NCTS Workshop on Quantum Condensation (QC13)
2013/08/29

Symmetry-protected topological phases and gapped vector-spin-chirality phases in a dimerized spin-1/2 XXZ zigzag chain

RIKEN

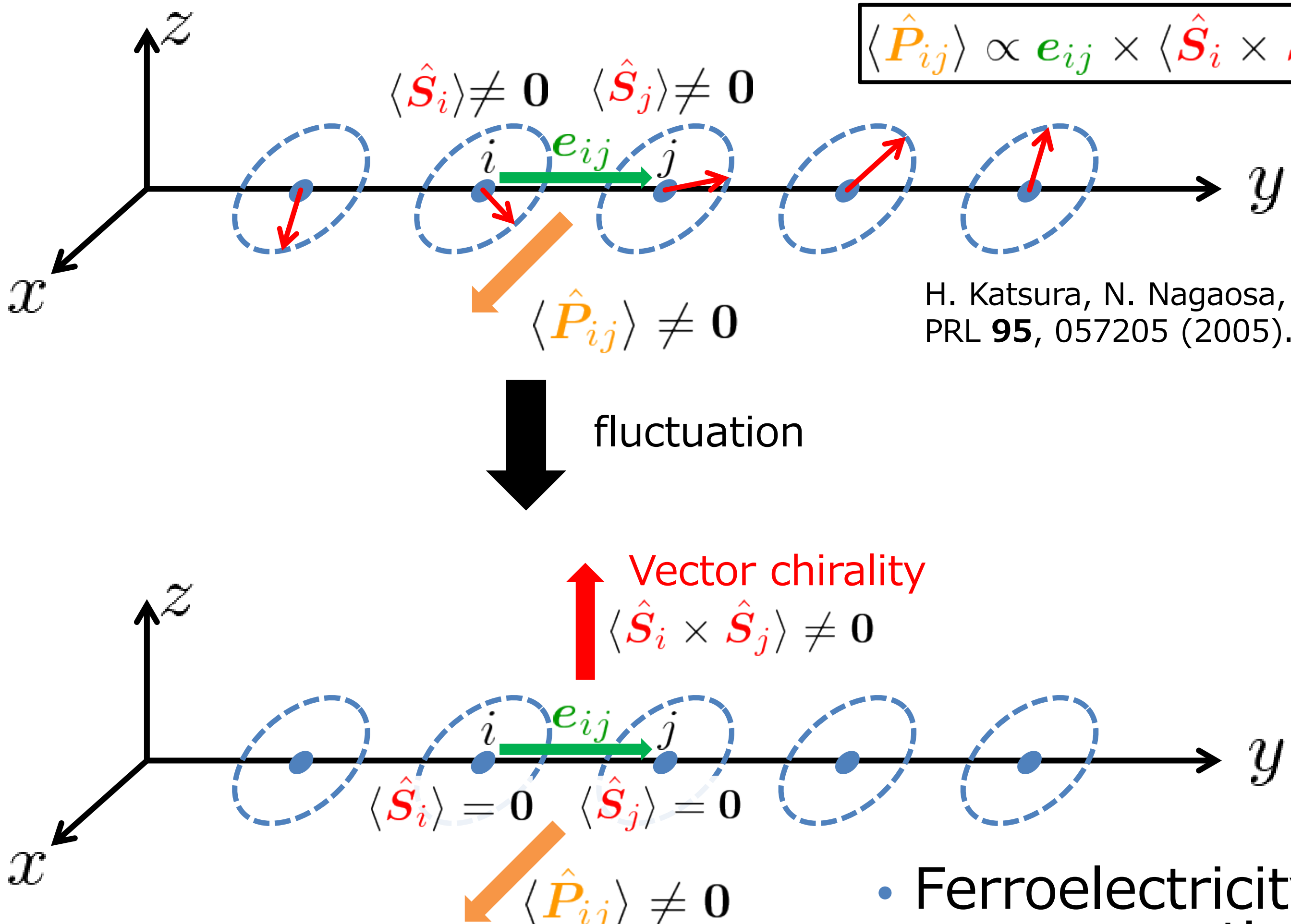
Hiroshi Ueda

Collaborator: Shigeki Onoda (RIKEN)

H.U. and S.O., arXiv:1308.5747

Introduction: Spiral magnet and ferroelectricity

$$\boxed{\langle \hat{\boldsymbol{P}}_{ij} \rangle \propto \boldsymbol{e}_{ij} \times \langle \hat{\boldsymbol{S}}_i \times \hat{\boldsymbol{S}}_j \rangle}$$

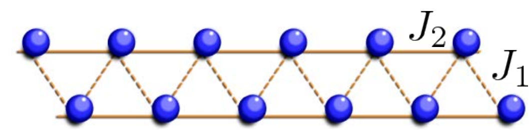


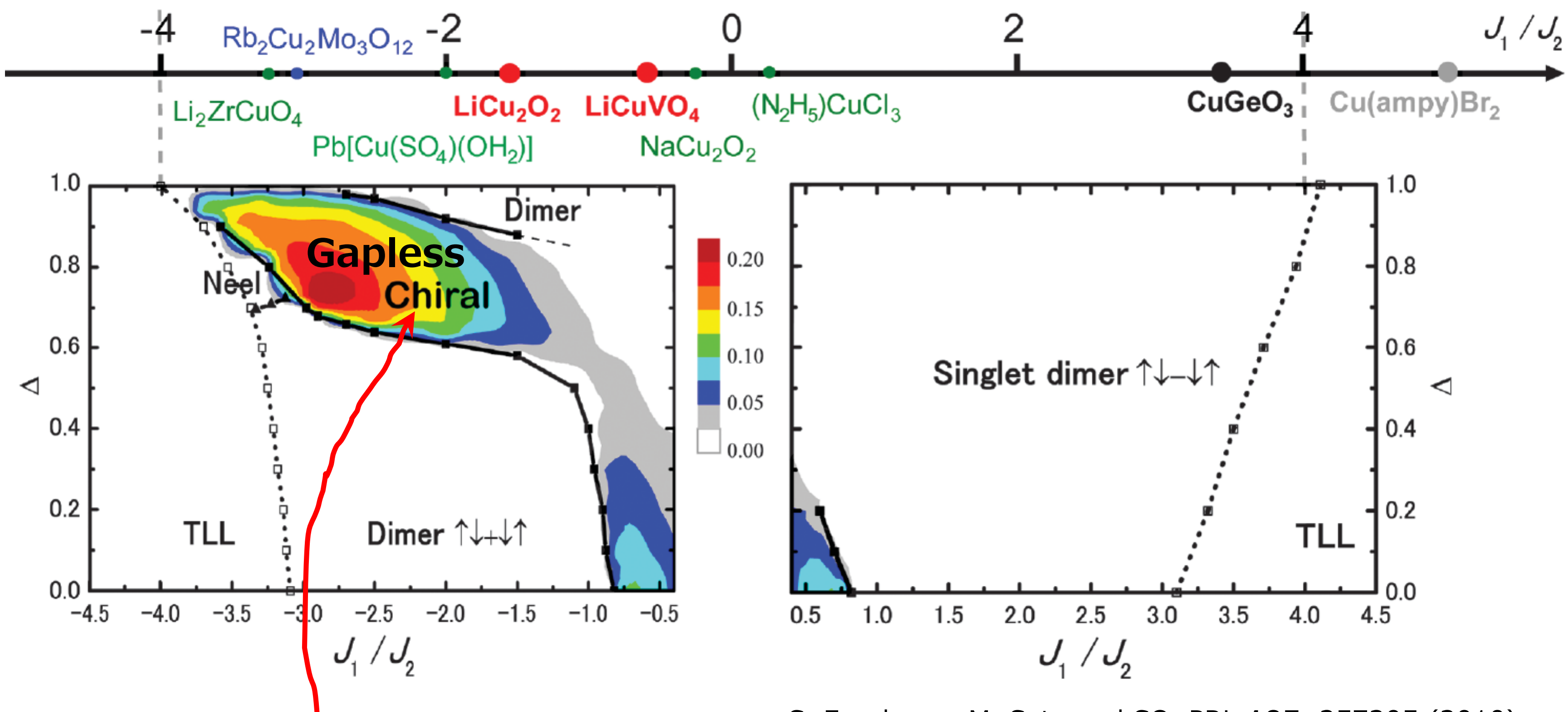
H. Katsura, N. Nagaosa, and A. V. Balastky, PRL **95**, 057205 (2005).

- Ferroelectricity without any magnetic spiral long-range order (LRO)

Vector-chiral (VC) order in quasi 1D system

$$\hat{\mathcal{H}}_{\mathrm{xxz}} = \sum_{\ell=1,2} J_\ell \sum_j \Big[\sum_{\mu=x,y} \hat{S}^\mu_j \hat{S}^\mu_{j+\ell} + \Delta \hat{S}^z_j \hat{S}^z_{j+\ell} \Big]$$





$$\langle \hat{\kappa}^z_{j+1/2} \rangle = \langle (\hat{\boldsymbol{S}}_j \times \hat{\boldsymbol{S}}_{j+1})^z \rangle \neq 0$$

S. Furukawa, M. Sato and SO, PRL **105**, 257205 (2010).

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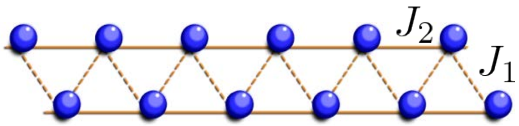

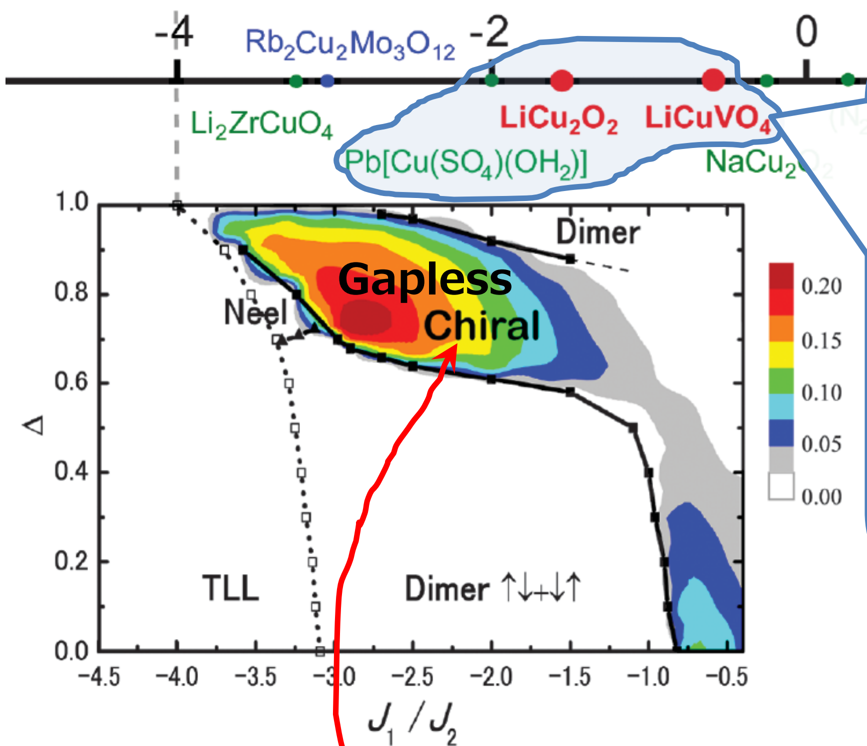

✓ Emergence of a spiral spin long range order (LRO)

Spin excitation gap is required for VC LRO w/o spiral spin LRO.

$$\langle \hat{\kappa}^z_{j+1/2} \rangle = \langle (\hat{\boldsymbol{S}}_j \times \hat{\boldsymbol{S}}_{j+1})^z \rangle \neq 0$$

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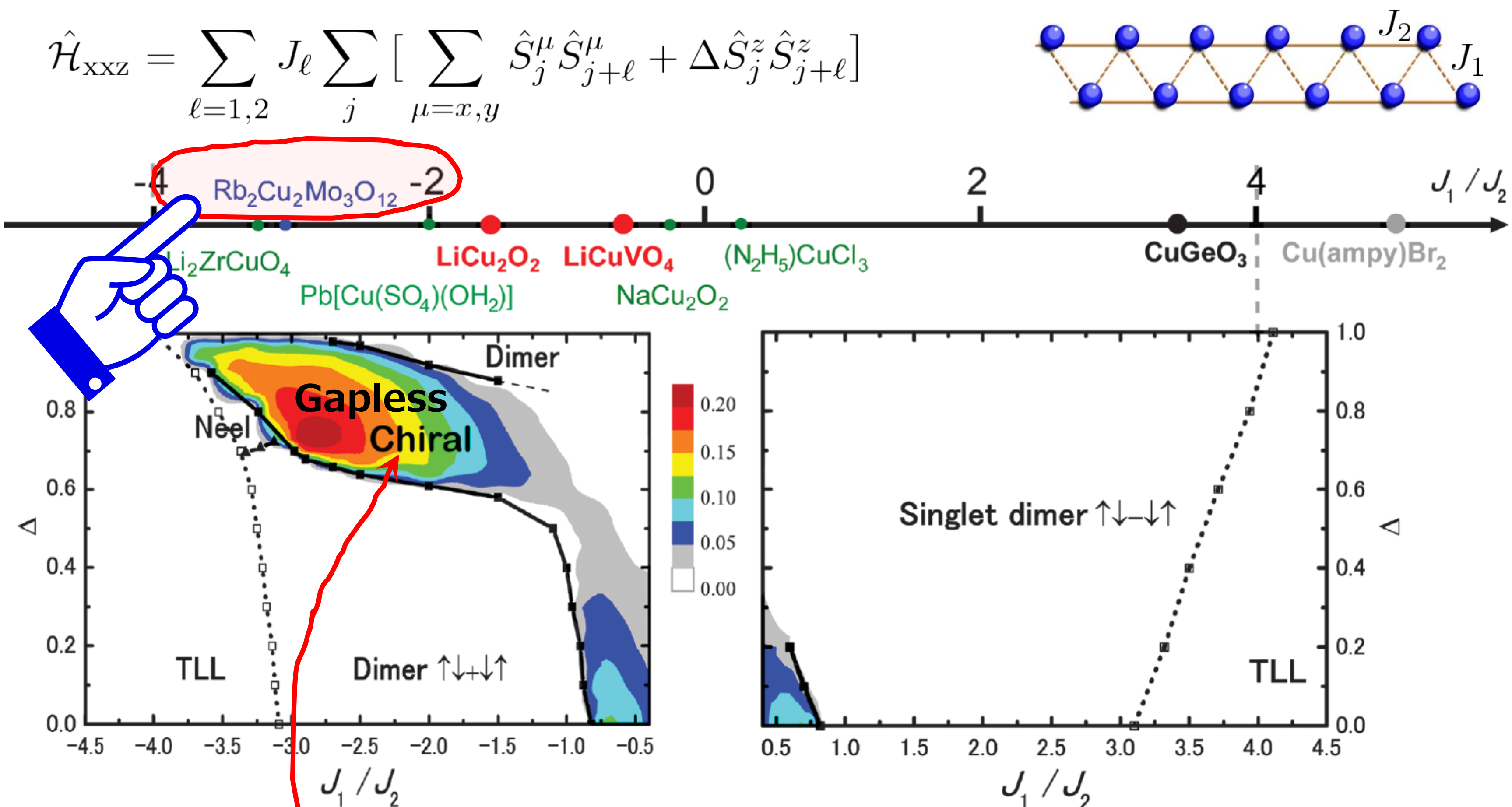

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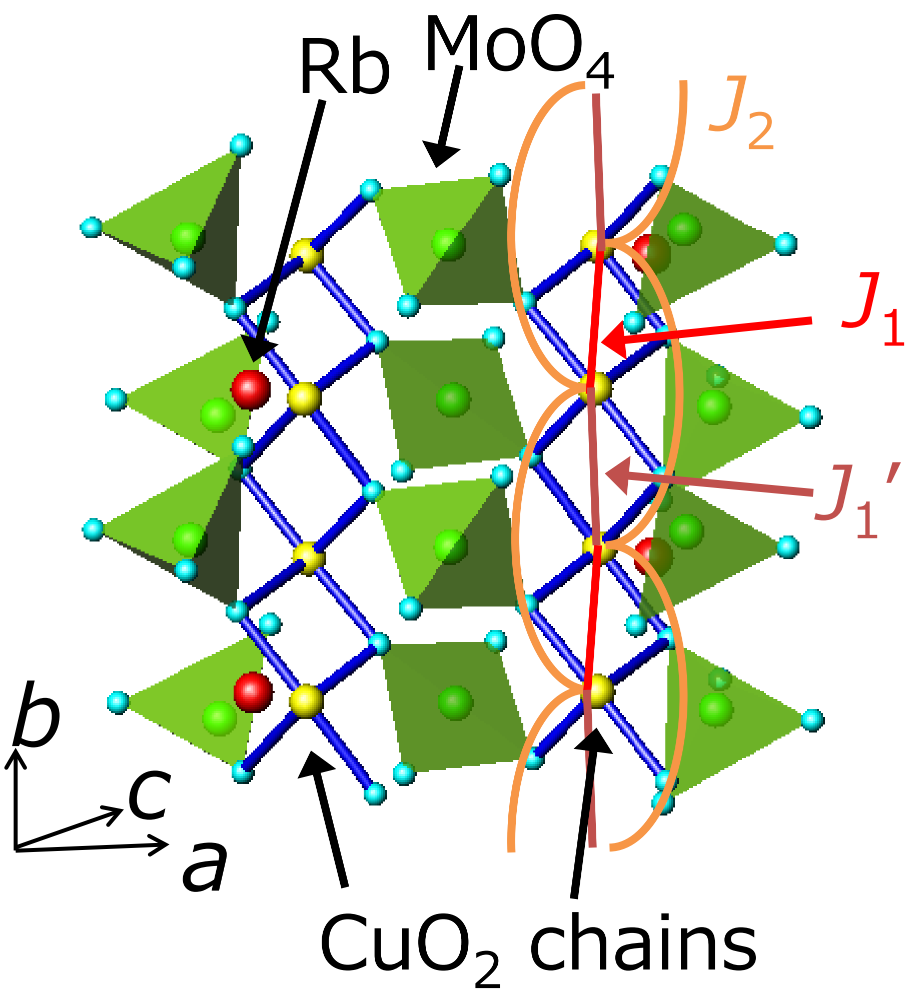
Field-induced ferroelectric system $Rb_2Cu_2Mo_3O_{12}$



By courtesy of Yanagisawa *et al*.

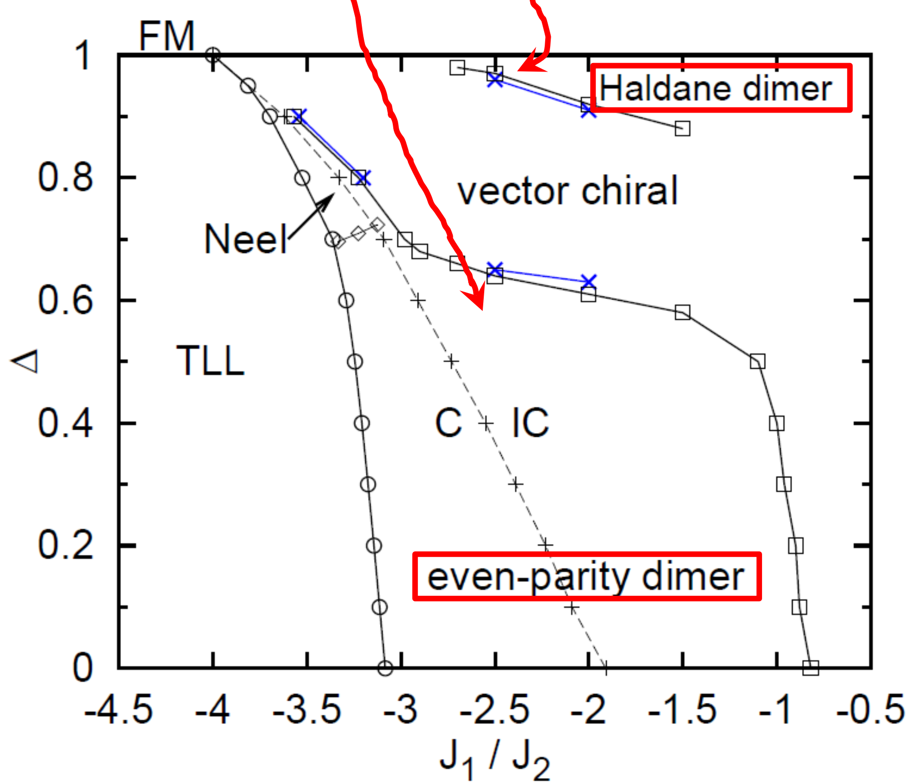
- Buckling of CuO_2 plane
  ➔ bond alternation
  Solodovnikov et al. (1997)

- $J_1/J_2 \sim -2.7$ (J_1 = -138K, J_2 = 51K)
  $$\mathcal{H} = \sum_{\ell=1,2} J_\ell \sum_j \hat{\boldsymbol{S}}_j \cdot \hat{\boldsymbol{S}}_{j+\ell}$$
- No magnetic order (T>2K)
  Hase et al. (2004)

- Field-induced ferroelectricity (T<8K)
  ➔ possible VC LRO w/o spin spiral
  Yasui et al. (2013)

Field-induced ferroelectric system $Rb_2Cu_2Mo_3O_{12}$

Two candidate ground states:



S. Furukawa, M. Sato, SO, and A. Furusaki, PRB **86**, 094417 (2012).

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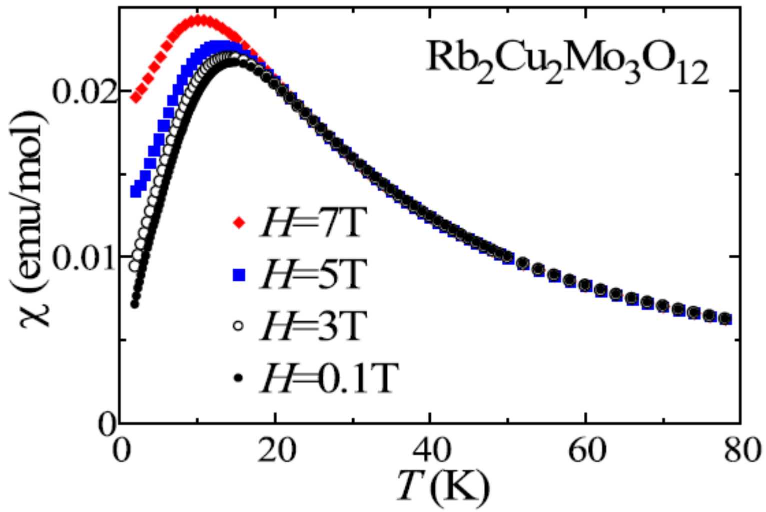

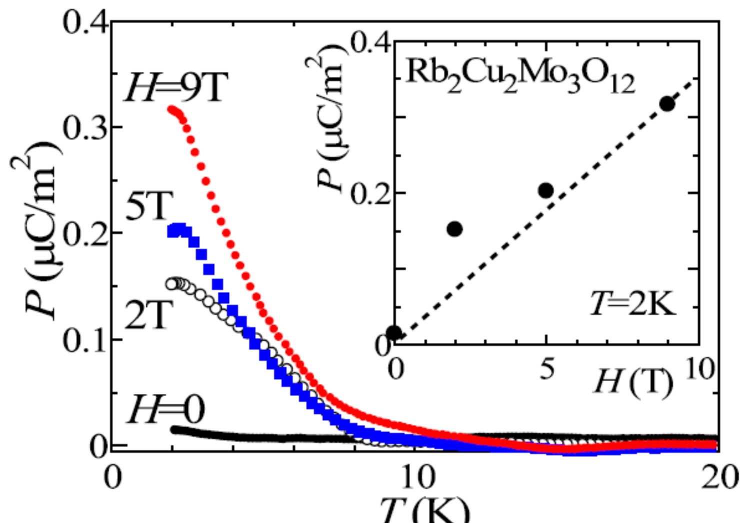

Y. Yasui *et al.*, J. Appl. Phys. **113**, 17D910 (2013).

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Main goals

✓Theoretical

- ✓ Propose a model which has gapped VC phases w/o any spiral spin LRO over a wide region of its parameter space.
  Key: Bond alternation
- ✓ Understand the model under low-magnetic field.
  Key: Staggered scalar chirality
- ✓ Understand symmetry-protected topological (SPT) phases.
  Key: Neel LRO

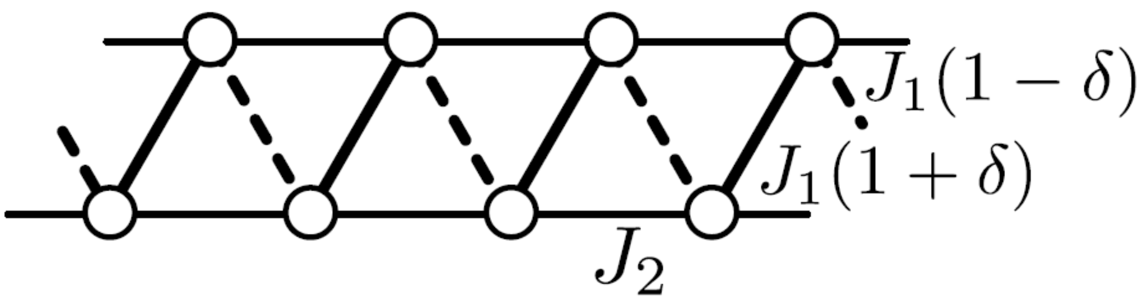
✓Experimental

- ✓ Find a new type of ferroelectric transition
  - ✓ $Rb_2Cu_2Mo_3O_{12}$: Weak bond alternation
  - ✓ spin gap: ~ 0.2 meV ⇔ ~2 T
  - ✓ Ferroelectric transition at H ~0.1 T

Zero Field Case

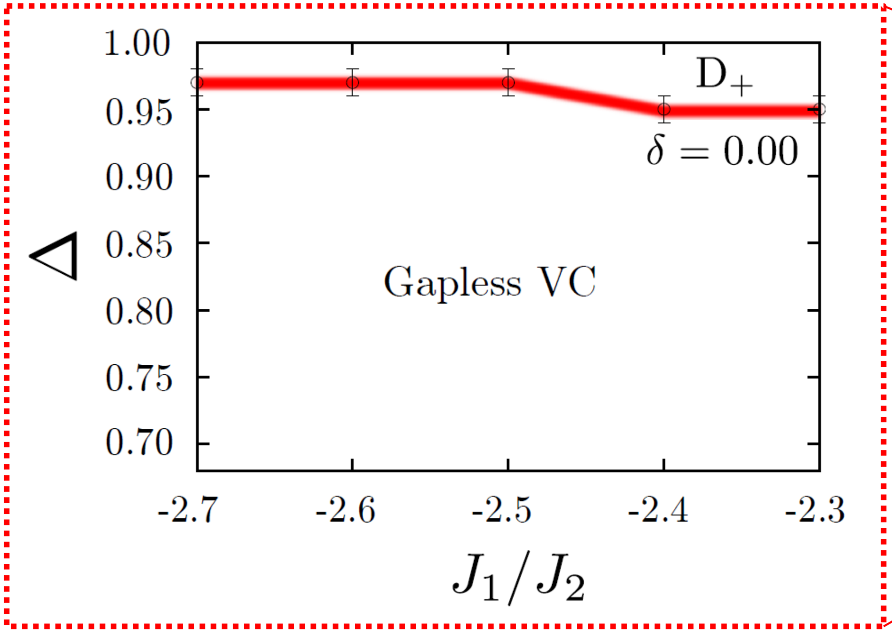
$$\hat{\mathcal{H}}_{\delta\mathrm{xxz}} = J_1 \sum_j (1-(-1)^j\delta)\left[\sum_{\mu=x,y} \hat{S}_j^\mu \hat{S}_{j+1}^\mu + \Delta \hat{S}_j^z \hat{S}_{j+1}^z\right] + J_2 \sum_j \left[\sum_{\mu=x,y} \hat{S}_j^\mu \hat{S}_{j+2}^\mu + \Delta \hat{S}_j^z \hat{S}_{j+2}^z\right]$$

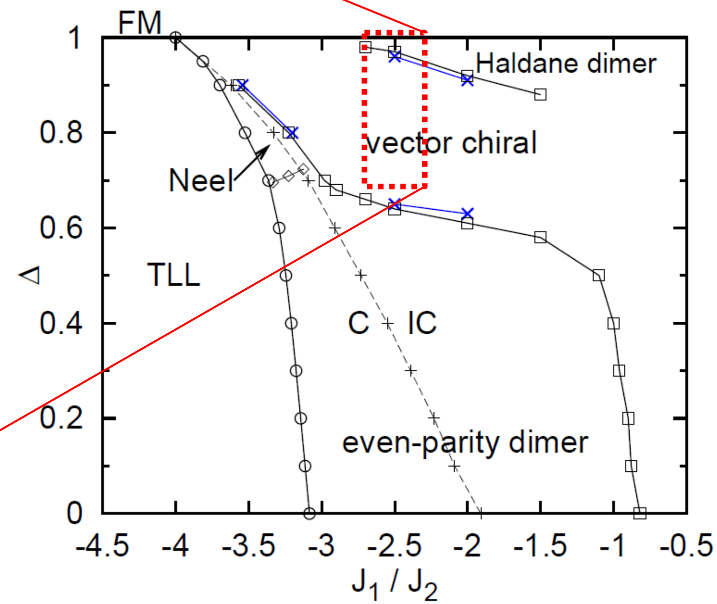
$$(\, J_1 < 0 \,, \quad \delta \geq 0 \,, \quad 0 \leq \Delta \leq 1 \,)$$



Phase diagrams (δ=0)

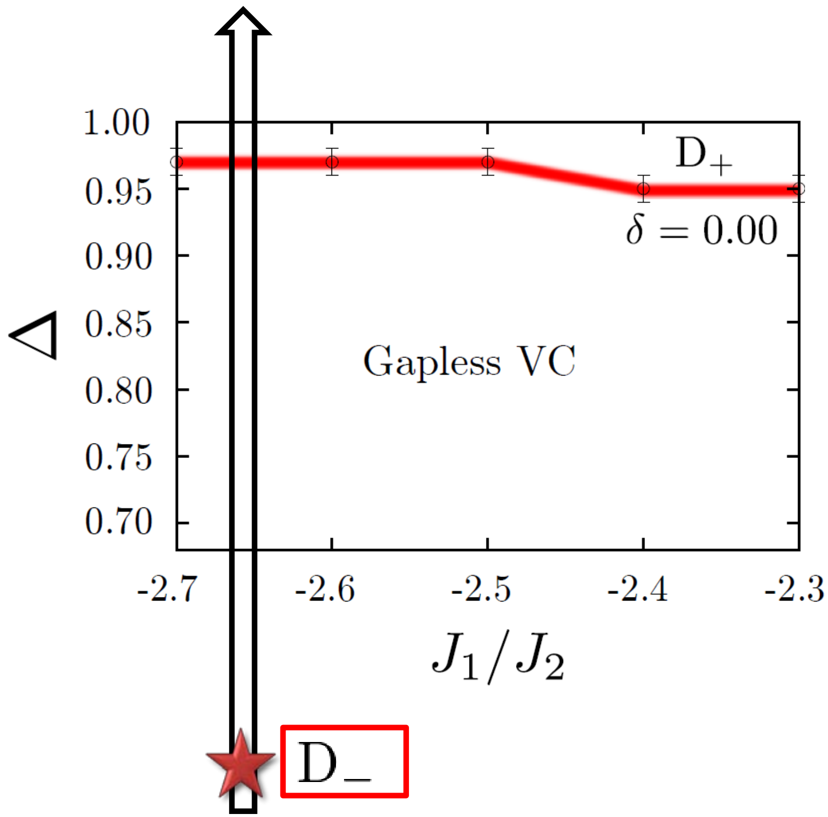
- Numerical Detail
  - DMRG (White, 1993)
  - # of kept state *m* up to 500
  - # of spin *N* up to 320





S. Furukawa, M. Sato, SO, and A. Furusaki, PRB **86**, 094417 (2012).

Phase diagrams (δ=0)



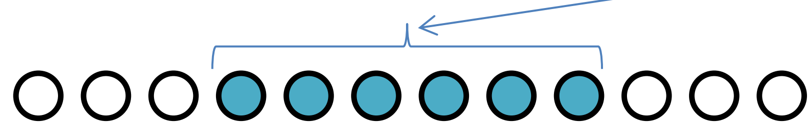
✓Even-parity dimer (D_-) phase

Dimer LRO: Gapped phase

$$\hat{D}_j^\mu = (-1)^j\left(\hat{S}_{j-1}^\mu \hat{S}_j^\mu - \hat{S}_j^\mu \hat{S}_{j+1}^\mu\right),$$

$$\left(\mathrm{Ave}_j\langle \hat{D}_j^x\rangle\right)\left(\mathrm{Ave}_j\langle \hat{D}_j^z\rangle\right) < 0,$$

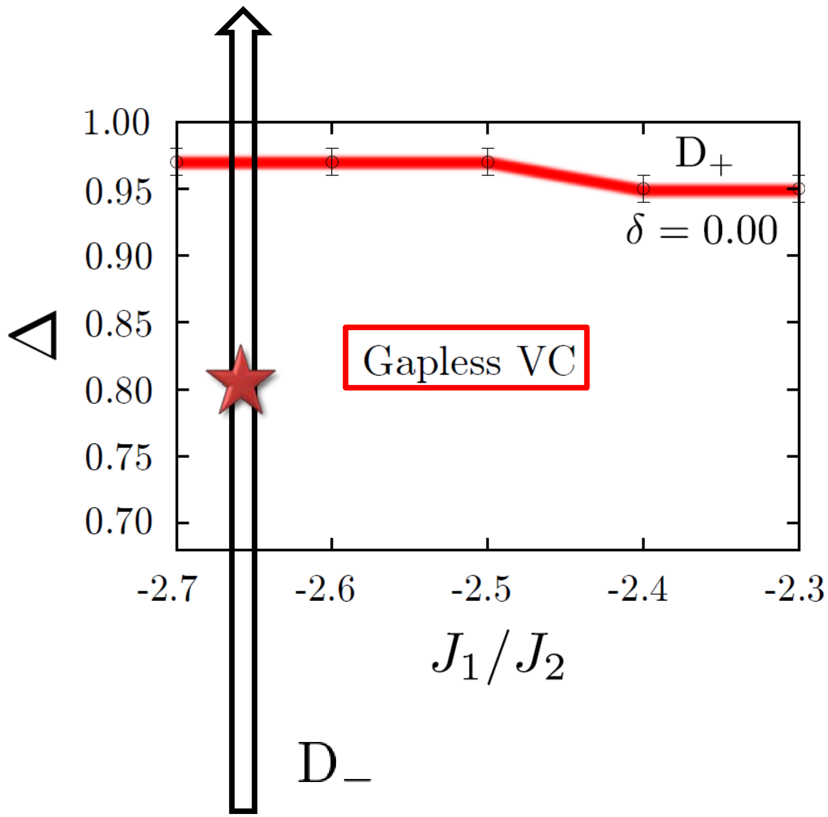
a spatial average only over $N/2$ spins located at



for excluding the boundary effects[1].

[1] T. Hikihara *et al.*, PRB **78**, 144404 (2008).

Phase diagrams (δ=0)



✓Gapless VC phase

Gapless phase

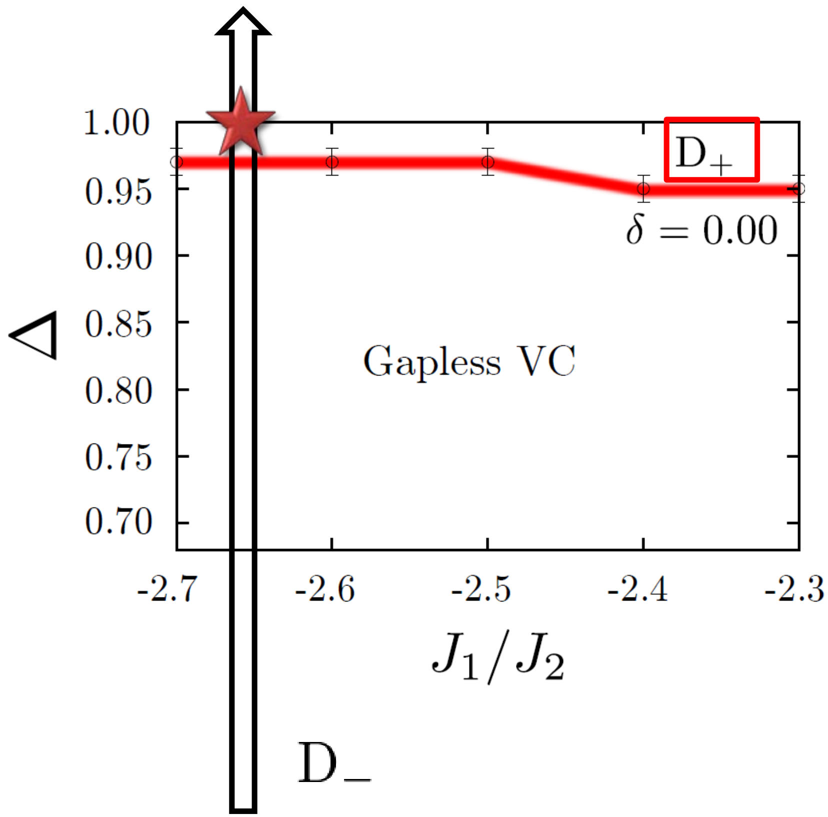
$$\mathrm{Ave}_j\langle \hat{D}_j^x\rangle = 0, \ \mathrm{Ave}_j\langle \hat{D}_j^z\rangle = 0$$

VC LRO

$$\hat{\kappa}_{j+1/2}^z = (\hat{\boldsymbol{S}}_j \times \hat{\boldsymbol{S}}_{j+1})^z,$$

$$\mathrm{Ave}_j\langle\hat{\kappa}_{j+1/2}^z\rangle \neq 0,$$

Phase diagrams (δ=0)

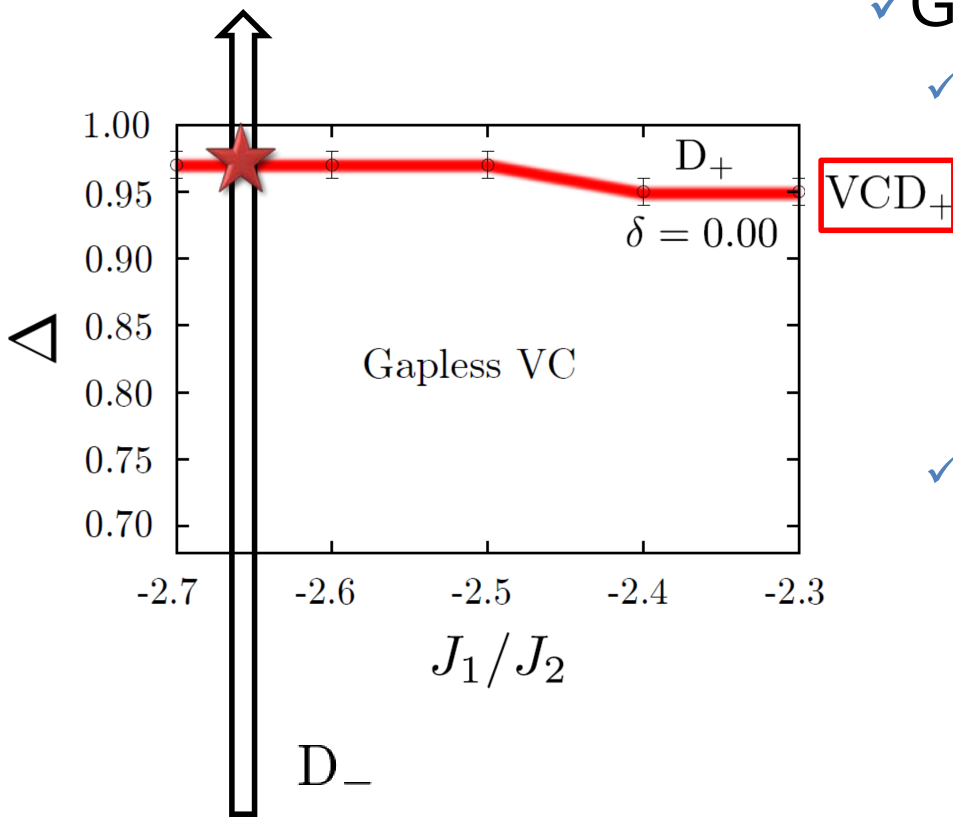


✓Haldane-dimer (D+) phase

Dimer LRO: Gapped phase

$$\left(\mathrm{Ave}_j \langle \hat{D}_j^x \rangle\right)\left(\mathrm{Ave}_j \langle \hat{D}_j^z \rangle\right) > 0,$$

Phase diagrams (δ=0)



[*]

- ✓Gapped VC dimer phases
  - ✓VCD_+ phase

$$\left(\mathrm{Ave}_j\langle\hat{D}^x_j\rangle\right)\left(\mathrm{Ave}_j\langle\hat{D}^z_j\rangle\right) > 0,$$

$$\mathrm{Ave}_j\langle\hat{\kappa}^z_{j+1/2}\rangle \neq 0$$

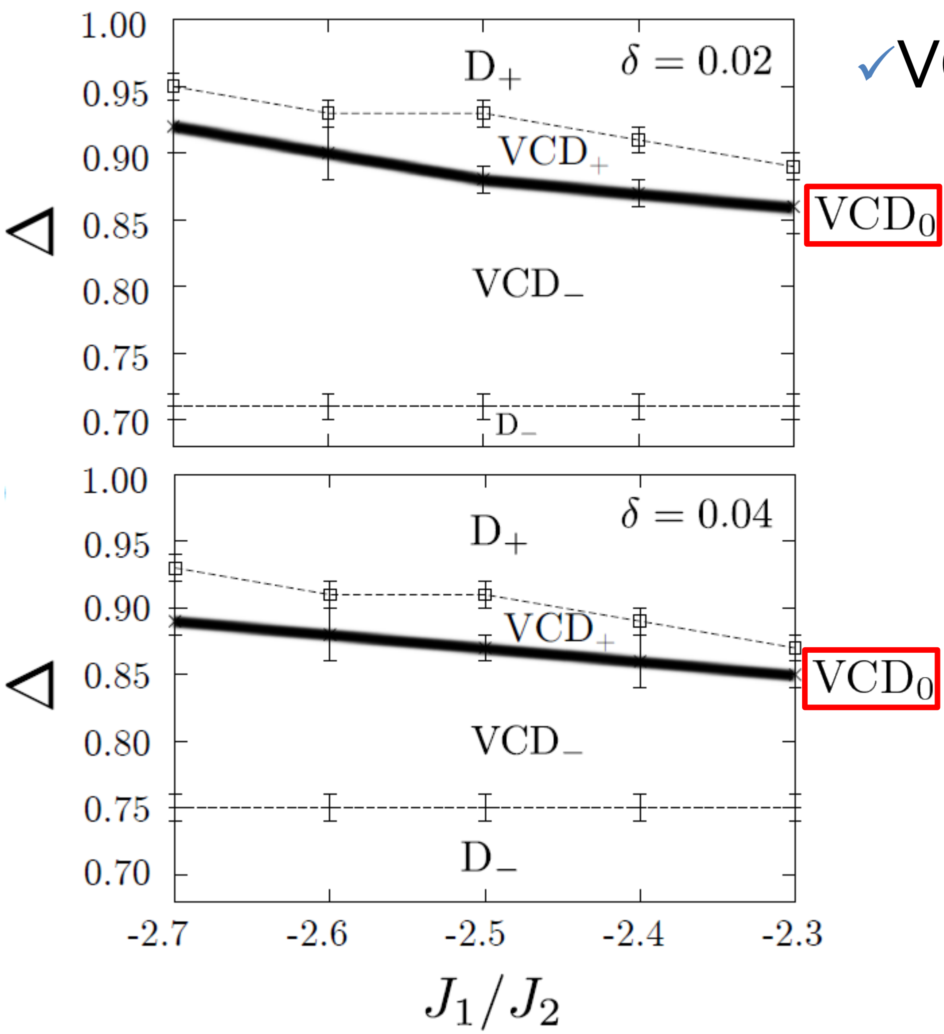
  - ✓VCD_- phase

$$\left(\mathrm{Ave}_j\langle\hat{D}^x_j\rangle\right)\left(\mathrm{Ave}_j\langle\hat{D}^z_j\rangle\right) < 0,$$

$$\mathrm{Ave}_j\langle\hat{\kappa}^z_{j+1/2}\rangle \neq 0$$

[*] S. Furukawa, M. Sato, SO, and A. Furusaki, PRB **86**, 094417 (2012).

Phase diagrams (δ>0)



✓VCD_0 region

Gapless nature

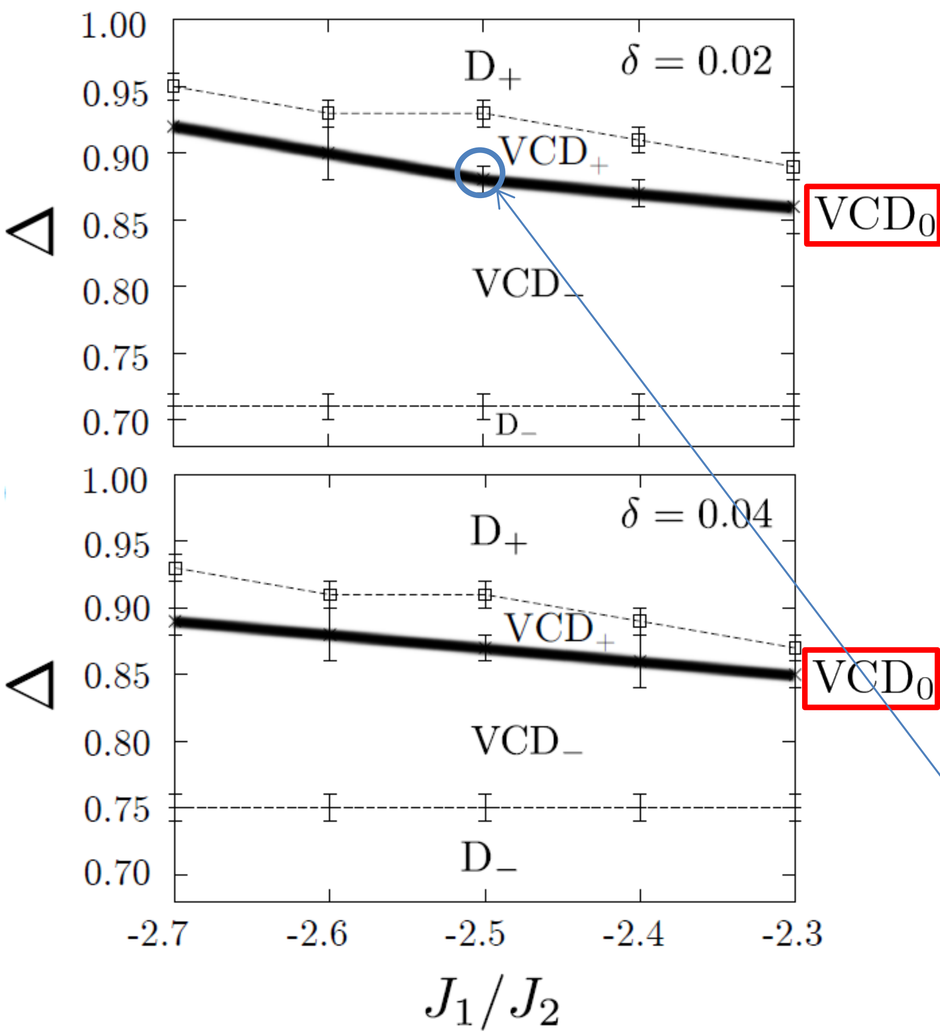
$$(\mathrm{Ave}_j\langle\hat{D}^x_j\rangle)(\mathrm{Ave}_j\langle\hat{D}^z_j\rangle) = 0,$$

where $\mathrm{Ave}_j\langle\hat{D}^x_j\rangle \neq 0,\ \mathrm{Ave}_j\langle\hat{D}^z_j\rangle = 0.$

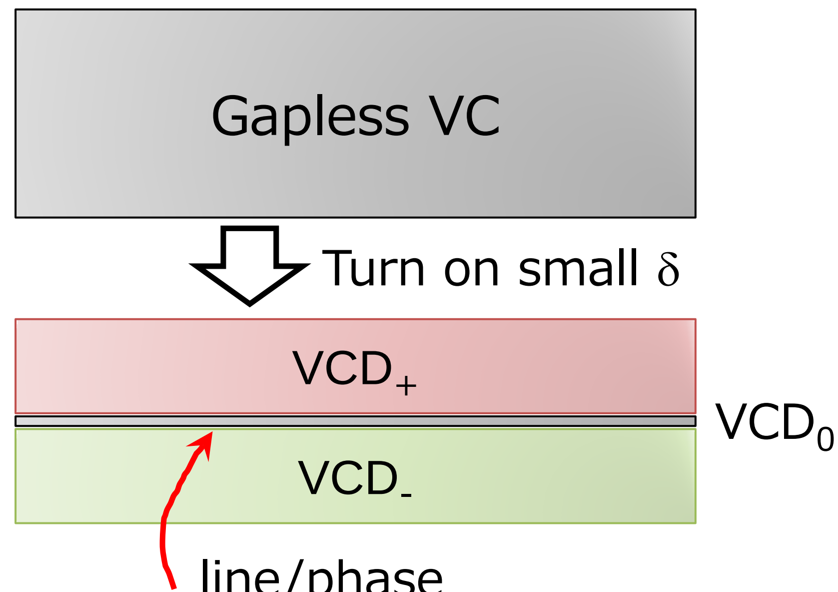
VC LRO

$$\mathrm{Ave}_j\langle\hat{\kappa}^z_{j+1/2}\rangle \neq 0$$

Phase diagrams (δ>0)



✓Effect of δ



N=320: $\Delta = 0.882$

N→∞ : narrower than

$$0.879 \leq \Delta \leq 0.883$$

Abelian bosonization analysis

Start from decoupled XXZ chains:

1. J_1 coupled two chain: $\mathcal{H}_+ + \mathcal{H}_- + \mathcal{H}_{\rm int}$

$$\mathcal{H}_\pm = \sum_{\nu=\pm} \frac{v_\nu}{2}\left[K_\nu(\partial_x\theta_\nu)^2 + K_\nu^{-1}(\partial_x\phi_\nu)^2\right]$$

2. Mean field decoupling of the $\pm$ sector (valid in VC, Neel, and/or dimer phases)

3. Self-consistent solution to two sine-Gordon problems

for $\left\{ \begin{array}{c} \langle \sin\sqrt{4\pi}\phi_+ \rangle \\ \langle \cos\sqrt{4\pi}\phi_+ \rangle \end{array} \right\}$ and $\left\{ \begin{array}{c} \langle \sin\sqrt{4\pi}\theta_- \rangle \\ \langle \cos\sqrt{4\pi}\theta_- \rangle \end{array} \right\}$

This analysis for δ=0: Nersesyan. *et al*., (1998)
S. Furukawa, M. Sato, SO, and A. Furusaki, PRB **86**, 094417 (2012).

VCD$_\pm$ Phase

- Absence of Neel LRO: $\langle \sin\sqrt{4\pi}\phi_+\rangle = 0$
- VC LRO: $\langle \sin\sqrt{4\pi}\theta_-\rangle \neq 0$
- z-component of dimer LRO: $\langle \cos\sqrt{4\pi}\phi_+\rangle \neq 0$
- x, y-component of dimer LRO: $\langle \cos\sqrt{4\pi}\theta_-\rangle \neq 0$

✓Transition from VCD$_+$ to VCD$_-$

⟺ Sign changing of $\langle \cos\sqrt{4\pi}\phi_+\rangle$

$\propto J_1\Delta\delta$ $\qquad \propto J_1$

Required conditions

$$\langle \cos\sqrt{4\pi}\phi_+\rangle_0 = C(K_+)\left(\frac{\gamma_\delta^{z+}+\gamma_1\langle\cos\sqrt{4\pi}\theta_-\rangle_0}{v_+/a^2}\right)^{\frac{1}{2K_+^{-1}-1}}$$

$$\left|\frac{\gamma_\delta^{z+}+\gamma_1\langle\cos\sqrt{4\pi}\theta_-\rangle_0}{v_+/a^2}\right| \geq \left[C(K_+)K_-\frac{(\gamma_{\mathrm{tw}}^{-+})^2}{v_+v_-/a^2}\right]^{\frac{2K_+^{-1}-1}{2(K_+^{-1}-1)}}$$

for absence of Neel LRO

VCD$_\pm$ Phase

- Absence of Neel LRO: $\langle \sin\sqrt{4\pi}\phi_+\rangle = 0$
- VC LRO: $\langle \sin\sqrt{4\pi}\theta_-\rangle \neq 0$
- z-component of dimer LRO: $\langle \cos\sqrt{4\pi}\phi_+\rangle \neq 0$
- x, y-component of dimer LRO: $\langle \cos\sqrt{4\pi}\theta_-\rangle \neq 0$

✓Possibilities:

(1) An accidental direct continuous transition

$\Leftrightarrow$ $\gamma_\delta^{z+} + \gamma_1\langle \cos\sqrt{4\pi}\theta_-\rangle = 0,\ K_+ = 1$ are satisfied at a single point.

(2) Gapless VCD$_0$ phase (ϕ_+ is unlocked.)

(3) Neel LRO at a transition point

(4) VCND phase sandwiched by VCD$_\pm$ phases

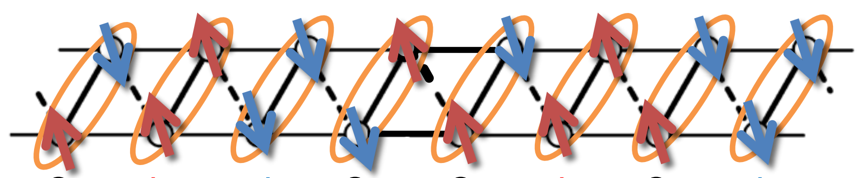
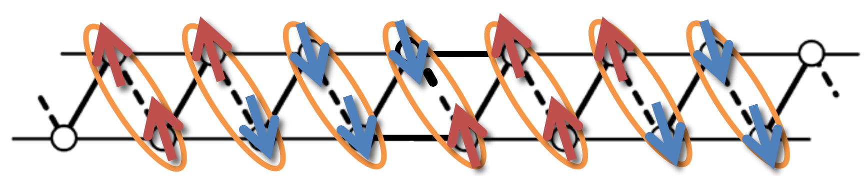
String correlation functions

$$C_N^{(O_\ell^z)}(2r) = \mathrm{Ave}_j \langle \hat{O}^z_{2j+\ell,2j+\ell+2r} \rangle \quad (\ell = 1, 2),$$

where $$\hat{O}^z_{j,j+2r} = -(\hat{S}^z_j + \hat{S}^z_{j+1}) \exp(i\pi \sum_{k=2}^{2r-1} \hat{S}^z_{j+k}) (\hat{S}^z_{j+2r} + \hat{S}^z_{j+2r+1}).$$

E. H. Kim *et.al*, PRB **62**, 14965 (2000), and references therein.

Distinction of two dimer phases:

Phase	LRO	A particular spin configuration
D_+ VCD_+	$\lim_{r\to\infty} C_N^{(O_1^z)}(2r) > 0$ $\lim_{r\to\infty} C_N^{(O_2^z)}(2r) = 0$	 $S^z_{2j+1} + S^z_{2j+2}$: 0 1 -1 0 0 1 0 -1
D_- VCD_-	$\lim_{r\to\infty} C_N^{(O_1^z)}(2r) = 0$ $\lim_{r\to\infty} C_N^{(O_2^z)}(2r) > 0$	 $S^z_{2j+2} + S^z_{2j+3}$: 1 0 -1 0 1 0 -1

Order parameter and Entanglement Entropy

✓ J_1/J_2 = -2.5, δ = 0.02

Entanglement Entropy:

$$S^{\mathrm{vN}} = -\mathrm{Tr}_A[\rho_A \log \rho_A]$$

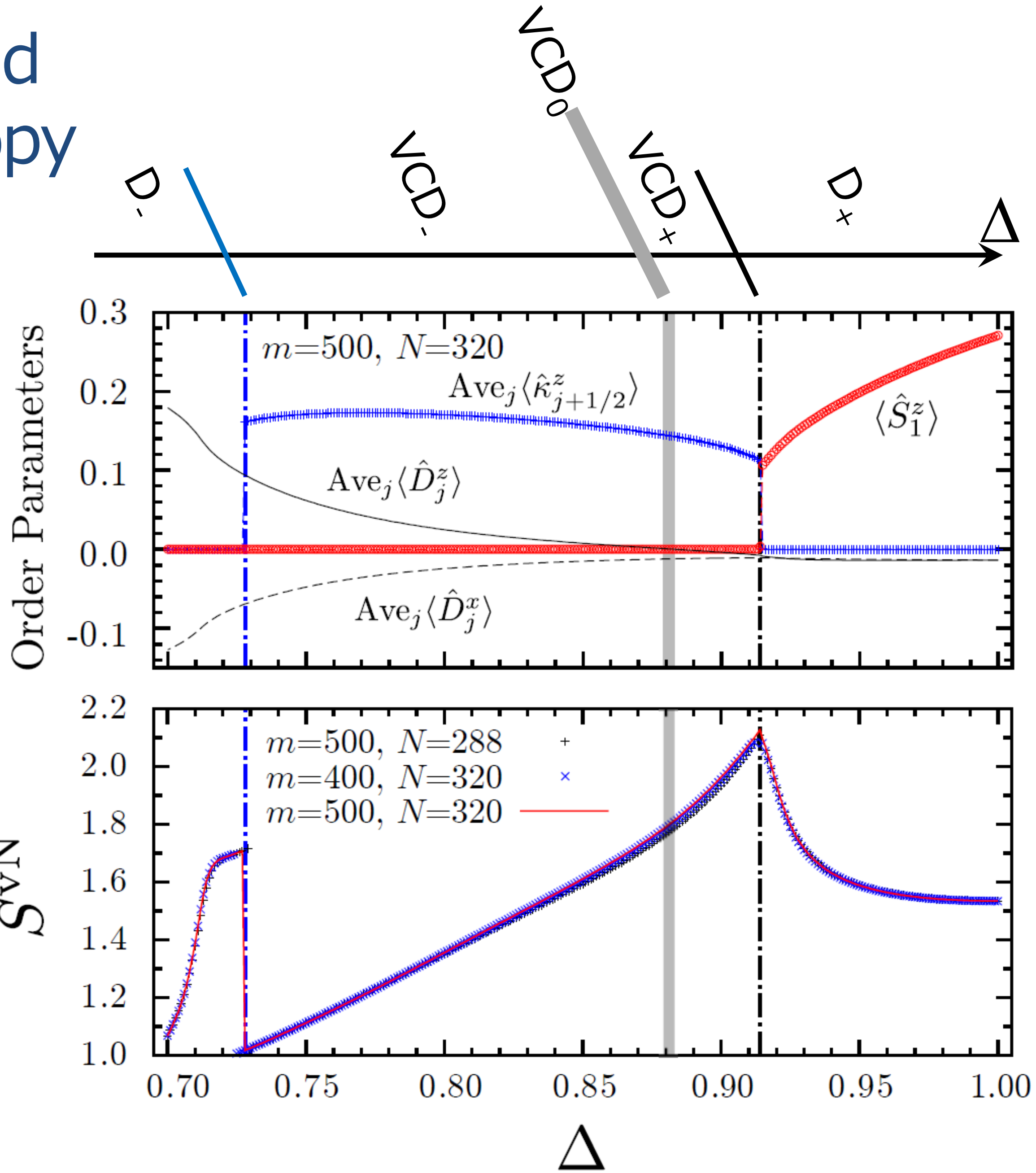
around critical:

$$S^{\mathrm{vN}} = \frac{c}{6} \log \frac{\xi}{\pi} + S_0$$

Critical:

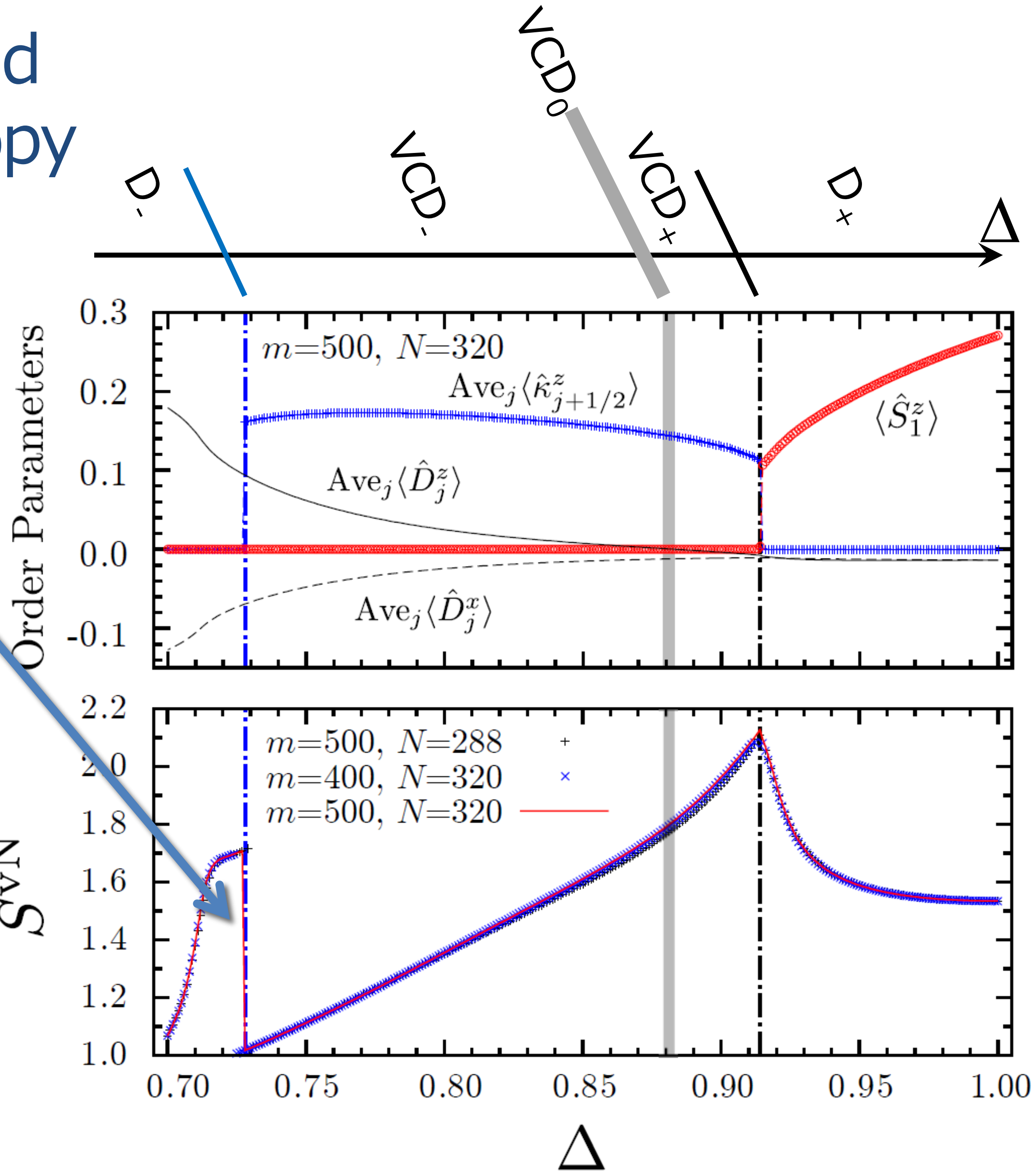
$$S^{\mathrm{vN}} = \frac{c}{6} \log \frac{N}{\pi} + S_0$$

c: central charge



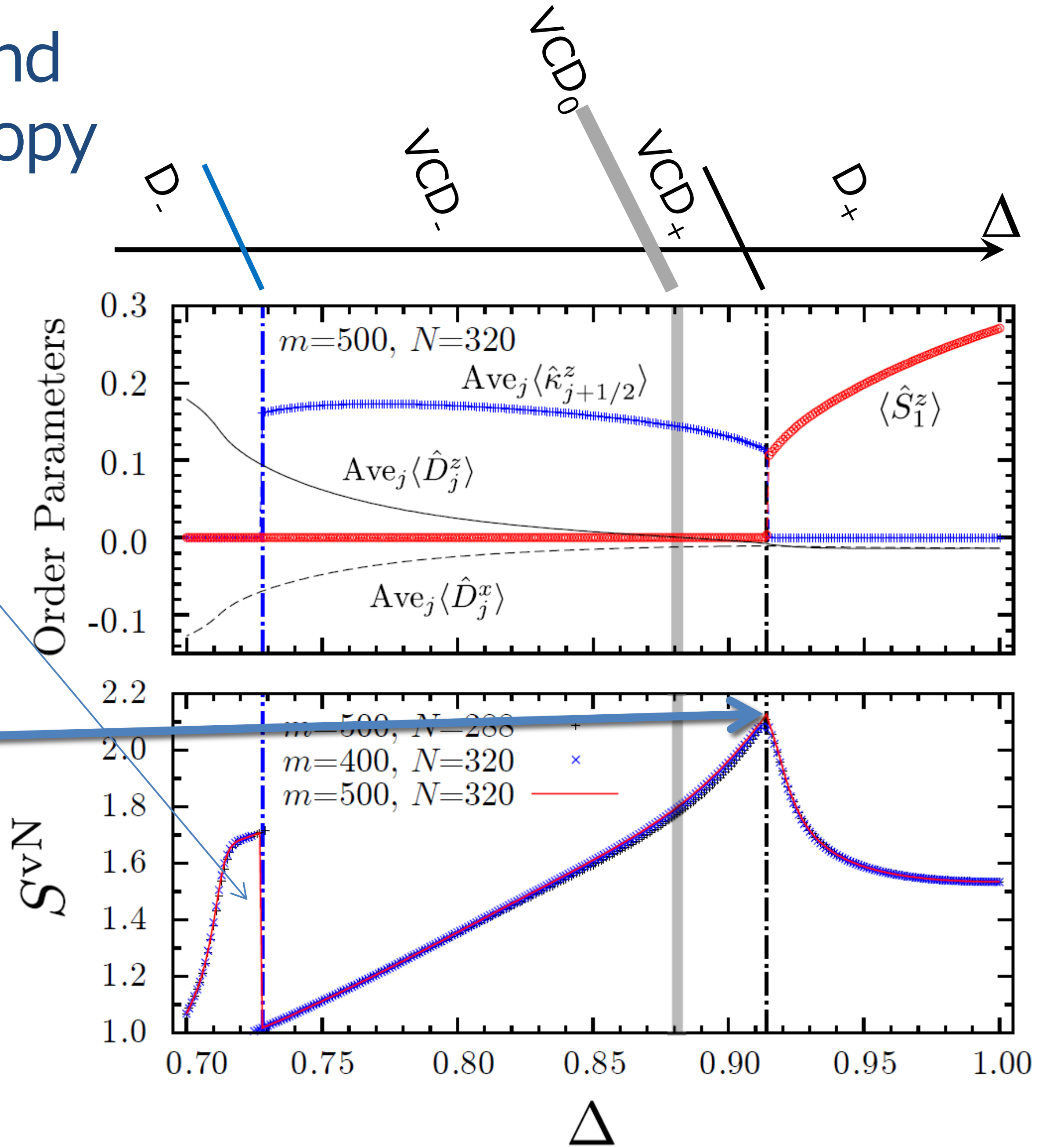
Order parameter and Entanglement Entropy

- ✓ $J_1/J_2 = -2.5$, $\delta = 0.02$
- ✓ Z_2 symmetry
  VC LRO: Breaking



Order parameter and Entanglement Entropy

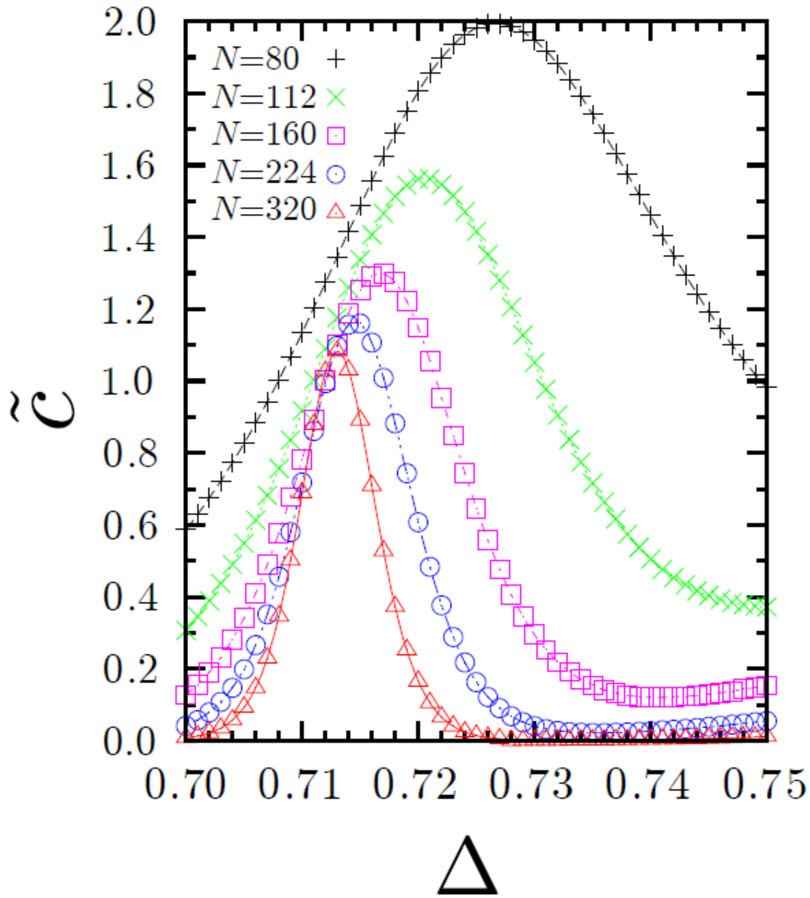
- ✓ J_1/J_2 = -2.5, δ = 0.02
- ✓ Z_2 symmetry
  VC LRO: Breaking
- ✓ Z_2 symmetry
  VC LRO: Recovering
  Edge spin: Breaking

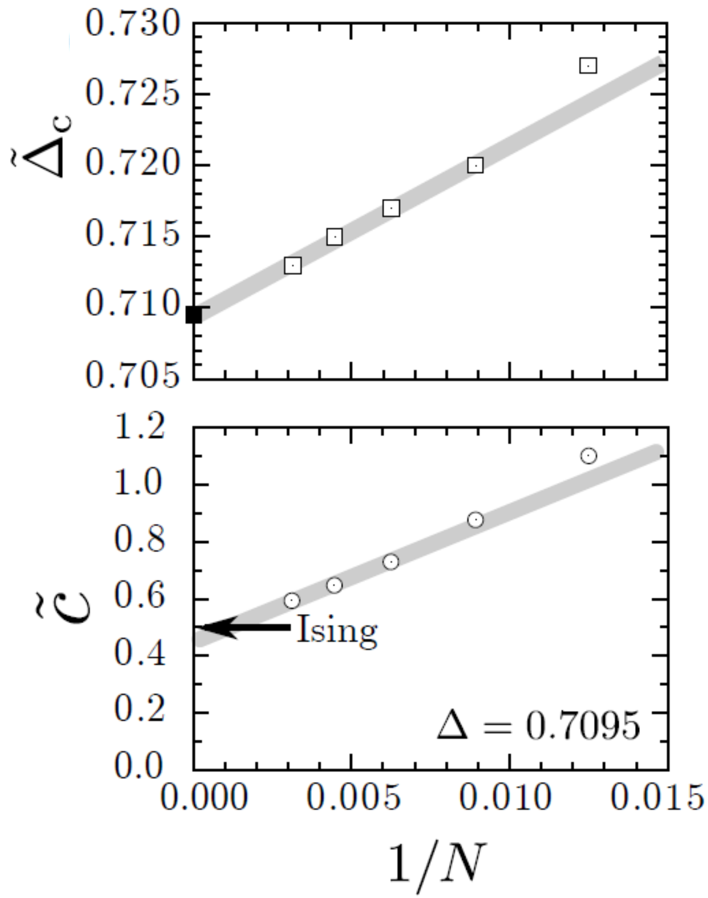


Criticality at the D_-VCD_ boundary

$$S_A(N,\ell) = \frac{\tilde{c}}{6}\log\left[\frac{N}{\pi}\sin\frac{\pi\ell}{N}\right] + S_0$$

P. Calabrese and J. Cardy, J. Stat. Mech. (2004) P06002.

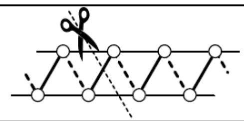
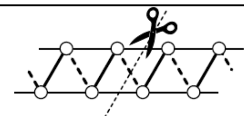
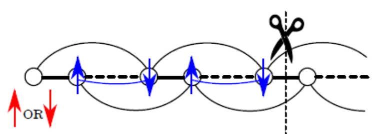
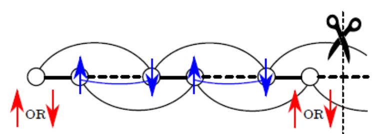
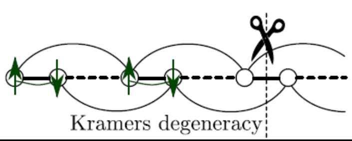
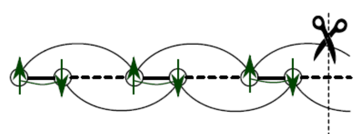


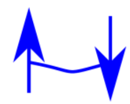


Entanglement Spectrum

$$S^{\mathrm{vN}} = -\mathrm{Tr}_A[\rho_A \log \rho_A] = \sum_i \zeta_i \exp(-\zeta_i)$$

ζ_i : Entanglement Spectrum

	Degeneracy of ζ_1	
Phase		
D_+	2 	4 
D_-	2 	1 

: like $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$

(odd-parity dimer)

: like $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$

(even-parity dimer)

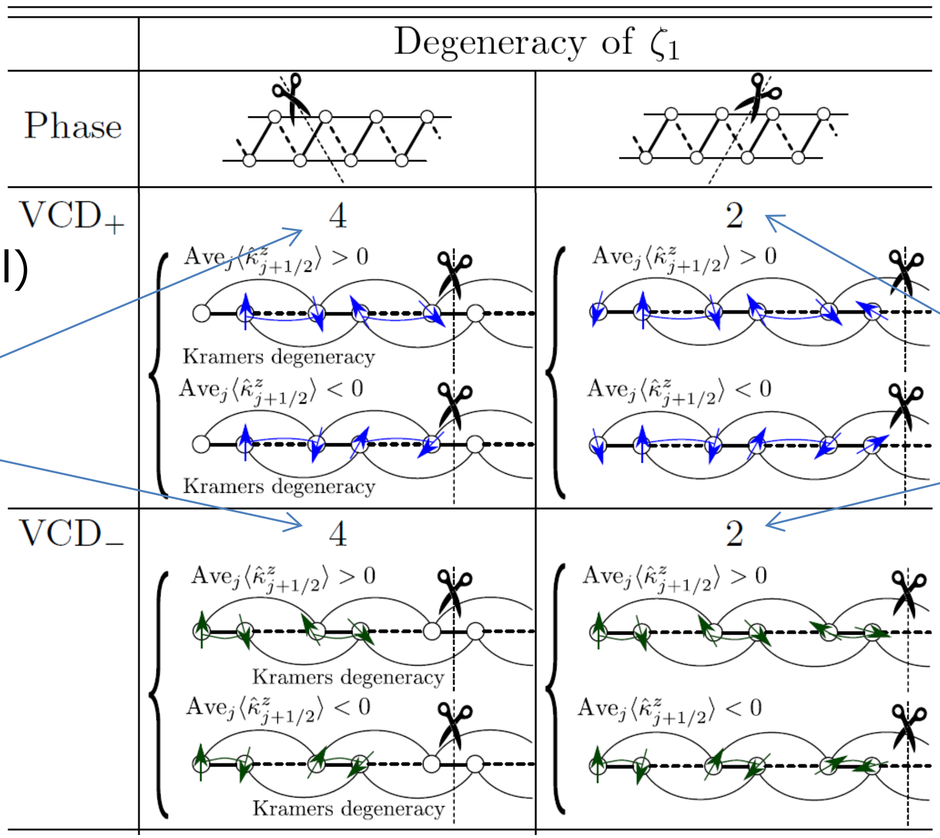
D_+ and D_- are SPT phases distinct in the absence of the Neel LRO.

Entanglement Spectrum

2 (Time reversal)

×

2 (VC LRO)

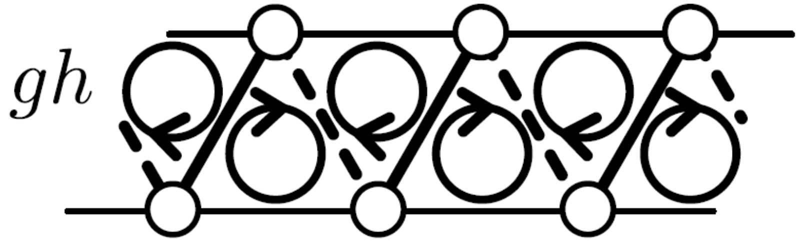


2 (VC LRO)

VCD+ and VCD- have different string orders.
➔ Distinct SPT?

Low-field case without Magnetization

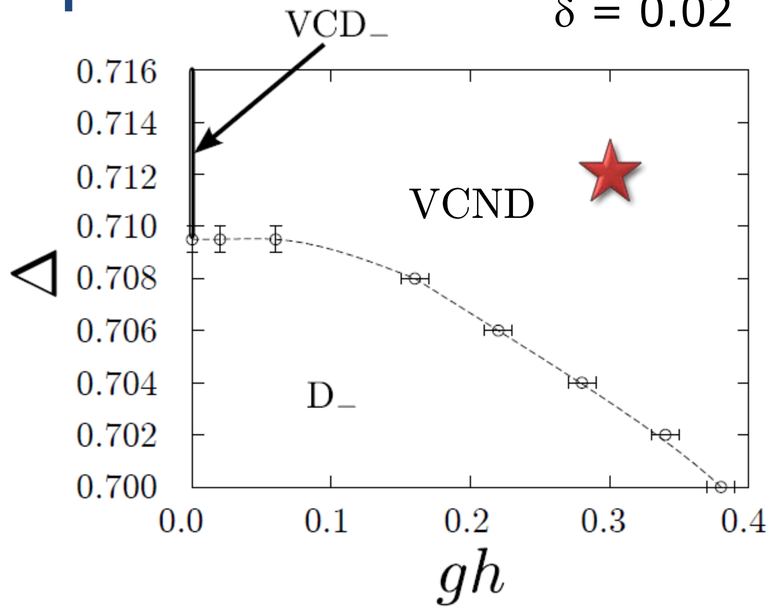
$$\hat{\mathcal{H}}_{\rm ssc} = gh \sum_j (\hat{\boldsymbol{S}}_{2j-1} - \hat{\boldsymbol{S}}_{2j+2}) \cdot \hat{\boldsymbol{S}}_{2j} \times \hat{\boldsymbol{S}}_{2j+1}$$



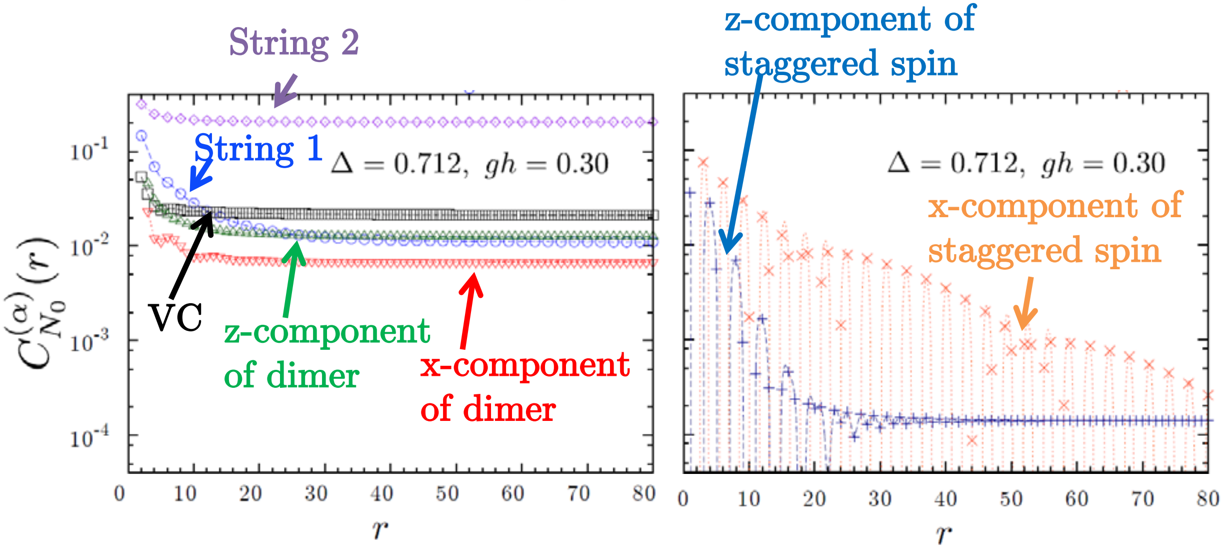
VC Neel Dimer (VCND) phase

J_1/J_2 = -2.5
δ = 0.02

$$\hat{\mathcal{H}}_{\delta\mathrm{xxz}} + \hat{\mathcal{H}}_{\mathrm{ssc}}$$



Correlation functions at ★ .



Bosonization analysis

VCND Phase

- Neel LRO: $\langle \sin\sqrt{4\pi}\phi_+ \rangle \neq 0$
- VC LRO: $\langle \sin\sqrt{4\pi}\theta_- \rangle \neq 0$
- z-component of Dimer LRO: $\langle \cos\sqrt{4\pi}\phi_+ \rangle \neq 0$
- xy-component of Dimer LRO: $\langle \cos\sqrt{4\pi}\theta_- \rangle \neq 0$

Associated with Neel LRO

$\propto$ J$_1$

Associated with VC LRO

$$\langle \sin\sqrt{4\pi}\phi_+ \rangle_1 = \left(\frac{\gamma_{\mathrm{tw}}\gamma'_{\mathrm{ssc}}}{v_+ K_+} - \gamma_{\mathrm{ssc}} \right) \langle \sin\sqrt{4\pi}\theta_- \rangle_0$$

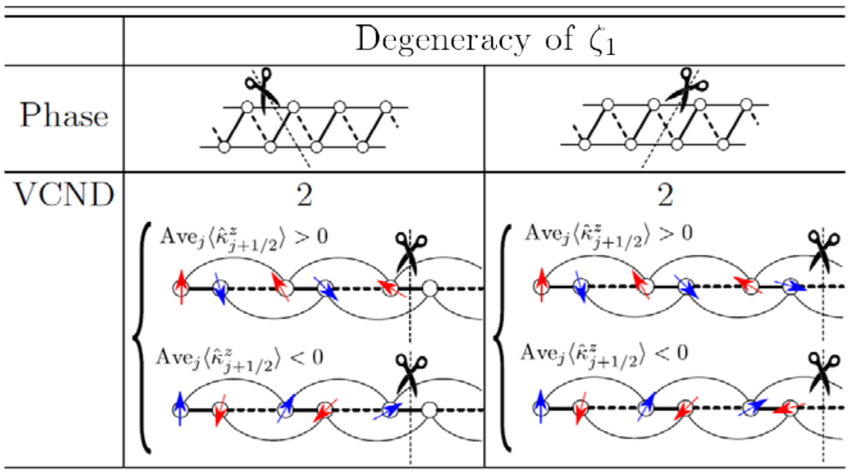
at finite field

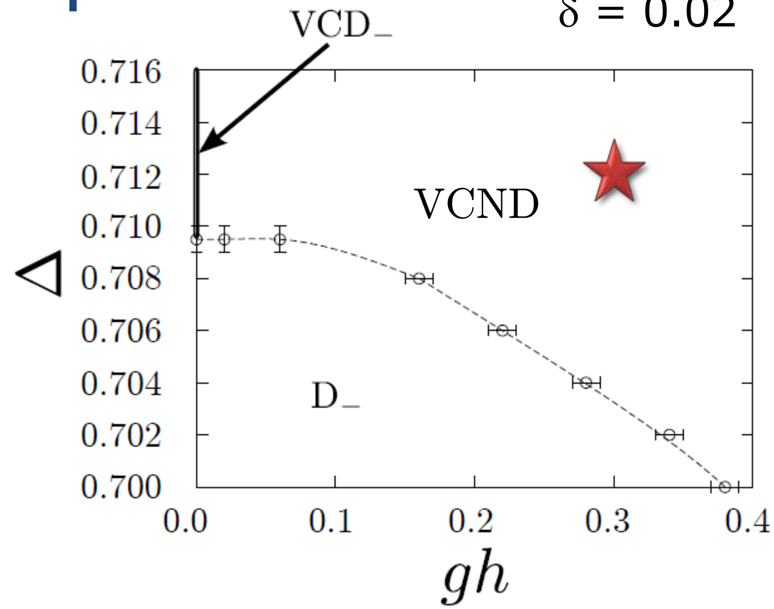
at zero filed

$\propto$ gh

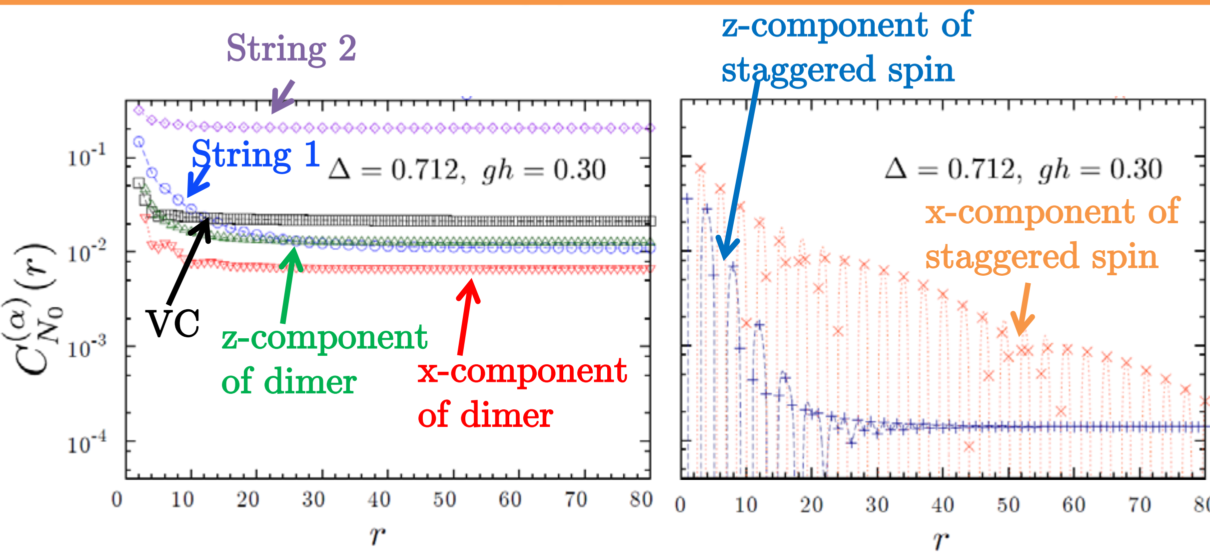
VC Neel Dimer (VCND) phase

$J_1/J_2 = -2.5$
$\delta = 0.02$





Correlation functions at ★ .

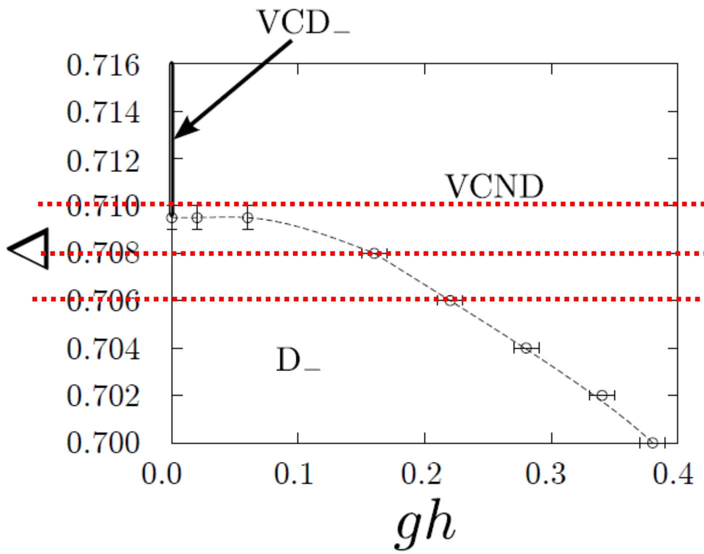


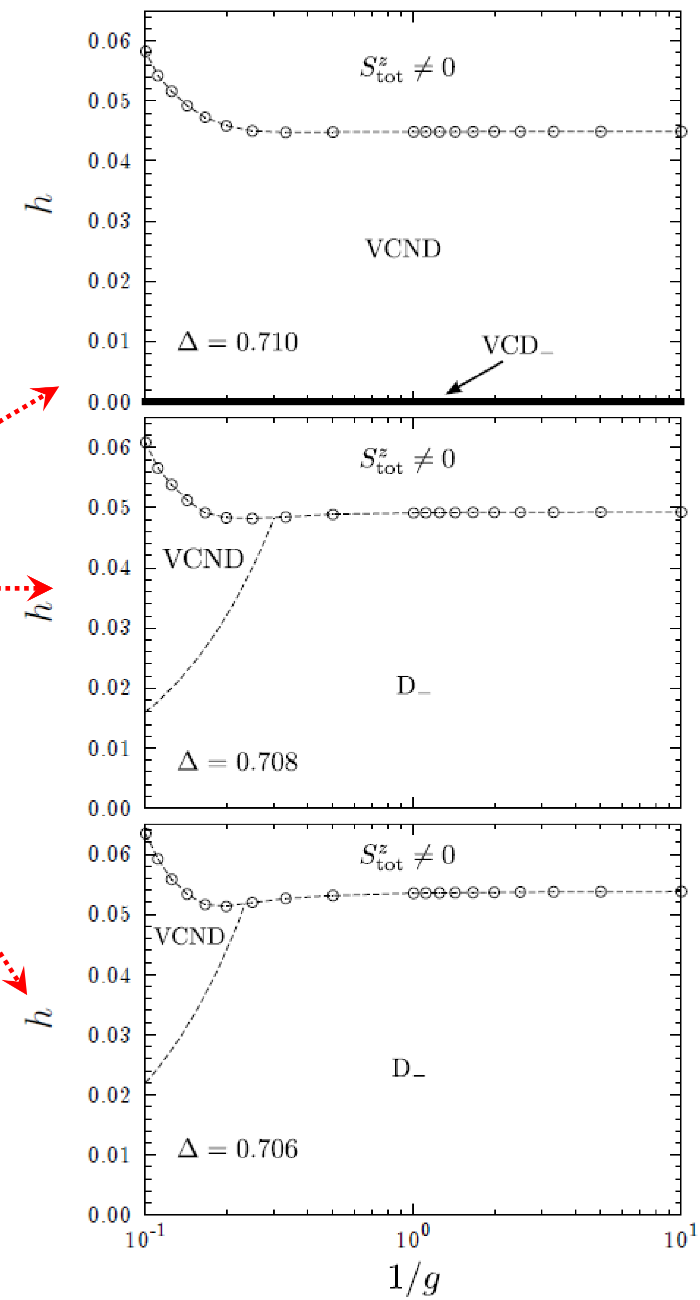
Case at moderately large magnetic field: Zeeman interaction

$$\hat{\mathcal{H}}_Z = -h\sum_j \hat{S}_j^z$$

Field induced VCND Phase

Phase diagram without $\hat{\mathcal{H}}_Z$:



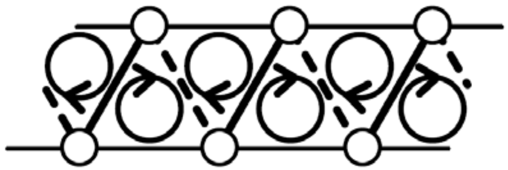


- ✓ If the system starts from D_+

➔ The field Induced VCND does not appear.

Summary

✓Investigate $\hat{\mathcal{H}}_{\delta \mathrm{xxz}} + \hat{\mathcal{H}}_{\mathrm{ssc}} + \hat{\mathcal{H}}_{Z}$



✓Gapped phases:

- ✓Dimer phases at zero-filed
- ✓Gapped vector chiral dimer phase at weak field

✓A possible relevance to experiments of $Rb_2Cu_2Mo_3O_{12}$

- ✓Our model: Bond alternation of J_1: 2 %,

  Spin gap: ~ 0.02 J_2

- ✓$Rb_2Cu_2Mo_3O_{12}$: J_1 = -138K, J_2 = 51K

  Alternation of the Cu-O-Cu angles: ~1 % @ 300K

  (Intensity of the alternation may increase at a low-T.)

  Spin gap: 0.2meV ⇔ ~2K ~ 0.04 J_2

Thank you for your attention!

謝謝！