Advances in the boundary O(N) universality class



New perspectives on Quantum Field Theory with Boundaries Impurities, and Defects Nordita, Stockholm, 4 August 2023

Boundary critical phenomena

In the vicinity of a second-order phase transitions:

- Power-laws, universality
- Renormalization Group:

 $\mathcal{K} \to \mathcal{R}(\mathcal{K}) \to \mathcal{R}(\mathcal{R}(\mathcal{K})) \dots$

- Real systems: surfaces
- RG: bulk vs surface couplings Cardy book (1996)





Reviews: Binder (1983); Diehl (1986)

→Rich bulk-surface phase diagram

 \rightarrow Surface UC determine the critical Casimir force Fisher, de Gennes (1978)

A renewed interest: quantum spin models

PRL 118, 087201 (2017)

PHYSICAL REVIEW LETTERS

week ending 24 FEBRUARY 2017

Unconventional Surface Critical Behavior Induced by a Quantum Phase Transition from the Two-Dimensional Affleck-Kennedy-Lieb-Tasaki Phase to a Néel-Ordered Phase

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¹International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China ²Collaborative Innovation Center of Quantum Matter, Beijing 100871, China (Received 30 November 2016; revised manuscript received 13 January 2017, published 21 February 2017)

- Bulk: quantum phase transition in the O(3) UC in d = 2 + 1
- Unexpected boundary exponents



A renewed interest: quantum spin models



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(Received 3 May 2022; revised 15 November 2022; accepted 15 November 2022; published 2 December 2022)

A renewed interest: Conformal Field Theory



Reexamining the boundary O(N) universality class

PHYSICAL REVIEW LETTERS 126, 135701 (2021)

Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class

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Sci Post Select

SciPost Phys. 12, 131 (2022)

Boundary criticality of the O(N) model in d = 3 critically revisited

Max A. Metlitski

Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

PHYSICAL REVIEW LETTERS 128, 215701 (2022)

Boundary Criticality of the 3D O(N) Model: From Normal to Extraordinary

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1 Surface critical behavior of the 3D O(N) model

 \bigcirc O(N): from Normal to Extraordinary

3 Line defect

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The 3D O(N) universality class

• Simplest model of classical magnets Liquid-vapor, uniaxial ferromagnets (N = 1), superfluid ⁴He (N = 2), isotropic magnets (N = 3), chiral transition QCD (N = 4), ... Pelissetto. Vicari (2002)

- Numerous investigations: field-theory, high-T expansion, MC, ...
- Conformal Bootstrap in d = 3Rigorous results, very precise

CB with boundaries Recent developments

McAvity, Osborn (1995) Liendo, Rastelli, van Rees (2013) Gliozzi, Liendo, Menieri, Rago (2015) Billó, Gonçalves, Lauria, Menieri (2016) Padayasi, Krishnan, Metiltski, Gruzberg, Meineri (2022)





Bulk coupling K_{bulk} vs Surface coupling K_{surface}



- Surf. trans.: usual d = 2 phase transition
- Ordinary: new surf. exponent

$$egin{aligned} &\langle \phi(\mathbf{x})\phi(0)
angle \sim rac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}} \ &\Delta_{\hat{\phi}} = (1+\eta_{\parallel})/2 = & 1.2751(6) \ & ext{Hasenbusch (2011)} \end{aligned}$$

• Special: multicritical point, relevant surface exponent + $\eta_{||}$

• Extraordinary: ordered

Bulk coupling K_{bulk} vs Surface coupling K_{surface}



- Surface transition: Berezinskii-Kosterlitz-Thouless
- Ordinary transition

$$egin{aligned} &\langle \phi(\mathbf{x})\phi(0)
angle \sim rac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}}, \ &\Delta_{\hat{\phi}} = (1+\eta_{\parallel})/2 = & 1.2286(25) \ & {}_{ ext{FPT (2013)}} \end{aligned}$$

• Extraordinary: ordered? first/second order?

Deng, Blöte, Nightingale (2005)

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• Extraordinary: "extraordinary-log" phase

$$\langle ec{\phi}({f x}) \cdot ec{\phi}(0)
angle \sim rac{1}{(\log {f x})^q}$$

Metlitski (2020); Hu, Deng, Lv (2021)

Bulk coupling K_{bulk} vs Surface coupling K_{surface}



- No surface transition
- Ordinary transition

$$\begin{split} \langle \phi(\mathbf{x})\phi(\mathbf{0})\rangle &\sim \frac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}},\\ \Delta_{\hat{\phi}} &= (1+\eta_{\parallel})/2 = \underset{\scriptscriptstyle \mathsf{FPT (2013)}}{1.194(3)} \end{split}$$

• Surface transition shifted to $K_{surface} \rightarrow \infty$ Only the ordinary UC Krech (2000)

Bulk coupling K_{bulk} vs Surface coupling K_{surface}



- No surface transition
- Ordinary transition

$$egin{aligned} &\langle \phi(\mathbf{x})\phi(\mathbf{0})
angle \sim rac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}}, \ &\Delta_{\hat{\phi}} = (1+\eta_{\parallel})/2 = rac{1.194}{_{
m FPT\ (2013)}} \end{aligned}$$

• "KT-like" special transition at finite K_{surface}

Deng, Blöte, Nightingale (2005)

Bulk coupling K_{bulk} vs Surface coupling K_{surface}



- No surface transition
- Ordinary transition

$$\begin{split} \langle \phi(\mathbf{x})\phi(\mathbf{0})\rangle &\sim \frac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}},\\ \Delta_{\hat{\phi}} &= (1+\eta_{\parallel})/2 = \underset{\text{FPT (2013)}}{1.194(3)} \end{split}$$

• Special: standard transition, relevant surface exponent + $\eta_{||}$

 $\Delta_{\hat{s}} = 1.64(1) \ \Delta_{\hat{\phi}} = 0.2635(10)$

• Extraordinary-log phase Correlations: power of a log Logarithmic violation FSS

Model

• $\phi^4 N = 3$ lattice model, $L \times L \times L$ lattice, open b.c. z-direction

$$\begin{aligned} \mathcal{H} &= -\beta \sum_{\langle i \ j \rangle} \vec{\phi}_i \cdot \vec{\phi}_j - \beta_{s,\downarrow} \sum_{\langle i \ j \rangle_{s\downarrow}} \vec{\phi}_i \cdot \vec{\phi}_j \\ &- \beta_{s,\uparrow} \sum_{\langle i \ j \rangle_{s\uparrow}} \vec{\phi}_i \cdot \vec{\phi}_j + \sum_i \vec{\phi}_i^2 + \lambda (\vec{\phi}_i^2 - 1)^2 \end{aligned}$$

- Heisenberg UC; $\lambda = \lambda^* = 5.17(11)$ improved Hasenbusch (2020) \rightarrow leading bulk scaling corrections suppressed
- MC simulations at $\lambda = \lambda^*$, $\beta = \beta_c(\lambda^*)$, $\beta_{s,\downarrow} = \beta_{s,\uparrow} = \beta_s$
- Scan the surface observables on β_s

(Goal: surface transition?)

Surface Binder ratio $U_4 = \langle M_s^4 \rangle / \langle M_s^2 \rangle^2$



Surface Binder ratio $U_4 = \langle M_s^4 \rangle / \langle M_s^2 \rangle^2$



Special surface transition

• Finite-Size Scaling analysis of U₄

Hasenbusch (1999); FPT, PRE 84, 025703R (2011); Review: FPT, PRE 105, 034137 (2022)

$$U_4 = f((\beta_s - \beta_{s,c})L^{\gamma_{\rm sp}})$$

Special phase transition on the surface of a 3D Heisenberg UC

$$y_{\rm sp} = 0.36(1)$$
 $\Delta_{\hat{s}} = 2 - y_{\rm sp} = 1.64(1)$

$$\langle \vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(0)
angle_{\text{surf}} \sim \frac{1}{|\mathbf{x}|^{1+\eta_{\parallel}}} \quad \eta_{\parallel} = -0.473(2) \quad \Delta_{\hat{\phi}} = \frac{1+\eta_{\parallel}}{2} = 0.2635(10)$$

Quantum spin models with unexpected boundary η_{\parallel} : accidentally close to the special transition (?)

• $\beta_s > \beta_{s,c}$: extraordinary phase

1 Surface critical behavior of the 3D-O(N) model

 \bigcirc O(N): from Normal to Extraordinary

Line defect

Bulk coupling K_{bulk} vs Surface coupling K_{surface}



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angle \sim rac{1}{|\mathbf{x}|^{2\Delta_{\hat{\phi}}}} \ &\Delta_{\hat{\phi}} = (1+\eta_{\parallel})/2 = & 1.2751(6) \ & ext{Hasenbusch (2011)} \end{aligned}$$

• Special: multicritical point, relevant surface exponent + $\eta_{||}$

• Extraordinary: ordered

O(N) Normal Universality Class

- 3D O(N) model + surface field \vec{h} \rightarrow ordered surface
- Ising UC: binary critical mixture A + B $\phi \sim c_A - c_{A,c}$
- Adsorption preference on surfaces

Fluid Interface Tensions near Critical End Points

Michael E. Fisher and Paul J. Upton^(a)

PRL 65, 3405 (1990)

de-

scribes criticality of wall free energies at the so-called extraordinary surface transition^{1,7} (which, however, in the laboratory is more normal than the "ordinary" transition).





Hertlein, Helden, Gambassi, Dietrich, Bechinger (2008) From: Balibar, Nature News&Views (2008)

Critical adsorption

Adsorption layer governed by $\sim \xi$

$$m(z) = a|t|^{\beta} P_{\pm}(z/\xi), \ t = \frac{T - T_c}{T_c}$$

$$P_+(ilde{z}_+ o \infty) \sim e^{- ilde{z}_+}$$

$$P_{-}(ilde{z}_{-}
ightarrow\infty)-1\sim e^{- ilde{z}_{-}}$$

$$P_{\pm}(\tilde{z}_{\pm}
ightarrow 0) = c_{\pm}\tilde{z}^{-eta/
u}$$

MC: $c_{+} = 0.844(6)$ FPT, S. Dietrich, JSTAT P11003 (2010) FT: $c_{+} = 0.94(4)$ Flöter, Dietrich (1995) Exp.: $c_{+} = 1.60(42)$ $c_{+} = 0.77(19)$ $c_{+} = 1.14(29)$ $c_{+} = 0.91(26)$ $c_{+} = 1.05(9)$ $c_{+} = 1.02(10)$ $c_{+} = 1.25(9)$ $c_{+} = 0.84(15)$

>)9 5

Flöter, Dietrich (1995)

$$c_{+} = 0.787^{+0.00}_{-0.01}$$

Carpenter, Law, Smith (1999)



Carpenter, Law, Smith (1999) Review: Law, Prog. Surf. Sc. (2001)

Normal Universality Class: O(N > 1) model

- O(N)-symmetric bulk, at criticality
- Introduce a surface field \vec{h} \rightarrow ordered surface Broken $O(N) \rightarrow O(N-1)$ $\vec{\phi} = (\vec{\varphi}, \sigma) \qquad \vec{\varphi} \perp \vec{h} \qquad \sigma \parallel \vec{h}$
- Longitudinal vs transverse surface correlations

J. Phys. A: Math. Gen., Vol. 10, No. 11, 1977. Printed in Great Britain. @ 1977

Critical behaviour of semi-infinite systems

A J Bray and M A Moore Department of Theoretical Physics, The University, Manchester, M13 9PL, UK \vec{h}

X

 $egin{aligned} &\langle \sigma(\mathbf{x})\sigma(\mathbf{y})
angle_c \sim |\mathbf{x}-\mathbf{y}|^{-2d} \ &\langle ec{arphi}(\mathbf{x})ec{arphi}(\mathbf{y})
angle \sim |\mathbf{x}-\mathbf{y}|^{-(2d-2)} \end{aligned}$

Normal Universality Class: O(N > 1) model

- O(N)-symmetric bulk, at criticality
- Introduce a surface field \vec{h} \rightarrow ordered surface Broken $O(N) \rightarrow O(N-1)$ $\vec{\phi} = (\vec{\varphi}, \sigma) \qquad \vec{\varphi} \perp \vec{h} \qquad \sigma \parallel \vec{h}$
- Longitudinal vs transverse surface correlations



 \bar{h}

x

Boundary CFT for the Normal UC

• O(N) broken to O(N-1)

Boundary operators are representations of O(N-1)

• Spectrum of the CFT:

- Displacement operator D, $\Delta_D = d$. O(N 1)-scalar
- Tilt operator t^i , $\Delta_t = d 1 O(N 1)$ -vector

• On the boundary, $ec{\phi}=(ec{arphi},\sigma)$





Longitudinal/transverse correlation:
 D and tⁱ are the lowest operators

From Normal to Extraordinary

• Boundary Operator Product Expansion $z \rightarrow 0$

$$\sigma(\mathbf{x}, z) = \frac{a_{\sigma}}{(2z)^{\Delta_{\phi}}} + b_{\mathrm{D}}(2z)^{3-\Delta_{\phi}}\mathrm{D}(\mathbf{x}) + \dots$$
$$\varphi^{i}(\mathbf{x}, z) = b_{\mathrm{t}}(2z)^{2-\Delta_{\phi}}\mathrm{t}^{i}(\mathbf{x}) + \dots$$

• Universal parameter lpha Metlitski (2020)

$$\alpha \equiv \frac{\pi}{2} \left(\frac{a_{\sigma}}{4\pi b_{\rm t}} \right)^2 - \frac{N-2}{2\pi}$$

 \vec{h}

• When $\alpha > 0$: extraordinary-log phase $\langle \vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(0) \rangle \sim \frac{1}{(\log \mathbf{x})^q} \qquad q = \frac{N-1}{2\pi\alpha}$

 $lpha({\sf N}=2)>$ 0: extraordinary-log phase Hu, Deng, LV (2021)

- Large-N: α < 0: extraordinary-log phase survives for N < N_c
- ullet Generalized to plane defect: always lpha > 0 Krishnan. Metlitski (2023)

Extraordinary-log phase

Log-power two-point function

$$\langle \vec{\phi}(\mathbf{x}) \cdot \vec{\phi}(\mathbf{0}) \rangle \sim \frac{1}{(\log \mathbf{x})^q} \qquad q = \frac{N-1}{2\pi lpha}$$

• Logarithmic violation of FSS

 $U_4 - 1 \propto 1/(\ln L)^2$ $(\xi/L)^2 \simeq A + \alpha/2 \ln L$ $\Upsilon L \simeq A + 4\alpha/N \ln L$

 $U_4 = \langle M_s^4 \rangle / \langle M_s^2 \rangle^2$: Binder ratio ξ : finite-size correlation length Υ : helicity modulus (spin stiffness)

• On a standard fixed point: U_4 , ξ/L , $\Upsilon L \sim \text{const}$

Extraordinary phase MC N = 3, $\beta_s = 1.5$



From Normal to Extraordinary

• Boundary Operator Product Expansion $z \rightarrow 0$

$$\sigma(\mathbf{x}, z) = \frac{a_{\sigma}}{(2z)^{\Delta_{\phi}}} + b_{\mathrm{D}}(2z)^{3-\Delta_{\phi}}\mathrm{D}(\mathbf{x}) + \dots$$
$$\varphi^{i}(\mathbf{x}, z) = b_{\mathrm{t}}(2z)^{2-\Delta_{\phi}}\mathrm{t}^{i}(\mathbf{x}) + \dots$$

• Universal parameter lpha Metlitski (2020)

$$\alpha \equiv \frac{\pi}{2} \left(\frac{a_{\sigma}}{4\pi b_{\rm t}} \right)^2 - \frac{N-2}{2\pi}$$

When $\alpha > 0$: extraordinary-log phase $N < N_c$, $N_c \ge 2$

(Goal: determine a_{σ} , b_t for N = 2, 3)

MC simulations: normal UC

• ϕ^4 N-components lattice model, $L \times L \times L$ lattice, open b.c. z-dir.

$$\mathcal{H} = -\beta \sum_{\langle i , j \rangle} \vec{\phi}_i \cdot \vec{\phi}_j + \sum_i [\vec{\phi}_i^2 + \lambda (\vec{\phi}_i^2 - 1)^2] \\ -\beta_s \sum_{\langle i , j \rangle_s} \vec{\phi}_i \cdot \vec{\phi}_j - \vec{h}_s \cdot \sum_{i \in s} \vec{\phi}_i$$

• O(N) UC: $\lambda = \lambda^*$ improved

 \rightarrow leading *bulk* scaling corrections suppressed

• MC simulations at $\lambda = \lambda^*$, $\beta = \beta_c(\lambda^*)$, $\beta_{s,\downarrow} = \beta_{s,\uparrow} = \beta$, $h_s > 0$.

Lattice to CFT

• Expand lattice observables in terms of CFT fields

Bulk: $\phi_{lat}^{i} \propto \phi^{i} + \dots$ Surface: $\sigma_{lat} \propto \sigma + \dots$, $\varphi_{lat}^{i}(x) \propto t^{i} + \dots$

Lattice to CFT

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Bulk: $\phi_{lat}^{i} \propto \phi^{i} + \dots$ Surface: $\sigma_{lat} \propto \sigma + \dots$, $\varphi_{lat}^{i}(x) \propto t^{i} + \dots$

• Fits of MC two-point functions \rightarrow fix normalization

 $\langle \phi^{i}(0)\phi^{j}(x)\rangle = \delta^{ij}|x|^{-2\Delta_{\phi}} \qquad \langle t^{i}(0)t^{j}(x)\rangle = \delta^{ij}|x|^{-4}$

Lattice to CFT

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 $\bullet\,$ Fits of MC two-point functions $\to\,$ fix normalization

 $\langle \phi^i(0)\phi^j(x)\rangle = \delta^{ij}|x|^{-2\Delta_{\phi}} \qquad \langle t^i(0)t^j(x)\rangle = \delta^{ij}|x|^{-4}$

• From the Boundary OPE

$$\langle \sigma(z) \rangle \simeq \frac{a_{\sigma}}{(2(z+z_0))^{\Delta_{\phi}}} \left[1 + B\left(\frac{z+z_0}{L}\right)^3 \right]$$
$$\vec{\varphi}(0,z)\vec{\varphi}(0,0) \rangle \simeq \frac{16(N-1)b_{\mathbf{t}}}{(2(z+z_0))^{2+\Delta_{\phi}}} \left[1 + B_{\varphi}\left(\frac{z+z_0}{L}\right)^3 + C(z+z_0)^{-2} \right]$$

• Fits of MC data \rightarrow universal BOPE a_{σ} , $b_{\rm t}$

Comparison with Conformal Bootstrap



TCB = Truncated Conformal Bootstrap

Padayasi, Krishnan, Metlitski, Gruzberg, Meineri, SciPost (2022)

Summary O(N) Normal UC

Normal expl. symmetry-breaking a_{σ}, b_t BOPE Extraordinary-log no symmetry-breaking Log. behavior $\alpha(a_{\sigma}, b_t)$

Summary O(N) Normal UC

Normal expl. symmetry-breaking a_{σ}, b_t BOPE Extraordinary-log no symmetry-breaking Log. behavior $\alpha(a_{\sigma}, b_t)$

Ν	MCnormal	MC _{extraordinary}	Truncated CB ^a
2	0.300(5)	0.27(2) ^b	0.3567
3	0.190(4)	0.15(2)*	0.2236

^aPadayasi, Krishnan, Metlitski, Gruzberg, Meineri (2022)

b_{Hu, Deng, Lv} (2021)

D Surface critical behavior of the 3D-O(N) model

2 O(N): from Normal to Extraordinary

3 Line defect

Other boundaries: line defect

• Line defects in critical models

Hanke (2000); Vasilyev, Eisenriegler, Dietrich (2013); Eisenriegler, Burkhardt (2016); Cuomo, Komargodski, Mezei (2022); Cuomo, Komargodski, Mezei, Raviv-Moshe (2022); Gimenez-Grau, Lauria, Liendo, van Vliet (2022); Gimenez-Grau (2022); Giombi, Helfenberger, Khanchandani (2022); Pannell, Stergiou (2023); Bianchi, Bonomi, de Sabbata (2023); Aharony, Cuomo, Komargodski, Mezei, Raviv-Moshe (2023)

 O(N) model, symmetry-breaking field on line defect

 N = 1: critical adsorption on elongated colloids FPT, Assaad, Wessel, 2017



Pinning-field approach

- Local ordering field, coupled to the order parameter Assaad, Herbut, 2013
- Symmetry-breaking: order parameter ≠ 0 in finite V Enhanced numerical stability
- Extrapolate the order parameter $V
 ightarrow \infty$



Correlations along the defect

VOLUME 84, NUMBER 10

PHYSICAL REVIEW LETTERS

6 March 2000

Critical Adsorption on Defects in Ising Magnets and Binary Alloys

Andreas Hanke*

For N = 1 (Ising), via an "interpolation" of ε -expansion

$$\langle \phi(x)\phi(y)\rangle_c \sim |x-y|^{-2\Delta_\sigma}, \qquad \Delta_\sigma \simeq 1.385(25)$$

Lattice model N = 1

Classical Blume-Capel model

$$\mathcal{H} = -K \sum_{\langle i , j \rangle} S_i S_j + D \sum_i S_i^2 - h_0 \sum_{i \in line} S_i$$
$$S_i = -1, 0, 1$$

• Continuous phase transition in Ising UC

• Suppressed scaling corrections at D = 0.655(20) Hasenbusch, 2010 \Rightarrow improved model

Goal: determine Δ_{σ}

Monte Carlo determination of Δ_{σ}

• We simulate an improved model in the Ising UC

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} S_i S_j + D \sum_i S_i^2 - h_0 \sum_{i \in line} S_i, \qquad S_i = -1, 0, 1$$

We take $h_0 = \infty \rightarrow$ fixed spins

Finite-Size Scaling analysis of local magnetization and susceptibility

Δ_{σ}	Method
1.52(6)	MC
1.385(25)	FT Hanke (2000)
1.55(14)	arepsilon - arepsilon Xp. Cuomo, Komargodski, Mezei (2022)
1.542	Large—N Cuomo, Komargodski, Mezei (2022)

 A renewed interest in boundary critical phenomena Advances in boundary conformal field theory Boundary exponents, universal Boundary OPE coefficients

 Reexamination of the classical 3D O(N) surface critical behavior New extraordinary-log UC ↔ Normal UC

Summary & Outlook

• Many other geometries are of current interest:

- Line defects
- Plane defects Krishnan, Metlitski (2023); Giombi, Liu (2023)
- Anisotropies on the boundary Diehl, Eisenriegler (1984); Trépanier (2023)

Quantum critical models

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 FPT, M. Metlitski, Phys. Rev. Lett. 128, 215701 (2022)
- Line defect (a.k.a. pinning field)
 FPT, F. F. Assaad, S. Wessel, Phys. Rev. B 95, 014401 (2017)

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Thank you!