# Theoretical analysis of non-ordinary surface universality class

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# outline

- 1. Brief introduction to surface critical behavior (SCB) and field theory description of SCB in classical O(N) models
- 2. Numerical exploration of SCB of 2+1 D quantum systems with SU(2) symmetry
- 3. Surface phase transition of 2+1 D AKLT model when bulk stays at critical point
- Field theory description and renormalization group analysis of SCB of 2+1D quantum systems with O(2) symmetry (collaborator: Prof Long Zhang)

# d>3 Classical O(N) model



#### $K_{1,c}/K$

Schematic phase diagram of the classical O(N) model with boundaries. *K* and *K*<sub>1</sub> are the bulk and the surface coupling strengths, respectively.

K. Binder, in Phase Transitions and Critical Phenomena, edited by C. Domband J. L. Lebowitz, Vol. 8 (Academic Press, London, 1983).

H. W. Diehl, International Journal of Modern Physics B 11, 3503?3523 (1997), ISSN 1793-6578, cond-mat/9610143

J. Cardy, Scaling and Renormalization in Statistical Physics, Cambridge Lecture Notes in Physics (Cambridge University Press, 1996).

H. W. Diehl, in Phase Transitions and Critical Phenomena, edited by C. Domband J. L. Lebowitz(Academic, London, 1986), Vol. 10, pp. 75–267.

Normal universality class

$$H = -\sum_{i,j} K_{i,j} \,\vec{s}_i \cdot \vec{s}_j + \sum_{surface} \vec{h} \cdot \vec{s}_j$$



normal universality class =extraordinary universality class

describe surface critical behavior of class O(N) model by field theory

$$\mathcal{H} = \int_{\mathcal{M}} dV \mathcal{L}(oldsymbol{x}) + \int_{\mathcal{B}} dA \mathcal{L}_1(oldsymbol{x})$$

• The Lagrangian of bulk is:

$$egin{aligned} \mathcal{L}(oldsymbol{x}) &= rac{1}{2} [
abla \phi(oldsymbol{x})]^2 + \mathcal{U}[\phi(oldsymbol{x})] \ \mathcal{U}(\phi) &= rac{1}{2} au_0 \phi^2 + rac{1}{4!} u_0 |\phi|^4 \end{aligned}$$

• The Lagrangian of surface is

$$egin{aligned} \mathcal{L}_1(oldsymbol{x}) &= \mathcal{U}_1[\phi(oldsymbol{x})] \ \mathcal{U}_1(\phi) &= rac{1}{2}c_0\phi^2 - h_{1,0}\phi \end{aligned}$$

H. W. Diehl, in Phase Transitions and Critical Phenomena, edited by C. Domband J. L. Lebowitz(Academic, London, 1986), Vol. 10, pp. 75–267.





Phase diagram of the semi-infinite *n*-vector model (2.13) in the variables  $\tau(\sim T - T_c^b)$  and c(= -surface enhancement), as predicted by Landau theory.

# 3D O(N) model

• D=3,N=1: 3d classical Ising model, the phase diagram is the same.





D=3,N>2:there is no spontaneous symmetry break at boundary(Mermin Wagner theorem), thus only ordinary class exist?( right for the large N case)



study this model at its bulk critical point  $T = T_c$  and in the  $K_1/K \gg 1$  region, when the surface has a strong tendency to local order.

The surface layer can be described by:

$$S_n = \int d^{d-1} \mathrm{x}igg(rac{1}{2g} {(\partial_\mu ec{n})}^2 - ec{h} \cdot ec{n}igg), \quad ec{n}^2 = 1$$

The system without the outermost surface:  $S_{ordinary}$  The coupling of the surface layer to the next layer:

$$S_{n\phi}=- ilde{s}\int d^{d-1}\mathrm{x}ec{n}(\mathrm{x})\cdotec{\phi}(\mathrm{x},x_d=0)$$

The total action is:

$$S_{UV} = S_{\text{ordinary}} + S_n + S_{n\phi}$$
  $H = -\sum_{i,j} K_{i,j} \vec{s}_i \cdot \vec{s}_j$ 

M. A. Metlitski, Boundary criticality of the o(n) model in d=3 critically revisited, arXivpreprint arXiv:2009.05119(2020).





The RG equations of  $S = \frac{1}{2g} \int d^2 x (\partial_\mu \vec{n})^2$  are

$$rac{dg}{d\ell}=rac{N-2}{2\pi}g^2, \hspace{1em} ec{n}
ightarrow \left(1-rac{\eta_n(g)}{2}d\ell
ight)ec{n}, \hspace{1em} \eta_n=rac{N-1}{2\pi}g$$

• The fixed point is g=0, which means the fluctuations of  $\vec{n}$  are frozen. The coupling  $S_{n\emptyset}$  acts as a boundary symmetry breaking field for the bulk O(N) model. This term is relevant at the ordinary boundary fixed point and makes the boundary flow to the normal fixed point.

$$egin{aligned} S_{UV} &= S_{ ext{ordinary}} \,+ S_n + S_{n\phi} \ S_n &= \int d^{d-1} \mathrm{x} \Big( rac{1}{2g} (\partial_\mu ec n)^2 - ec h \cdot ec n \Big), &ec n^2 = 1 \ S_{n\phi} &= - ilde s \int d^{d-1} \mathrm{x} ec n (\mathrm{x}) \cdot ec \phi (\mathrm{x}, x_d = 0) \end{aligned}$$

# Near normal universality class

$$\begin{split} S_{UV} &= S_{\text{ordinary}} + S_n + S_{n\phi} \quad \underbrace{flow to}_{SIR} = S_{\text{normal}} + S_n - s \int d^{d-1} x \pi_i(x) \hat{\phi}_i(x) + \delta S \\ \vec{n} &= \left(\vec{\pi}, \sqrt{1 - \vec{\pi}^2}\right) \\ \sigma(x, x_d) &\sim \frac{a_{\sigma}}{(2x_d)^{\Delta_{\phi}}} + \mu_{\sigma}(2x_d)^{d-\Delta_{\phi}} \hat{\sigma}(x) + \dots, \quad x_d \to 0 \\ \phi_i(x, x_d) &\sim \mu_{\phi}(2x_d)^{d-1 - \Delta_{\phi}} \hat{\phi}_i(x) + \dots, \quad x_d \to 0 \\ \langle O^e(x) O^b(y) \rangle &= \frac{\delta^{ab}}{|x - y|^{2\Delta_O}} \qquad \langle O^e(x) \hat{O}^b(y) \rangle = \frac{\delta^{ab}}{|x - y|^{2\Delta_O}} \\ \delta_{\phi_i}^e &= d - 1, \, \Delta_{\widehat{\sigma}} = d \qquad \qquad s = \frac{\Gamma(d-1)}{(4\pi)^{\frac{d-1}{2}} \Gamma(\frac{d-1}{2})} \frac{a_{\sigma}}{\mu_{\phi}} \overset{d=3}{=} \frac{1}{4\pi} \frac{a_{\sigma}}{\mu_{\phi}} \end{split}$$

## RG results

$$rac{dg}{d\ell}=-lpha g^2 \quad lpha=rac{\pi s^2}{2}-rac{N-2}{2\pi} \quad \eta_n=rac{N-1}{2\pi}g$$

- N=2, $\alpha > 0$
- Correlation function of surface can be got by solving the callan-symanzik equation:



•  $N \rightarrow \infty, \alpha < 0$ 



• There should exist a critical vaule  $N_c$ , if  $N < N_c$ , extra-ordinary-log class exists.

# Near Nc

$$rac{dg}{d\ell}pprox a(N-N_c)g^2+bg^3, \quad a>0$$



Sceanrio 2 b<0

# summary



 $N < N_c \text{ or } N < N_{c2}$ 

 $N > N_c \text{ or } N > N_{c2}$ 



3D Classical O(N), N=2,3..Nc



2+1D quantum SU(2), U(1)?



$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle ij \rangle'} \mathbf{S}_i \cdot \mathbf{S}_j$$



$$\chi_{1,1} = -\frac{\partial^2 f_1}{\partial h_1^2} \sim L^{-(d+z-1-2y_{h_1})}$$

$$|C_{\parallel}(\mathbf{r})| \sim r^{-(d+z-2+\eta_{\parallel})}$$

 $|C_{\perp}(\mathbf{r})| \sim r^{-(d+z-2+\eta_{\perp})}$ 

	$J_c$	z	ν	η	β	$y_{h_1}$	$\eta_{\parallel}$	$\eta_{\perp}$
$J_{c1}$	1.064382(13)	1.0008(16)	0.7060(13)	0.0357(13)	0.3663(8)	0.810(20)	1.327(25)	0.680(8)
$J_{c2}$	0.603520(10)	1.001(5)	0.7052(9)	0.031(4)	0.3642(13)	1.7276(14)	-0.449(5)	-0.2090(15)
$J_{c3}$	-0.934251(11)	0.9999(13)	0.7052(15)	0.0365(10)	0.3659(9)	1.7802(16)	-0.561(4)	-0.2707(24)
3D O(3) field			0.7073(35)	0.0355(25)	0.3662(25)			
theory [25]								
3D classical						0.813(2)		
Heisenberg [15]								

L. Zhang and F. Wang, Phys. Rev. Lett. 118, 087201 (2017)

Realize three types of surface critical behavior of 3D O(3) universality class with different surface configurations



Columnar (left) and staggered (right) dimerized spin-1/2 Heisenberg models on the square lattice. J and J' are the exchange coupling strengths on the two types of bonds, and J' > J. In each model, two types of open boundaries (denoted by cut-1 and 2) cutting along the two dashed lines are considered in this work.

C. Ding, L. Zhang, and W. Guo, Phys. Rev. Lett. 120, 235701 (2018).

Surface critical exponents of the dimerized Heisenberg models with different surface cut configurations. Results of the decorated square lattice at the trivial phase-Néel QCP ( $J_{c1}$ ) and the AKLT-Néel QCP ( $J_{c2}$ ) [10], the 3D classical Heisenberg model [7], and the field theoretic results for the ordinary (ord.) and the special (sp.) transitions from various techniques, including  $\epsilon = 4 - d$  expansion [22,23],  $\epsilon = d - 2$  expansion [24], massive field theory [25,26], and conformal bootstrap [27], and the anomalous dimensions of transverse (trans.) and longitudinal (long.) correlations from the scaling arguments and the large-*n* expansion of O(*n*) models at the extraordinary (ext.) transition [13,14] are also listed for comparison.

Class	Model	$y_{h1}$	$\eta_{\parallel}$	$\eta_{\perp}$
Ord.	Column, cut-1	0.840(17)	1.387(4)	0.67(6)
	Stagger, cut-1	0.830(11)	1.340(21)	0.682(2)
	Deco.sq., $J_{c1}$	0.810(20)	1.327(25)	0.680(8)
	3D classical	0.813(2)		
	$\epsilon = 4 - d \exp$ .	0.846	1.307	0.664
	$\epsilon = d - 2 \exp$ .		1.39(2)	
	Massive field	0.831	1.338	0.685
	Bootstrap	0.831		
Sp.	Column, cut-2	1.7339(12)	-0.445(15)	-0.218(8)
	Deco.sq., $J_{c2}$	1.7276(14)	-0.449(5)	-0.2090(15)
	$\epsilon = 4 - d \exp$ .	1.723	-0.445	-0.212
Ext.	Stagger, cut-2		1.004(13)	-0.5050(10)
	Scaling, trans.		3	3/2
	Scaling, long.		5	$(5 + \eta)/2$



Configuration	$\eta_{\parallel}$	$\eta_{\perp}$	$y_{h_1}$
CD-N	1.30(2)	0.69(4)	0.84(1)
DAF-N	1.29(6)	0.65(3)	0.832(8)
PAF-N	1.33(4)	0.65(2)	0.82(2)
CD-D	-0.50(1)	-0.27(1)	1.740(4)
DAF-D	-0.50(1)	-0.228(5)	1.728(2)
PAF-D	-0.517(4)	-0.252(5)	1.742(1)



Configuration	Spin S	$\eta_{\parallel}$	$\eta_{\perp}$	$y_{h_1}$
Nondangling	1	1.32(2)	0.70(2)	0.80(1)
000	1/2	1.30(2)	0.69(4)	0.84(1)
Dangling	1	-0.539(6)	-0.25(1)	1.762(3)
	1/2	-0.50(1)	-0.27(1)	1.740(4)

L. Weber and S. Wessel, Phys. Rev. B 100, 054437 (2019).

L. Weber, F. ParisenToldin, and S. Wessel, Phys. Rev. B 98, 140403 (2018)



SCB class	Model/methods	Cuts	Spin S	$\eta_{\parallel}$	$\eta_{\perp}$	Yh1
Nonord. Ord.	CHC	<i>x</i> surface <i>y</i> surface	1 1	-0.57(2) 1.38(2)	-0.27(2) 0.69(2)	1.760(3) 0.79(2)

W. Zhu, C. Ding, L. Zhang, and W. Guo, Surface critical behavior of coupled haldanechains, Phys. Rev. B 103

surface phase transition of 2D AKLT model with SU(2) symmetry



C.-M. Jian, Y. Xu, X.-C. Wu, and C. Xu, SciPostPhys. 10, 33 (2021), 2004.07852

# Edge state

The 1d boundary of this AKLT state should be effectively described by an extended Heisenberg model

$$H = \sum_{j} J\vec{S}_{j} \cdot \vec{S}_{j+1} + \cdots$$

The boundary system is the  $SU(2)_1$  CFT described by the following Hamiltonian in the infrared limit

$$H_0 = \int dx \, \frac{1}{3 \cdot 2\pi} \left( \vec{J_L} \cdot \vec{J_L} + \vec{J_R} \cdot \vec{J_R} \right)$$

The relation between the microscopic operator  $\vec{S}$  and the low energy field is

$$\vec{S}(x) \sim \frac{1}{2\pi} \left( \vec{J}_L(x) + \vec{J}_R(x) \right) + (-1)^x \vec{n}(x)$$

Because the lattice Hamiltonian has a lower symmetry than the infrared theory  $H_0$ , another term is allowed in the low energy Hamiltonian:



#### Quantum critical modes couple to boundary fields



$$C_n(\mathbf{x}, 0)_{ab} = \langle \Phi^a(x, \tau) \Phi^b(0, 0) \rangle = \frac{\delta_{ab}}{(x^2 + \tau^2)^{3/2 - \epsilon_n}},$$
$$C_v(\mathbf{x}, 0) = \langle \Phi(x, \tau) \Phi(0, 0) \rangle = \frac{1}{(x^2 + \tau^2)^{3/2 - \epsilon_v}}$$

The boundary quantum critical modes couple to the fields at the boundary

$$\begin{split} \mathcal{S} &= \int d^2 \mathbf{x} \ g_n \vec{\Phi}(\mathbf{x}) \cdot \vec{n}(\mathbf{x}) + g_v \Phi(\mathbf{x}) v(\mathbf{x}) \\ &+ \int d^2 \mathbf{x} d^2 \mathbf{x}' \ \frac{1}{2} \Phi^a(\mathbf{x}) C_n^{-1}(\mathbf{x}, \mathbf{x}')_{ab} \Phi^b(\mathbf{x}') \\ &+ \int d^2 \mathbf{x} d^2 \mathbf{x}' \ \frac{1}{2} \Phi(\mathbf{x}) C_v^{-1}(\mathbf{x}, \mathbf{x}') \Phi(\mathbf{x}'), \end{split}$$

# RG equation

$$\beta(\lambda) = \frac{d\lambda}{d\ln l} = 2\pi\lambda^2 - \frac{\pi}{2}g_n^2 + \frac{\pi}{2}g_v^2,$$
  
$$\beta(g_n) = \frac{dg_n}{d\ln l} = \epsilon_n g_n - \frac{\pi}{2}\lambda g_n,$$
  
$$\beta(g_v) = \frac{dg_v}{d\ln l} = \epsilon_v g_v + \frac{3\pi}{2}\lambda g_v.$$

There is no general reason for  $\vec{\phi}, \phi$  to become critical simultaneously in the bulk. Hence let us ignore the  $\phi$  field first, and consider the coupled RG equation for  $\lambda$ ,  $g_n$  only. The beta functions have an new unstable fixed point at

$$(\lambda^*, g_n^*) = \left(\frac{2\epsilon_n}{\pi}, \frac{4\epsilon_n}{\pi}\right)$$





# Surface critical behavior of 2+1 D XXZ model



**Dangling chain** 

H.-H. Song and L. Zhang, in preparation.

# The surface layer

The surface layer is described by XXZ chain

$$H_{xxz} = \sum_{i=1}^{\infty} \frac{1}{2} (\sigma_i^+ \sigma_{i+1}^- + \sigma_i^- \sigma_{i+1}^+) + \frac{\Delta}{4} \sum_{i=1}^{\infty} \sigma_i^z \sigma_{i+1}^z$$

By bosonization method, the efficient theory of surface layer is

$$S_{xxz} = \int dz d\overline{z} \{ \frac{1}{K} \partial_z \phi \partial_{\overline{z}} \phi - v \cos(\sqrt{16\pi}\phi) \} \qquad v = \frac{\Delta}{4\pi^2 \alpha^2 K} , K = (1 + \frac{4\Delta}{\pi})^{-\frac{1}{2}}$$

RG equations of XXZ chain are

$$\frac{dv}{dl} = (2 - 4K)v$$
$$\frac{d\frac{1}{K}}{dl} = 8\pi^2 v^2$$



# Influence of bulk

The effective non-local dangling XXZ chain action can be written as

$$S_1 = S_{xxz} + S_{int}$$

The quantum critical modes couple to the fields at surface

$$S_{int} = \int dz d\overline{z} g_{xx} (n_1 \psi_1 + n_2 \psi_2) + g_z n_3 \psi_3 + \int dz d\overline{z} dw d\overline{w} \psi_a(z, \overline{z}) C_{(a,b)}^{-1}(z, \overline{z}, w, \overline{w}) \psi_b(w, \overline{w})$$



RG results:

1.ordinary  $v \to -\infty, K \to 0, g_z \to 0, g_{xx} \to 0$ 2.extraordinary(break z2 symmytry)

$$v \to \infty, K \to 0, g_z \to \infty, g_{xx} \to 0.$$

3.extraordinary(break O(2) symmytry)

$$v \to 0, K \to +\infty, g_z \to 0, g_{xx} \to +\infty$$

Z axis, and surface have long range order along Z axis

Easy-axis:strong interaction between bulk and surface along

Easy-plane:strong interaction between bulk and surface in X-Y plane, and that surface have long range order in X-Y plane

$$\langle e^{i\phi}e^{-i\phi}\rangle \sim 0$$
 and  $\langle e^{i\theta}e^{-i\theta}\rangle \sim 1$  as  $x - y \rightarrow \infty$ 

The surface layer is described by ladder

$$H_{ladder} = H_{\tau} + H_{\sigma} + H_{\sigma\tau}$$

$$H_{\sigma} = \sum_{j} \frac{1}{2} (\sigma_{j}^{+} \sigma_{j+1}^{-} + \sigma_{j}^{-} \sigma_{j+1}^{+}) + \frac{\Delta_{1}}{4} \sigma_{j}^{z} \sigma_{j+1}^{z}$$

$$H_{\tau} = \sum_{j} \frac{1}{2} (\tau_{j}^{+} \tau_{j+1}^{-} + \tau_{j}^{-} \tau_{j+1}^{+}) + \frac{\Delta_{2}}{4} \tau_{j}^{z} \tau_{j+1}^{z}$$

$$H_{\sigma\tau} = \sum_{j} \frac{\lambda_{xy}}{2} (\tau_{j}^{+} \sigma_{j}^{-} + \tau_{j}^{-} \sigma_{j}^{+}) + \frac{\lambda_{z}}{4} \tau_{j}^{z} \sigma_{j}^{z}$$

By bosonization method, the efficient theory of ladder is

$$S_{ladder,s} = \int dz d\overline{z} \{ \frac{1}{K_1} \partial_z \phi_s \partial_{\overline{z}} \phi_s + g_3 \cos(2\sqrt{2\pi}\phi_s) \}$$
$$S_{ladder,a} = \int dz d\overline{z} \{ \frac{1}{K_2} \partial_z \phi_a \partial_{\overline{z}} \phi_a + g_1 \cos(\sqrt{2\pi}\theta_a) + g_2 \cos(2\sqrt{2\pi}\phi_a) \}$$

**Dangling ladder** 



# Phase diagram of ladder

$$S^{+}(x) = \frac{1}{\sqrt{2\pi\alpha}} e^{i\sqrt{\frac{\pi}{2}}\theta_{s}(x)} [2i(-1)^{\frac{x}{a}} \sin(\sqrt{\frac{\pi}{2}}\theta_{a}(x)) + 2ie^{i\sqrt{2\pi}\phi_{s}(x)} \sin(\sqrt{\frac{\pi}{2}}\theta_{a}(x) + \sqrt{2\pi}\phi_{a}(x))]$$
  

$$\overrightarrow{S} = \overrightarrow{\sigma} - \overrightarrow{\tau}.$$
  

$$S^{z}(x) = 2\sqrt{\frac{2}{\pi}}\partial_{x}\phi_{a} - (-1)^{\frac{x}{a}} \frac{4}{\pi\alpha} \sin(\sqrt{2\pi}\phi_{s}) \sin(\sqrt{2\pi}\phi_{a})$$

$$S_{ladder,s} = \int dz d\overline{z} \{ \frac{1}{K_1} \partial_z \phi_s \partial_{\overline{z}} \phi_s + g_3 \cos(2\sqrt{2\pi}\phi_s) \}$$
$$S_{ladder,a} = \int dz d\overline{z} \{ \frac{1}{K_2} \partial_z \phi_a \partial_{\overline{z}} \phi_a + g_1 \cos(\sqrt{2\pi}\theta_a) + g_2 \cos(2\sqrt{2\pi}\phi_a) \}$$

Ising AF phase:  $g_2$  is more relevant and  $g_3$  is relevant Singlet phase:  $g_1$  is more relevant and  $g_3$  is relevant XY1 phase:  $g_1$  is more relevant and  $g_3$  is irrelevant XY2 phase:  $g_2$  is more relevant and  $g_3$  is irrelevant

#### Influence of bulk

The effective non-local dangling ladder action can be written as

 $S_2 = S_{ladder} + S_{L,int}$ 

The quantum critical modes couple to the fields at surface

$$S_{L,int} = \int dz d\overline{z} \sum_{i=\sigma,\tau} \left[ g_{xx}^i (n_1^i \psi_1 + n_2^i \psi_2) + g_z^i n_3^i \psi_3 \right] + \int dz d\overline{z} dw d\overline{w} \psi_a(z,\overline{z}) C_{(a,b)}^{-1}(z,\overline{z},w,\overline{w}) \psi_b(w,\overline{w}) d\overline{w} \psi_b(w,\overline{w}) d\overline{w}$$

RG results:

1.ordinary(singlet): no coupling, disorder surface

2.extraordinary(break z2 symmetry)(Ising-AF,XY2):strong interaction between bulk and surface along Z axis, and surface have long range order along Z axis

3.extraordinary(break O(2) symmetry)(XY1):strong interaction between bulk and surface in X-Y plane, and argue that surface have long range order in X-Y plane

# Thanks!