behavior — can be further improved by combining standard coupling and constraint (Bögli et al. '12)

$\chi_t \, \xi^2$ diverges just logarithmically, even if dislocations cost zero action. Still, $\langle q(x)q(y)\rangle|_{x \neq y}$ is a sensible top. quantity.
($\rightarrow$ study of θ-vacua, de Forcrand/Pepe/Wiese '12)

IV. The 2d XY Model (or O(2) Model)

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

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

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

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

BKT transition : essential phase transition (order ∞)

$$\xi(T \gtrsim T_{\rm c}) \propto \exp\left(\frac{\text{const.}}{(T - T_{\rm c})^{1/2}}\right) \ , \quad aT_{\rm c} = a/\beta_{\rm c} \simeq 1.1199(1)$$

(Hasenbusch '05)

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

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

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

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

$T_{\rm c}$ was estimated from energy cost for isolated vortices (or anti-vortices).

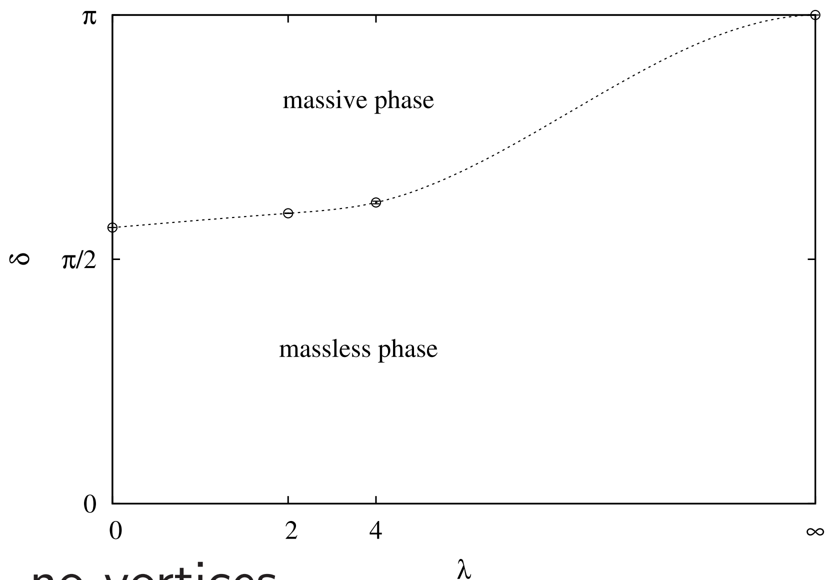
Topological lattice actions:

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

New type of *cluster algorithm* still applies at $\lambda > 0$. At fixed λ :
$\delta_c(\lambda = 0) = 1.7752(6)\,,\ \delta_c(\lambda = 2) = 1.8665(8)\,,\ \delta_c(\lambda = 4) = 1.9361(8)$

$$\xi(\delta \gtrsim \delta_c) \propto \exp\left(\frac{\text{const.}}{(\delta - \delta_c)^{1/2}}\right)$$

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

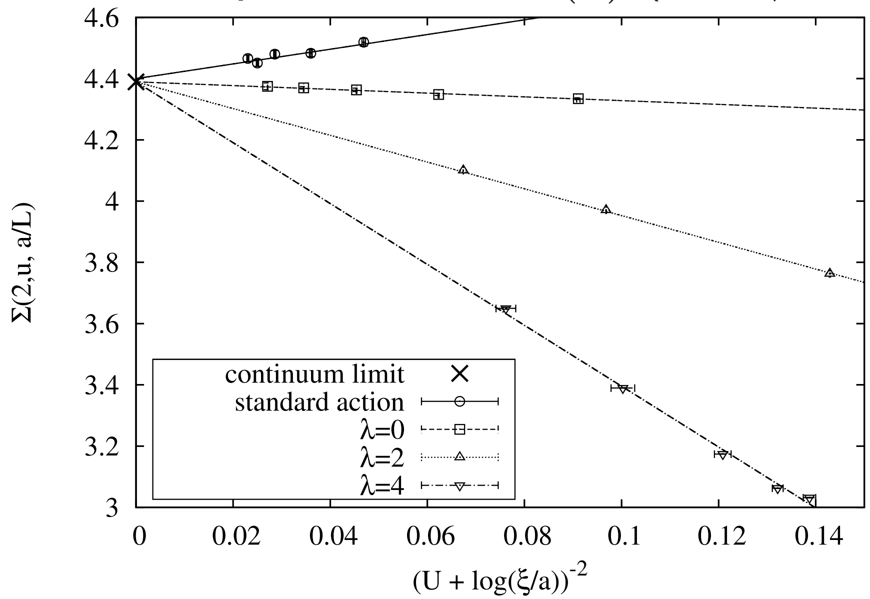


$\delta < \pi/2$ or $\lambda \to +\infty$: no vortices

Further evidence for BKT behavior:

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)



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

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

2. Dimensionless Helicity Modulus $\bar{\Upsilon}$

Twisted boundary conditions; $p(\alpha)$: probability for twist angle α

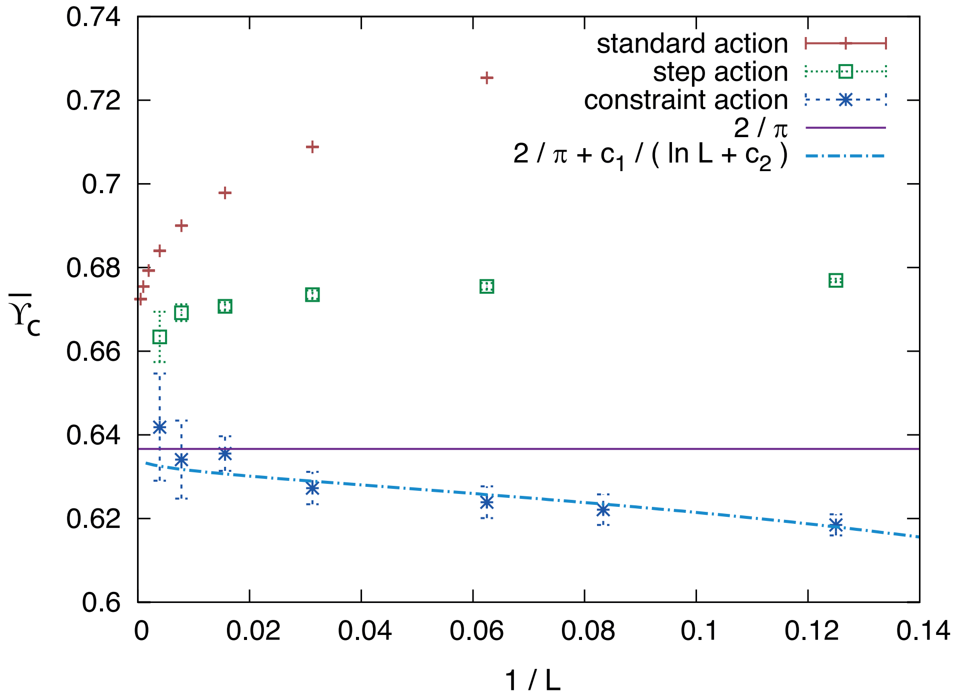
$$\bar{\Upsilon} = -\frac{\partial^2}{\partial^2 \alpha} \ln p(\alpha)|_{\alpha=0}$$

At BKT transition

$$\bar{\Upsilon}_{\rm c} = \frac{2}{\pi}$$

(Nelson/Kosterlitz '77)

Simulate with dynamical boundary conditions,
extract $\bar{\Upsilon}_{\rm c}$ from histogram for α.

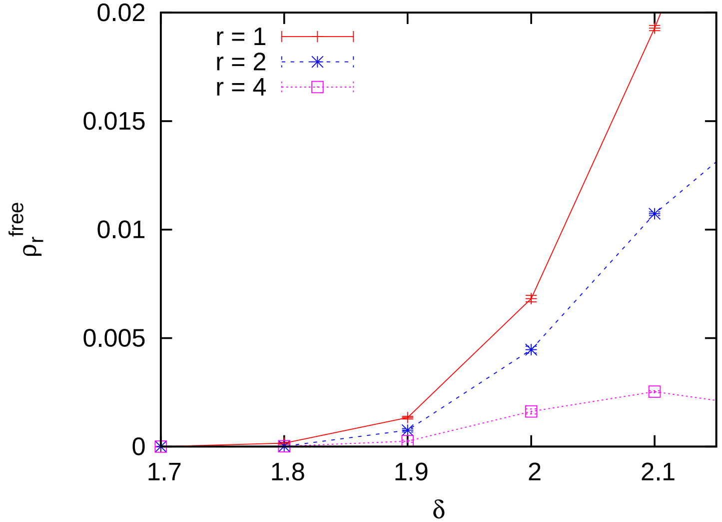


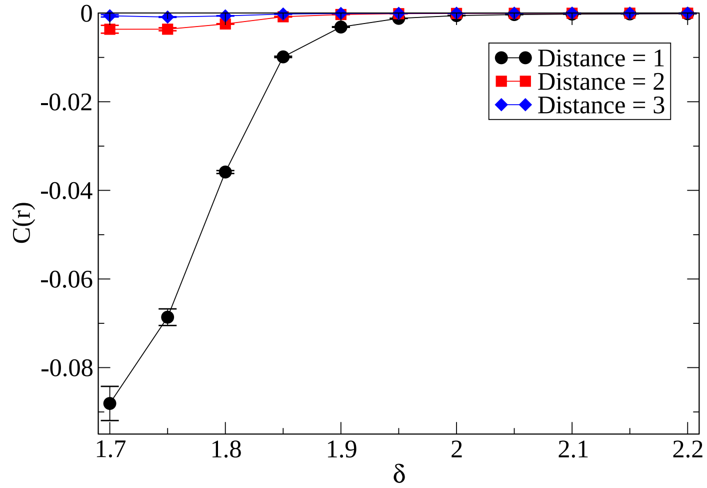
- Standard action: $\bar{\Upsilon}_c(L = 2048)$: 5.6 % off (Hasenbusch '05)
- Step action: $\bar{\Upsilon}_c(L = 256)$: 4.1 % off (Olsson/Holme '01)
- **Constraint action:** $\bar{\Upsilon}_c(L = 8)$: 2.8 % off, $L \geq 64$: correct!

Incredibly small finite size effects.

One of the **best numerical evidences** ever for a BKT transition !

Vortex–anti-vortex pair (un)binding mechanism is still valid:





Left: density of "free vortices" (no anti-vortex within distance r, or v.v.)

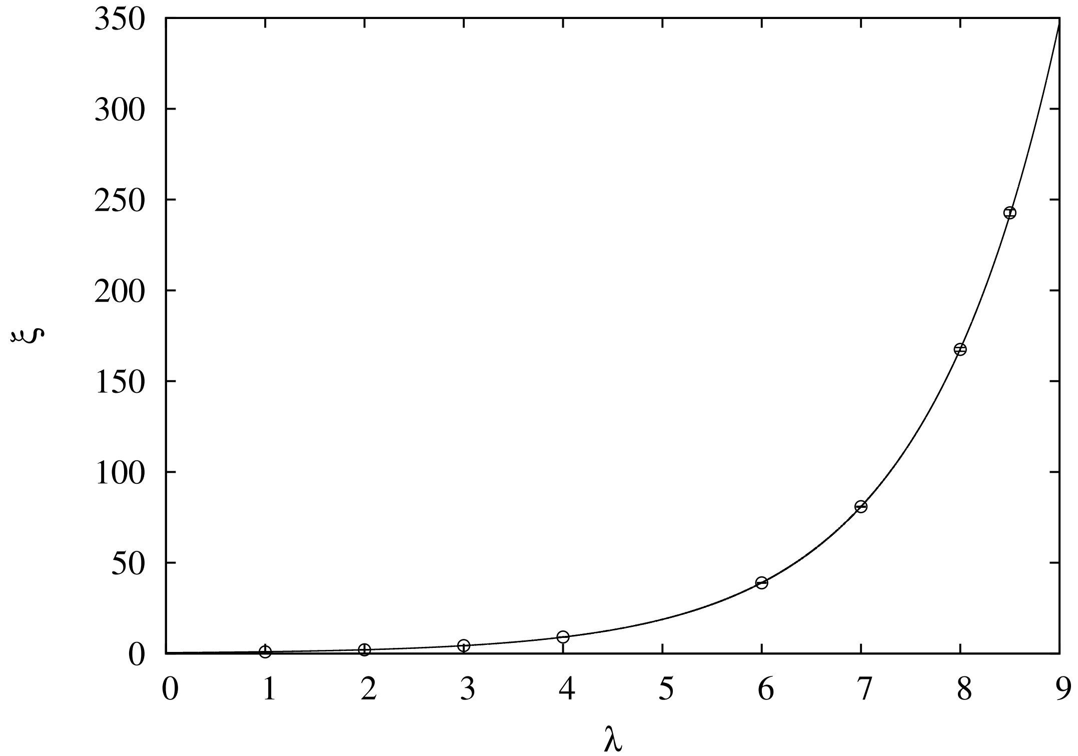
Right: vorticity correlation function $C(r) = \langle v_{\square,x} v_{\square,x+r} \rangle \big|_{|v_{\square,x}|=1}$

(Un)binding as a purely combinatorial effect, without any Boltzmann factor!

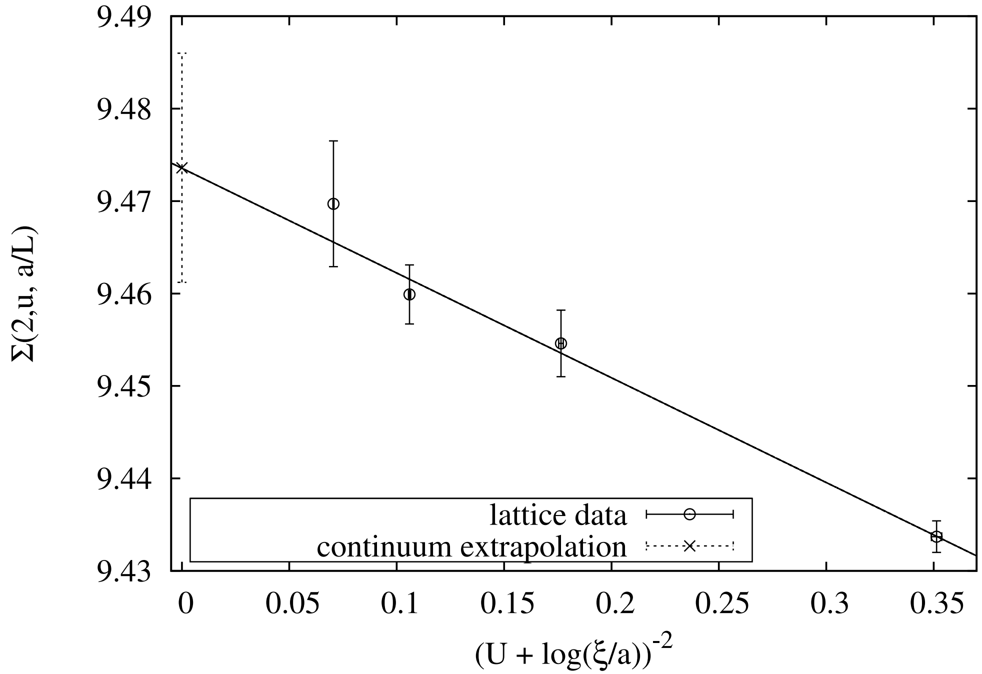
$\delta = \pi$: Pure Vortex Suppressing Action, upper axis in phase diagram:

good fit with (unexpected) ansatz

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



Step-2 SSF has extrapolation $\sigma(2, u = 6)_{\text{fit}} = 9.47(1)$



BKT value: $\sigma(2, u = 6)_{\text{BKT}} = 11.53$ (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.

Conclusions for the 2d XY Model

δ-constraint and $\lambda = 0$ or finite λ :
Phase transition at $\delta_c(\lambda)$, consistent with BKT behavior

SSF and $\chi_m \to \eta_c$ [2]:
large L extrapolation compatible with BKT prediction.

$\bar{\Upsilon}(\delta)$: gap at δ_c [3]. BKT prediction $\bar{\Upsilon}_c = 2/\pi$ confirmed with unprecedented precision: correct even without large-L extrapolation!

One of the most compelling numerical evidences for a BKT transition.

Vortex–anti-vortex pair (un)binding mechanism:
still applies, even without any energy requirement for free vortices.

$\lambda \to \infty$:
new transition in this model, not of BKT type, to be explored ...

Appendix A: **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 '97, Olsson/Holme '01)

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

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

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

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

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

(analytic: van Enter/Shlosman '02, numeric: $e.g.$ Ota/Ota '06, Shinha/Roy '10)

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

Appendix B: **Second Moment Correlation Length ξ_2**

(Connected) correlation function (or 2-point function):

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

ξ_2 is given by the magnetic susceptibility $\chi_m = \tilde{G}(0)$, and by $\tilde{G}$ at the minimal non-zero momentum, $\phi \doteq \tilde{G}(2\pi/L, 0)$:

$$\xi_2 \doteq \left(\frac{\chi_m - \phi}{4\phi \sin^2(\pi/L)} \right)^{1/2}$$

Can be measured conveniently without fit to exp. decay.

At large L: $\xi_2 \simeq \xi$ (up to < 0.1 %) (Caracciolo/Edwards/Pelissetto/Sokal '95)

Appendix C: **Correlation of top. charge density,** $\langle q(0)q(x)\rangle$**, with**

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

does have a finite cont. limit (at $x \neq 0$) ! (Balog/Niedermayer '97)

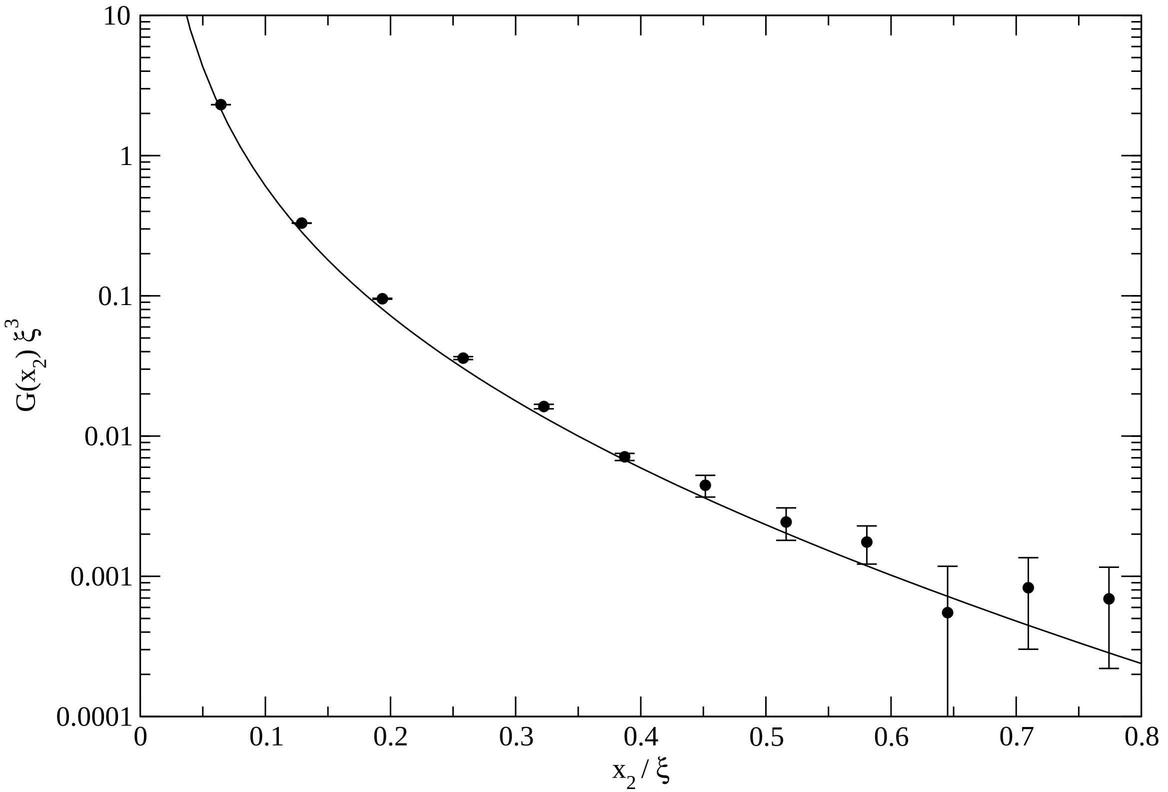
At $x = 0$: cancellation of power divergences, log. divergence persists.

Similar in QCD with chiral quarks, q defined with a chiral lattice Dirac operator. (Giusti/Rossi/Testa '04, Lüscher '04)

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

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

$G(x_2)\xi^3$ vs. x_2/ξ for **Constraint Action** (cluster algorithm)



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