Engineering Surface Critical Behavior of Quantum Critical Points

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# Outline

• Brief review of classical surface criticality

• Surface criticality of Quantum Critical points

 $\diamond$  Ordinary transition

♦ Special transition

 $\diamond$  Extraordinary transition

Conclusions

#### Classical surface critical behavior: schematic phase diagram

• 3D Ising as an example

 $\diamond i, j$ 

 When J<sub>s</sub> ∼ J, the surface remains disordered at T<sub>c</sub>, due to less coordination. The surface singularities are induced by the bulk criticality, ordinary

 $J_{c}^{*}/J$ 

 $J_{c}/J$ 

- If J<sub>s</sub>/J ≫ 1, the surface undergoes a 2D phase transition at a T<sub>cs</sub> > T<sub>c</sub>. At T<sub>c</sub>, the surface exhibits extra singularities, called extraordinary transition
- The surface  $T_{cs}$  and  $T_c$  merge at a fine-tuned surface coupling strength  $J_s^*$ , where both the 2D surface and 3D bulk are critical: multicritical special transition

#### Finite-size scaling

Total free energy

$$F = f_b V + f_1 A$$

$$f_b(t,h,\frac{1}{L}) = L^{-d} f_{bs}(tL^{y_t},hL^{y_h},1) + f_{ba}(t,h)$$

$$f_1(t,h,t_1,h_1,\frac{1}{L}) = L^{-(d-1)} f_{1s}(tL^{y_t},hL^{y_h},t_1L^{y_{t1}},h_1L^{y_{h1}},1) + f_{1a}(t,h,t_1,h_1)$$

with  $t_1 \sim J_s - J_s^*$ ,  $h_1$  the surface scaling fields

• surface susceptibility 
$$\chi_1 = \frac{\partial^2 f_1}{\partial h_1^2} = L^{d-1} m_1^2 / T$$

$$\chi_1(L) = L^{-2y_{h1}-d+1} f(tL^{y_t}, t_1L^{y_{t1}}, L^{y_i}) + \chi_{1a}$$

• ordinary at given 
$$J_s < J_s^*$$
:  $\chi_1 = c + bL^{2y_{h1}^{(o)} - d + 1}$   
with  $y_{t1}^{(o)} = -1$  irrelevant; Burkhardt and Cardy, 1987  
 $y_{h1}^{(o)} = 0.7249(6)$  Hasenbush, 2011

• special, scan  $J_s \sim J_s^*$ :  $\chi_1 = L^{2y_{h1}^{(s)} - d + 1}(a_0 + a_1(J_s - J_s^*)L_{r1}^{y_{r1}^{(s)}})$ with  $y_{r1}^{(s)} = 0.718(2)$  relevant;  $y_{h1}^{(s)} = 1.6465(6)$ Hasenbusch, 2012



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Deng, Blöte, Nightingale; PRE 2005

correlation functions

$$C_{\parallel}(r) = \langle S_{1,1,1} \cdot S_{1+r,1+r,1} \rangle$$
$$C_{\perp}(r) = \langle S_{1,1,1} \cdot S_{1,1,r+1} \rangle$$

We expect

$$C_{\parallel}(L/2) \propto rac{1}{L^{-(d-2+\eta_{\parallel})}}$$
  
 $C_{\perp}(L/2) \propto rac{1}{L^{-(d-2+\eta_{\perp})}}$ 

- Scaling relations
  - ► The scaling dimension of surface magnetization  $\Delta_s = (d 2 + \eta_{\parallel})/2$  satisfies  $\Delta_s + y_{h1} = d 1$ , therefore

$$\eta_{\parallel} = d - 2y_{h1}$$

Consider d − 2 + η<sub>⊥</sub> = Δ<sub>s</sub> + Δ<sub>b</sub>, and Δ<sub>b</sub> = (d − 2 + η)/2 is the scaling dimension of bulk magnetization, therefore

$$2\eta_{\perp}=\eta_{\parallel}+\eta$$

Quantum critical point and its surface critical behavior

- Surface critical behavior also sets in at quantum critical points
- We study the SCB of the dimerized spin-1/2 AFM Heisenberg models on the square lattice
- We realize all three types of SCB of 3D O(3) universality class by engineering the surface configurations, instead of adapting surface couplings as in the classical models

This is somehow a surprise: For 3D classical  $O(n \ge 3)$  model: the 2D surface has no symmetry breaking phase at finite temperature, thus no extraordinary or special transition

# dimerized spin-1/2 Heisenberg models

$$H = J \sum S_i \cdot S_j + J' \sum S_i \cdot S_j$$





adapting g = J'/J, from Néel ordered phase to the gapped dimerized phase

- 3D O(3) universality class
- Columnar model:  $(J'/J)_c = 1.9096(4)$
- Staggered model: (J'/J)<sub>c</sub> = 2.5196(2) debate on universality class resolved recently Fritz, Doretto, Wessel, Wenzel, Burdin and Vojta, PRB 2011 Ma, Weinberg, Shao, WG, Yao and Sandvik, PRL 2018
- two types of open boundaries: cut-1 and cut-2 realize three types of SCB of 3D O(3) universality class instead of adapting surface couplings as in the classical models

### Methods

- · Projective quantum Monte Carlo algorithm with valence bond basis
- Observables and scaling (D = d + z = 3: spacetime dimension)

$$\chi_1(L) \to m_{s1}^2(L)L = c + bL^{2y_{h1}-D}$$
, (special:  $c = 0, y_{h1}^{(s)}$ )

- $m_{s1}$ : staggered magnetization of the surface spins
- $y_{h1}$  is the scaling dimension of the surface staggered magnetic field  $h_1$
- c encodes the short-range nonuniversal contribution

$$|C_{\parallel}(L/2)| \sim L^{-1-\eta_{\parallel}}$$
$$|C_{\perp}(L/2)| \sim L^{-1-\eta_{\perp}}$$

- $\eta_{\parallel}$  and  $\eta_{\perp}$  are the surface anomalous dimensions
- Scaling relations

$$\eta_{\parallel} = D - 2y_{h1}, \quad 2\eta_{\perp} = \eta_{\parallel} + \eta$$

•  $\eta$  is the bulk anomalous dimension

### Cut-1 leads to Ordinary transition



The surface cut-1 in both models do not break any strong bonds

- The surface states remain gapped in the bulk disordered phases.
- The power-law correlation on the surface at the QCP is purely induced by the critical bulk states.
  - Columnar model  $\eta_{\parallel}^{(o)} = 1.387(4), \eta_{\perp}^{(o)} = 0.67(6), y_{h1}^{(o)} = 0.840(17)$ (consistent result obtained independently by Weber, Toldin and Wessel, PRB 2018)
  - ► Staggered model  $\eta_{\parallel}^{(o)} = 1.340(21), \eta_{\perp}^{(o)} = 0.682(2), y_{h1}^{(o)} = 0.830(11)$
  - Match ordinary transition of the 3D O(3) class: 3D classical model, 4-ε, 2+ε support the results of Ma et al PRL 2018
- Obey the scaling relations

### Cut-2 in the columnar model leads to Special transition



cut-2 breaks the strong bonds and leaves dangling bonds on the surface

These dangling bonds form a spin-1/2 AF Heisenberg chain

• power-law decay of  $C_{\parallel}$  and  $C_{\perp}$  with different exponents

we see power-law decay of 
$$m_{s1}^2$$
  
 $m_{s1}^2 L \sim L^{2y_{h1}^{(s)}-D}$ ,

$$|C_{\parallel}(L/2)| \sim L^{-1-\eta_{\parallel}^{(s)}}$$

$$|C_{\perp}(L/2)| \sim L^{-1-\eta_{\perp}^{(s)}}$$

• 
$$y_{h1}^{(s)} = 1.7339(12), \eta_{\parallel}^{(s)} = -0.445(15), \eta_{\perp}^{(s)} = -0.218(8)$$

# Special transition, cut-2 in the columnar model



- ► match 4 
  e calculation of classical models
- match the results of QCP from AKLT to Néel, Heisenberg model on the decorated square lattice
  - attributed to the gapless surface state of the SPT phase

#### Zhang and Wang, PRL 2017



Scaling relations satisfied

# Special transition, cut-2 in the columnar model



- The special transition was never anticipated in the 3D classical O(3) model: 2D surface cannot posses LRO or power-law corr. at finite T.
- Pure quantum origin: top  $\theta$  term of the S-1/2 AF H chain suppresses the topological defects and leads to a critical state at the ground state.

Similar to the AKLT-Neel QCP of the decorated square lattice model

Sp.	Column, cut-2	1.7339(12)	-0.445(15)	-0.218(8)		
	Deco.sq., J <sub>c2</sub>	1.7276(14)	-0.449(5)	-0.2090(15)		
	$\epsilon = 4 - d \exp$ .	1.723	-0.445	-0.212	Diehl and Dietrich, PLA, 19	980

This SCB class is a general consequence of the coexistence of the critical states both in the surface and the bulk

See also an independent work by Weber, Toldin and Wessel, PRB 2018

 Robustness of the critical surface states leaves the special transitions less fine tuned, compared with SCB in the 3D Ising model.

# Cut-2 in the staggered model leads to Extraordinary transition



#### *m*<sub>s1</sub>, *m*<sub>1</sub> extrapolate to nonzero values as *L* → ∞, both in the disordered phase and at the QCP, revealing the FI order on the surface

- ▶ In the bulk dimerized phase, extensive degeneracy of the dangling bonds is lifted by their effective FM coupling → FM order on this sublattice
- The AFM coupling to the other sublattice induces a weaker antiparallel magnetization on the other sublattice

# Cut-2 in the staggered model leads to Extraordinary transition



- $C_{\parallel}$  at QCP saturates with a power law:  $\eta_{\parallel}^{(e)} = 1.004(13)$ 
  - distinct from the FI spin chains where spin corr. drop exponentially.
  - It is induced by the bulk critical state; captures the surface singularity at the extr. transition
- $C_{\perp}$  at QCP follows a pure power-law decay:  $\eta_{\perp}^{(e)} = -0.5050(10)$ .
- Violate the scaling relation  $2\eta_{\perp} = \eta_{\parallel} + \eta_{\parallel}$ 
  - the general understand of extraordinary transition based on scaling theory is incomplete.

#### Conclusions

- We have studied the surface critical behavior of two dimerized Heisenberg models at their bulk critical points.
- We show that all three types of SCB are realized with certain surface configurations
  - · Gapped surface states in the bulk disordered phase lead to ordinary transition
  - Gapless surface states in the bulk disordered phase result into multicritical special transition even precluded in the classical models
  - We find a ferrimagnetic order on the surface cut-2 of the staggered model, which leads to an extraordinary transition, with surface anomalous dimensions violating the scaling relation

# Thank you for your attention