Topological Lattice Actions

I. Concept and 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 (SSF)

Topological susceptibility and charge density correlation

IV. 2d XY Model

Is there a Berezinsky-Kosterlitz-Thouless (BKT) 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, arXiv:1212.0579 [hep-lat] (to be published in JHEP)

I. Topological Lattice Actions: Concept and Motivation

Lattice studies usually start by discretizing some cont. Lagrangian $\Rightarrow$ UV regularization. Prototype:

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

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

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

Or: couplings beyond nearest neighbor sites.

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

Universality : Continuum limits of physical observables coincide.

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

Conditions : **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 the "goes without saying", *does it ?*

Here we discuss counter-examples: lattice actions without any classical limit. We probe how far universality really reaches.

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

We consider $O(N)$ models (non-linear σ-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.

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), since $\Pi_d[S^d] = \mathbb{Z}$ (winding number).

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

and $N = 2$ (XY model, relevant for superfluids)

or $N = 3$ (Heisenberg model, describes ferromagnets).

Simplest topological lattice action : **Constraint Action**

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

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

Deformations of a configuration (within the allowed set) do not cost any action

$\Rightarrow$ "topological lattice action" ($\neq$ lattice actions with discrete derivatives)

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

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"

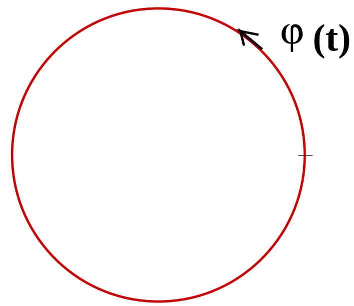
$$S[\vec{e}] = \lambda \sum_{\langle x,y,\dots\rangle} |q_{x,y,\dots}| \ , \qquad \lambda > 0 \ .$$

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

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.

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



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

1. Continuum:

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

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

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

$$\text{top. susceptibility} \quad \chi_t \;=\; \frac{1}{\beta}\,\langle Q^2\rangle = \cdots = \frac{1}{4\pi^2 I}\ , \quad \chi_t\,\xi = \frac{1}{2\pi^2}$$

2. Constraint Lattice Action

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

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

$E_n - E_0 = \frac{\delta^2}{6a} n^2 + \mathcal{O}(\delta^4) \to$ identify $I = 3a/\delta^2$. Scaling quantities:

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

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

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 localization in Euclidean time).
Violated by Constraint Action $\Rightarrow$ not relevant for continuum limit.

3. Q Suppressing Action

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

$$E_n - E_0 = \tfrac{1}{a\lambda^2} + \mathcal{O}(\lambda^{-4}) \;\longrightarrow\; I = \tfrac{a\lambda^2}{2}.$$

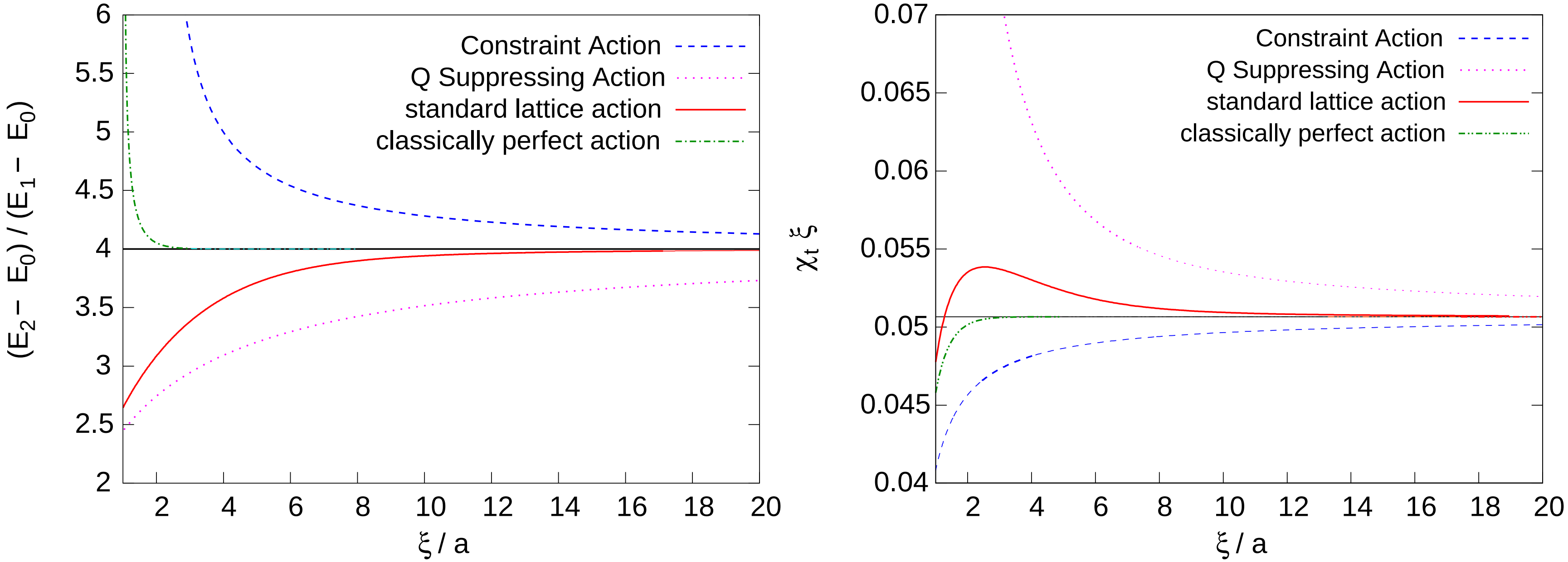
Again correct scaling, up to $\mathcal{O}(a)$ artifacts

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

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

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

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



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

Correct continuum limit !

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

III. The 2d O(3) Model

$\vec{e}(x) \in S^2$ with periodic b.c., topological, asymptotically free

1. Continuum

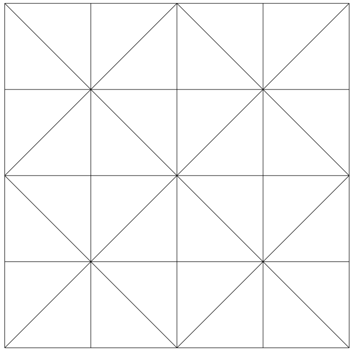
$$S[\vec{e}] = \frac{1}{2g^2} \int d^2x \; \partial_\mu \vec{e}\, \partial_\mu \vec{e} \; , \quad Q[\vec{e}] = \frac{1}{8\pi} \int d^2x \; \epsilon_{\mu\nu} \, \vec{e} \, (\partial_\mu \vec{e}\, \partial_\nu \vec{e}) \in \mathbb{Z}$$

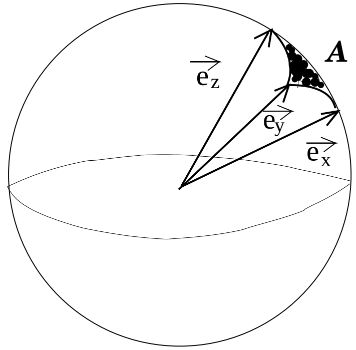
Schwarz inequality: $S[\vec{e}] \geq \frac{4\pi}{g^2} \, |Q[\vec{e}]|$

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 an $L \times L$ lattice, dim'less 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 are known analytically, *e.g.*

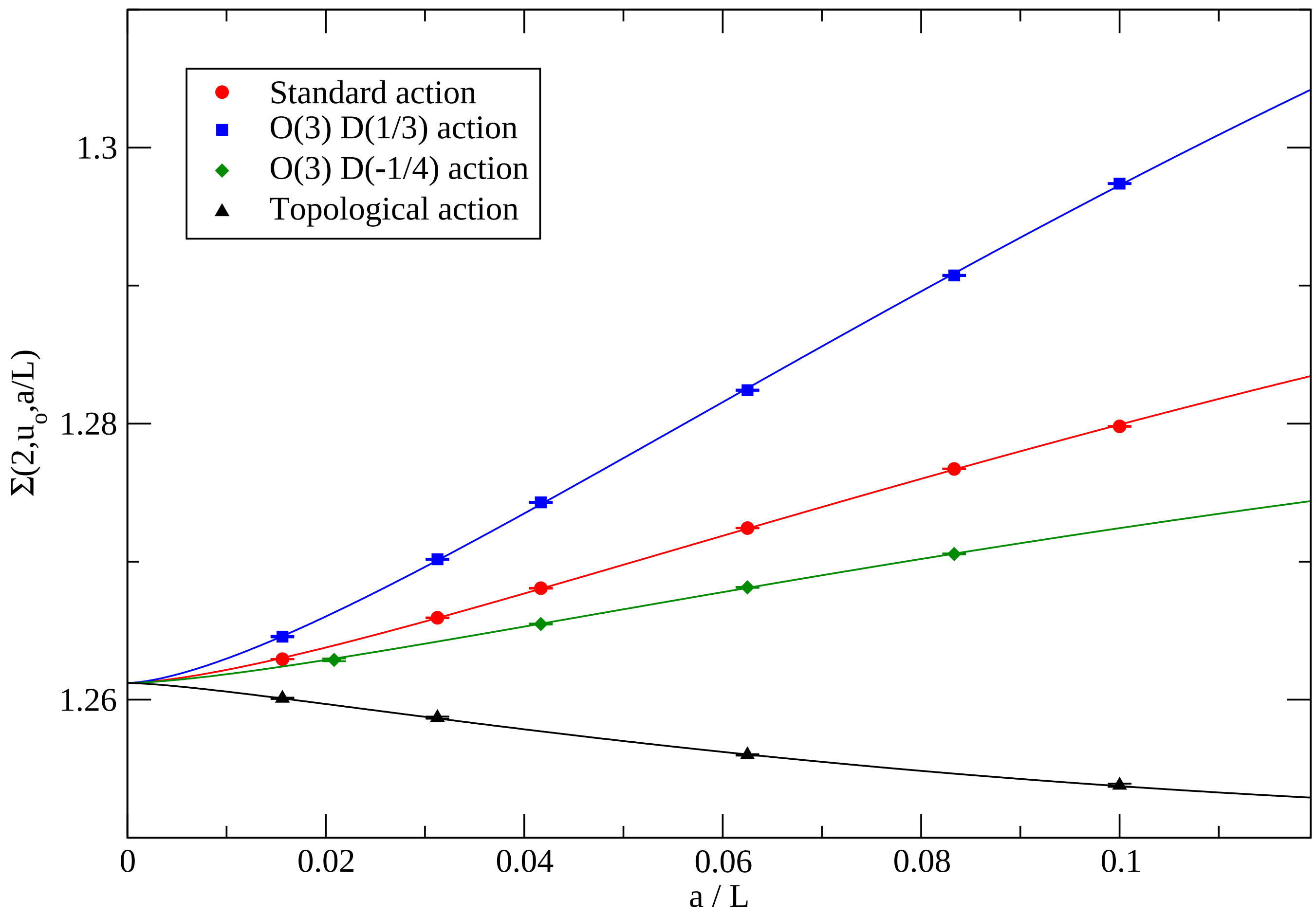
$$\sigma(2, u_0 = 1.0595) = 1.26121$$

(Balog/Niedermayer/Weisz '09)

Must be reproduced in the cont. 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 measure $\xi(2L)$).

High precision thanks to Wolff cluster algorithm !



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

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

(data from Balog/Niedermayer/Weisz '10)

Q Suppressing Action

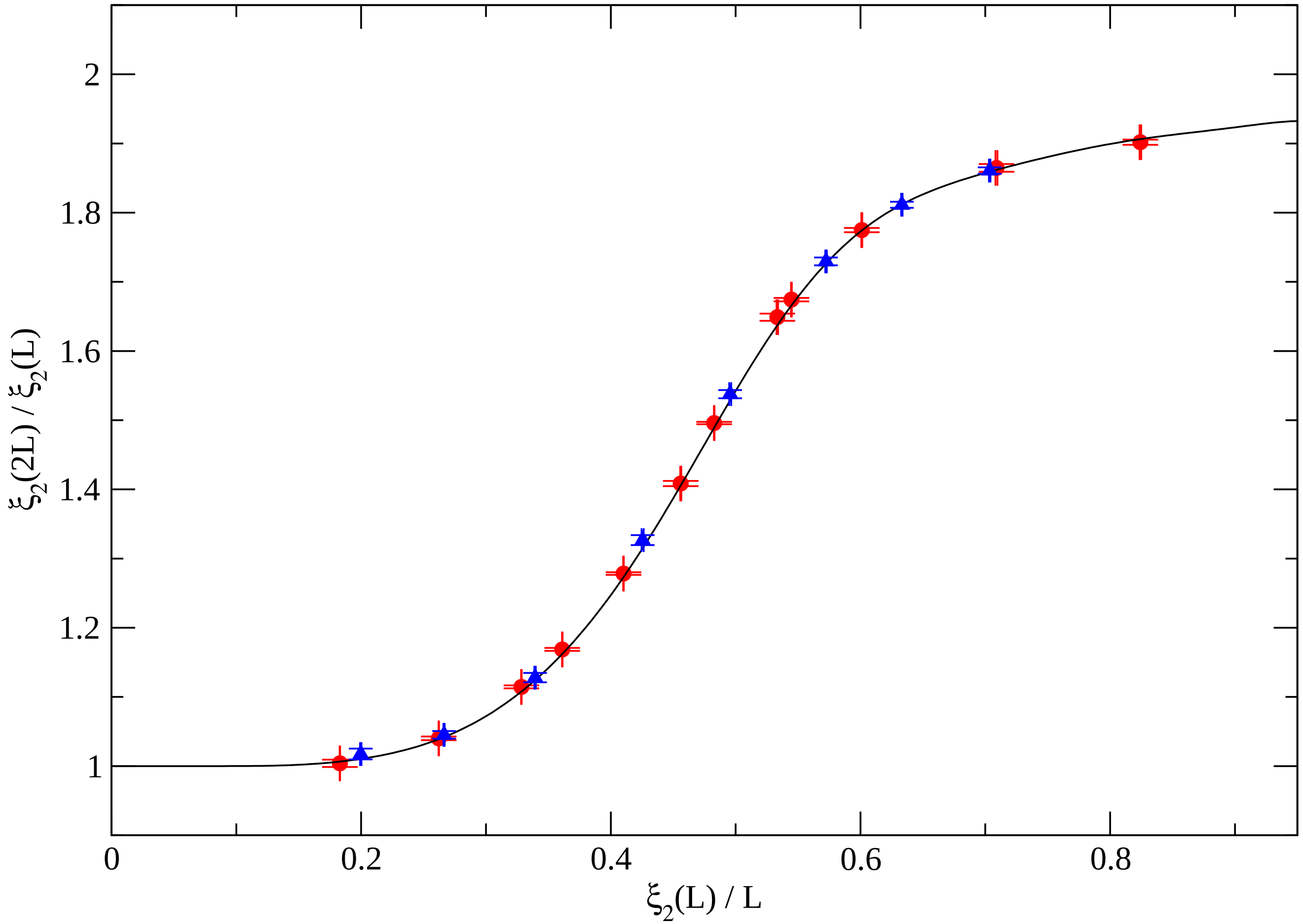
$$S[\vec{e}] = \lambda \sum_{\langle x,y,z \rangle} |A_{x,y,z}| \geq \lambda \left| \sum_{\langle x,y,z \rangle} A_{x,y,z} \right| = 4\pi\lambda\, |Q[\vec{e}]|$$

Metropolis simulation (cluster algorithm does not apply)

$\longrightarrow$ use "2^{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 : $\chi_t = \frac{1}{V}\langle Q^2 \rangle$

"Scaling term" $\chi_t\, \xi^2$ diverges in cont. limit
(small "dislocations" are not sufficiently suppressed)
Semi-classical consideration: $\chi_t\, \xi^2 \propto (\xi/a)^p, \quad p \simeq 0.9$ (Lüscher '82)

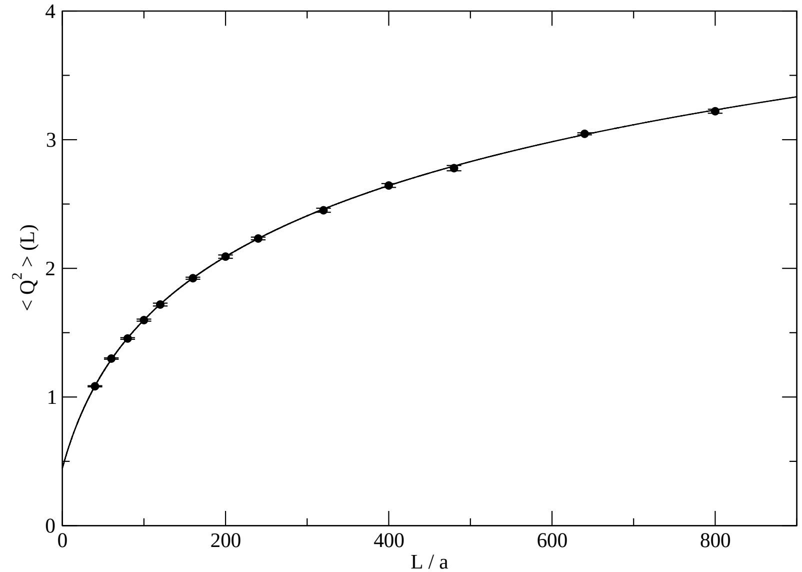
Study with "classically perfect action" which eliminates dislocations $\rightarrow$ log divergences (Blatter/Burkhalter/Hasenfratz/Niedermayer '96)

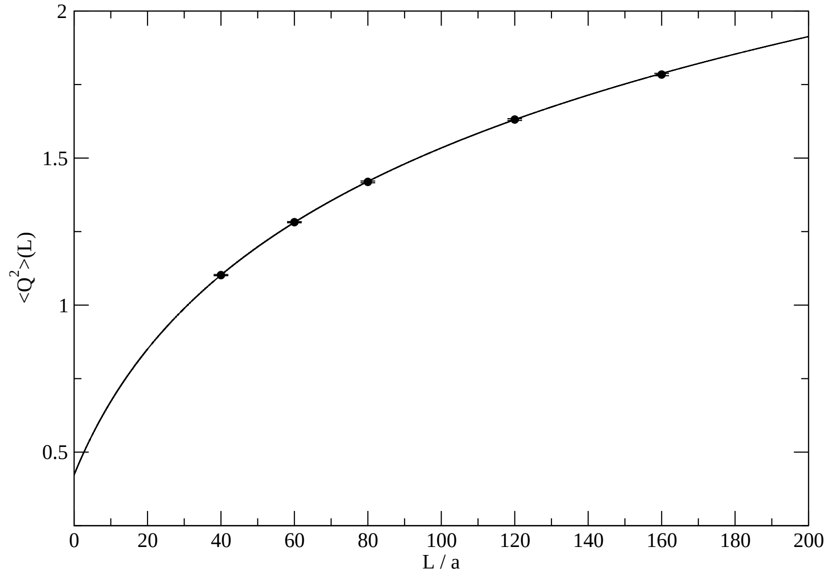
How about top. actions ?
E.g. Constraint Action does not suppress dislocations at all ...

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

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

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





Divergence in the cont. limit is **only logarithmic**, both for Constraint Action (left, **no** dislocation suppression) and Q Suppressing Action (right).

Therefore the 2d $O(3)$ model is sometimes considered "ill", at least regarding top. aspects, but . . .

the **correlation of top. charge density,** $\langle q(0)q(x)\rangle$, 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 $x \neq 0$) ! (Balog/Niedermayer '97)

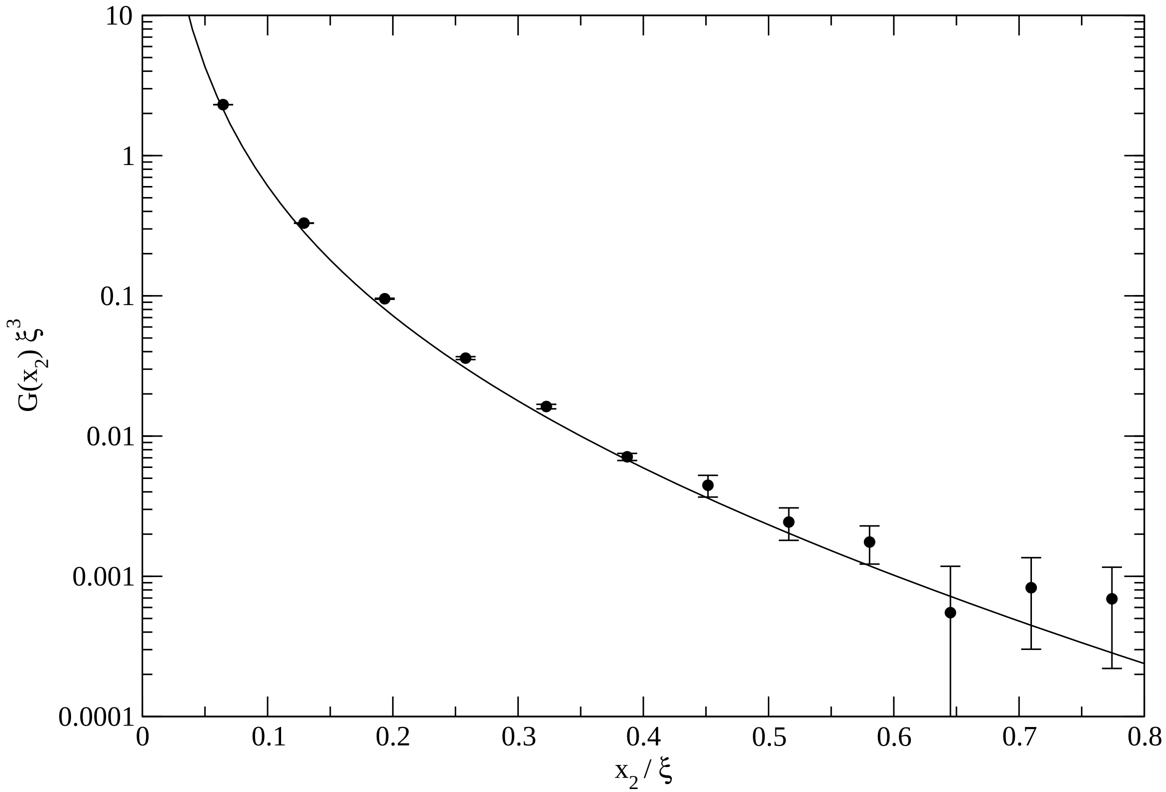
At $x = 0$: cancellation of power divergences, log. divergence persists.

Similar in QCD with chiral quarks, q defined with Ginsparg-Wilson Dirac operator (Giusti/Rossi/Testa '04, Lüscher '04)

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

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

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



Data are cont. extrapolated. Curve: prediction by Balog/Niedermayer '97

Conclusion for the 2d $\mathrm{O}(3)$ model

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

Lattice formulations do not need to start from classical cont. theory and discretize, universality includes much 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 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, sensible top. quantities exist in this model; we saw correlation of top. charge density $q(x)$ ($\longrightarrow$ study of θ-vacua, de Forcrand/Pepe/Wiese '12)

Analogue in lattice gauge theory: constraint plaquette value

(Fukaya et al. '06, W.B., Scorzato et al. '06)

IV. The 2d O(2) Model (or XY 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: (Berezinsky '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 ∞)

$$\xi(T \gtrsim T_c) \propto \exp\left(\text{const.}/[T - T_c]^{1/2}\right) \qquad aT_c = a/\beta_c \simeq 1.1$$

No global top. charge, but each plaquette $\square$ (corners $x_1, \dots, x_4$) has a **vortex number:**

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

BKT transition:

- $T > T_c$: isolated vortices condense, disorder the system, massive
- $T < T_c$: bound vortex–anti-vortex pairs, long-range order, massless

T_c can be estimated from energy cost for isolated vortices (or anti-vortices)

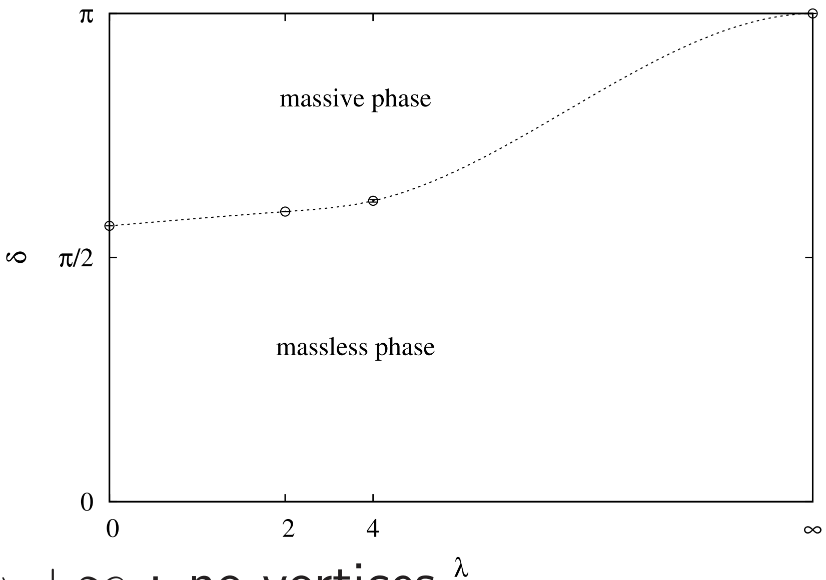
Topological lattice actions:

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

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

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

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

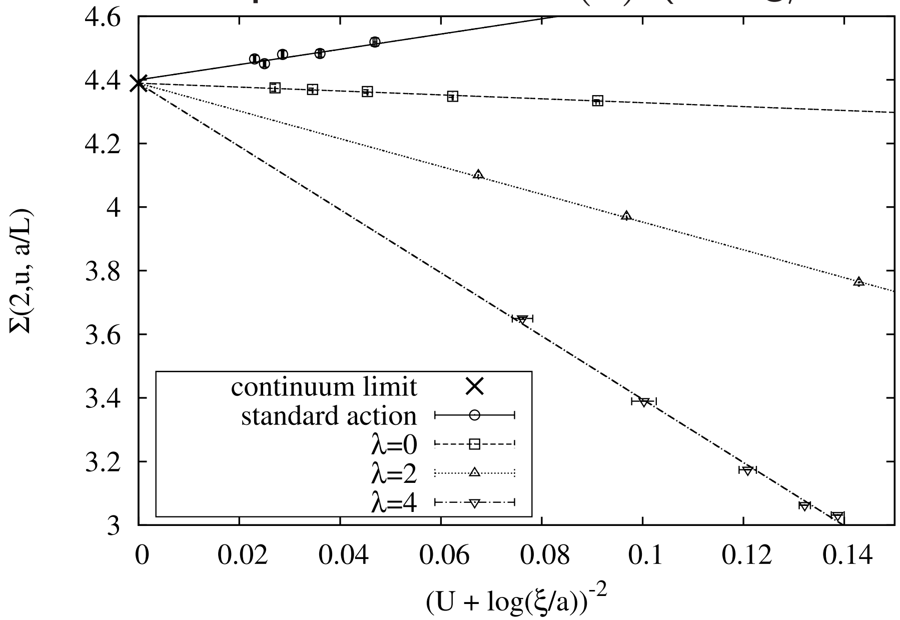


$\delta < \pi/2$ or $\lambda \to +\infty$: no vortices

Evidence for BKT universality behavior 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!

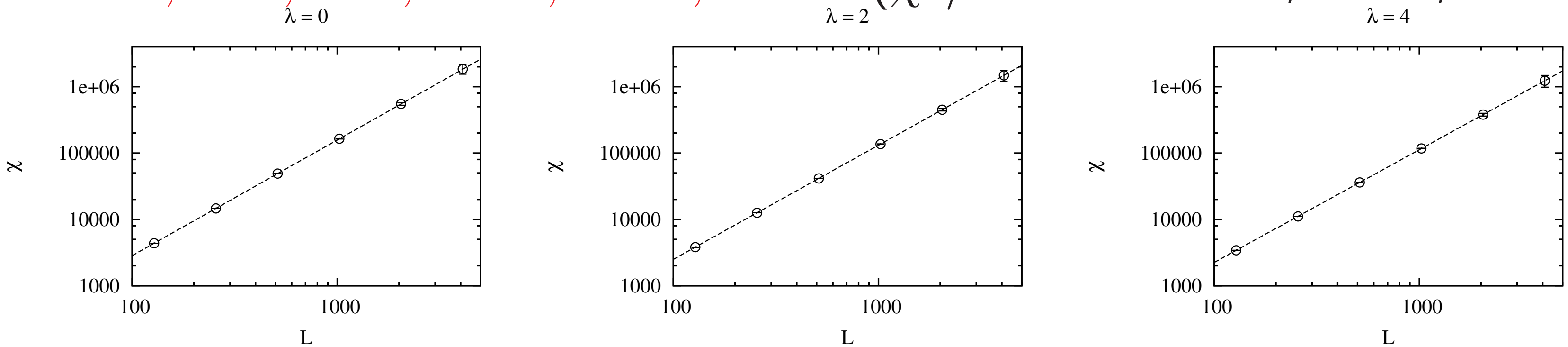
$c \simeq 2.6$ was claimed to be universal, but $c < 0$ for top. actions

2. Magnetic susceptibility in massless phase (near transition)

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

$$\eta_c = 1/4 \;, \quad r_c = -1/16 \qquad (\text{Kosterlitz } '74)$$

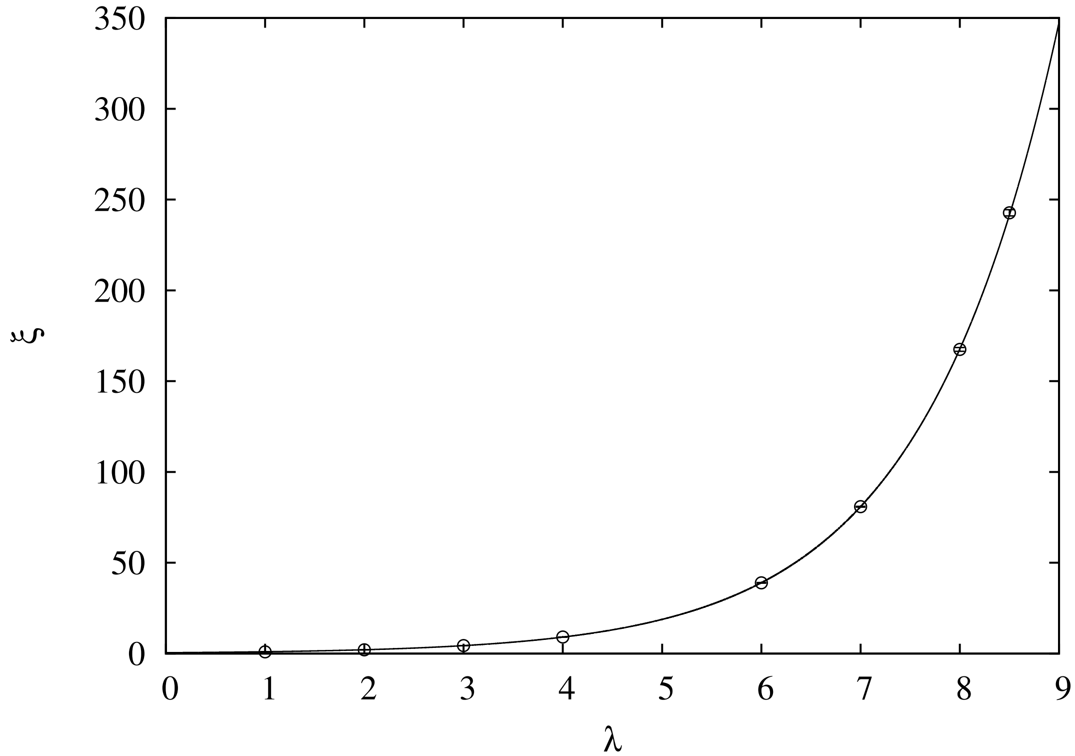
Fits with free parameters a_1, a_2 work very well, $e.g.$ for
$L = 128,\ 256,\ 512,\ 1024,\ 2048, 4096$ (χ^2/d.o.f. $=$ 0.084, 0.022, 0.131)



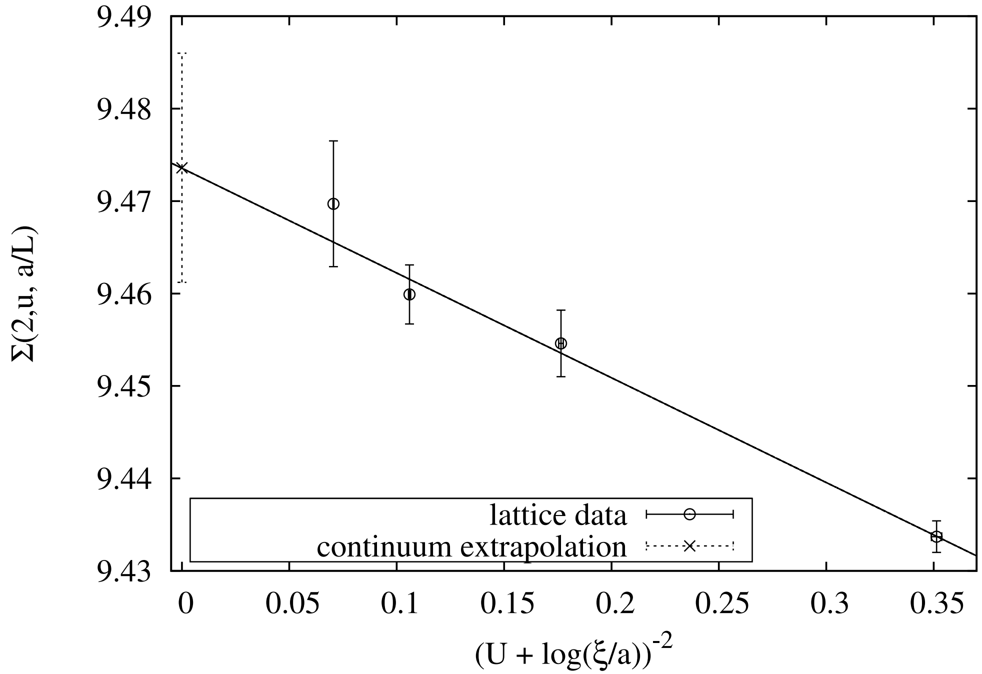
For Standard Action: similar results by Hasenbusch '05.
In general: direct determination of η_c, r_c difficult due to $\ln L$ effects.

$\delta = \pi$: 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 $\sigma(2, u = 6)_{\text{fit}} = 9.47(1)$



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.

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

  (Irving/Kenna '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)

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

$q = 1 \sim$ 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 transition at large λ unknown.