南京航空航天大学
NANJING UNIVERSITY OF AERONAUTICS AND ASTRONAUTICS

强关联电子体系中的量子磁性、量子物质和量子材料

罗强

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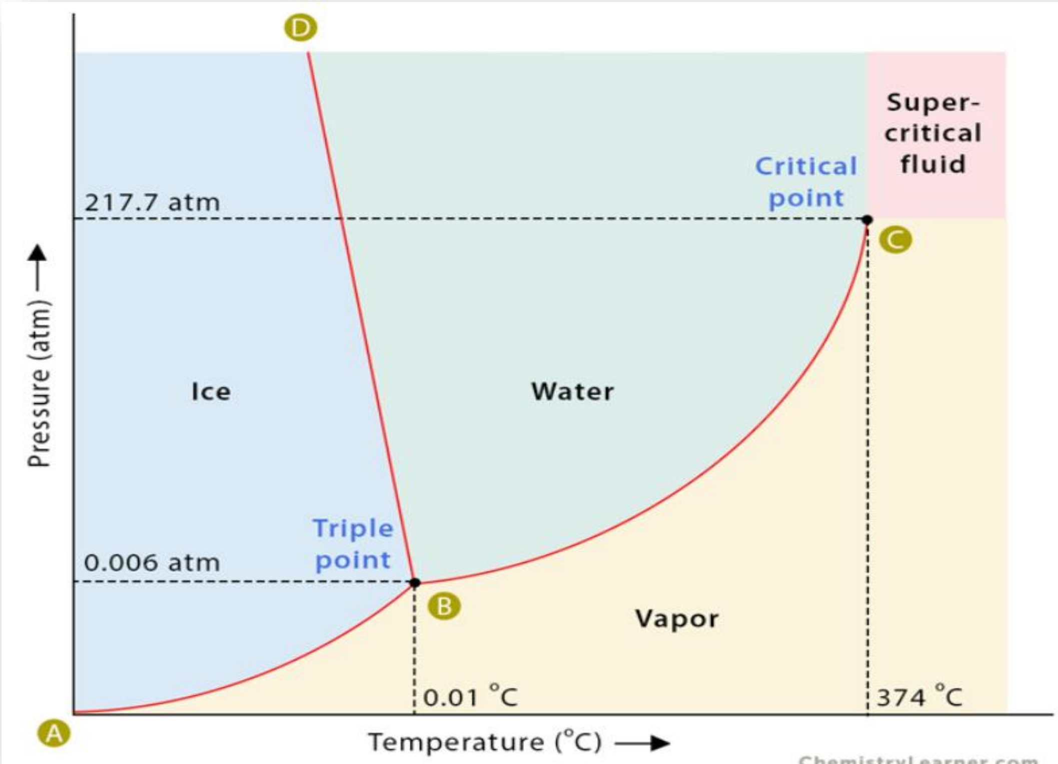
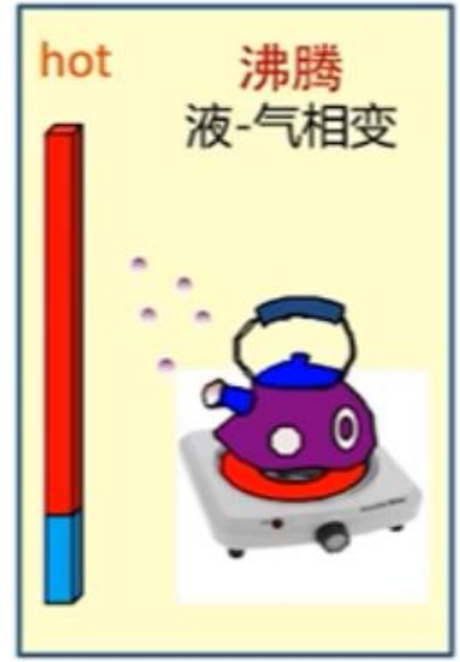
2024年6月13日

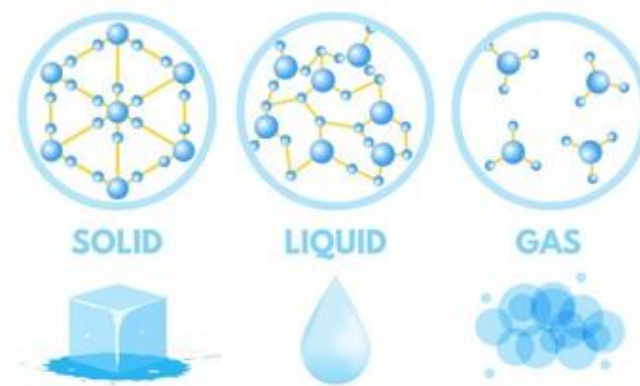
量子磁性与多体计算培训班

水：看似寻常无奇，实则暗藏乾坤

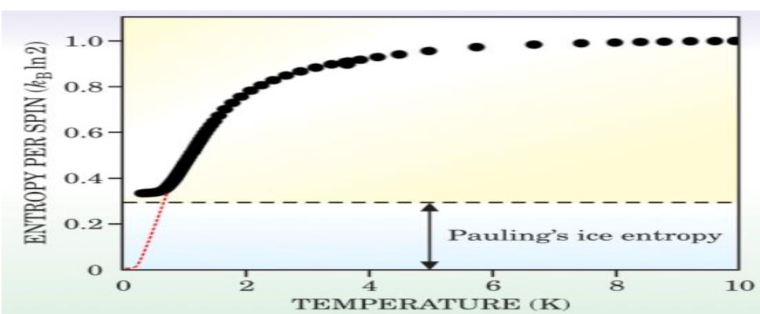


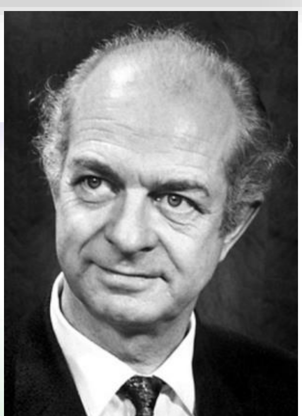
看点1：相与相变





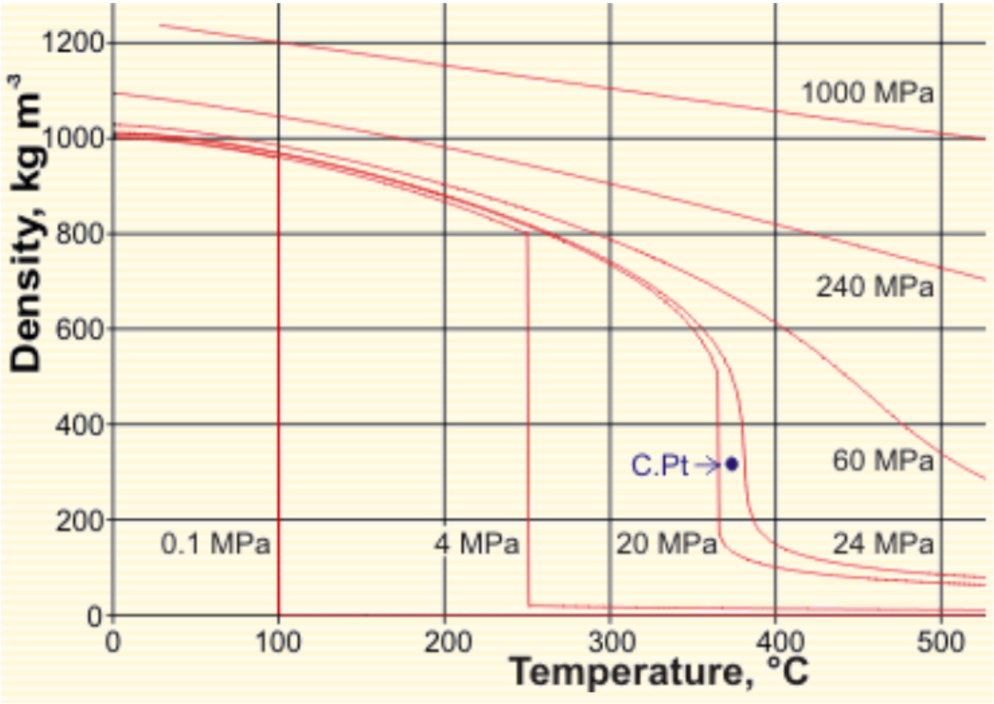
看点2：Pauling剩余熵





看点1：First-order liquid-gas transition

- There is a density jump at the liquid-gas transition, signifying a first-order phase transition.
- The density jump decreases at higher temperatures/pressures, and the first-order line ends at the liquid-gas critical point.



https://water.lsbu.ac.uk/water/water_density.html

isothermal compressibility

$$\kappa_T = -\left(\frac{\partial V}{\partial p}\right)_T \sim |p_c - p|^{-\gamma}.$$

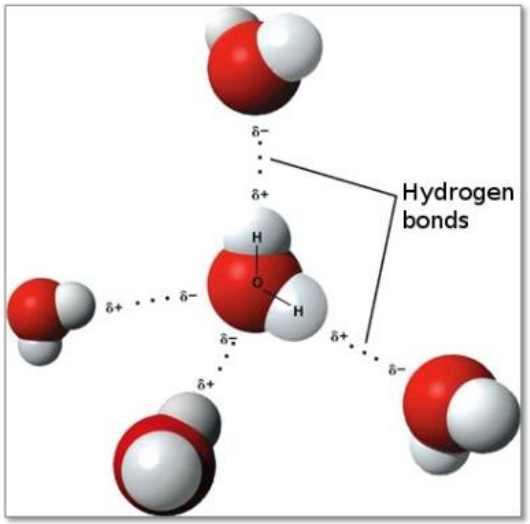
specific heat

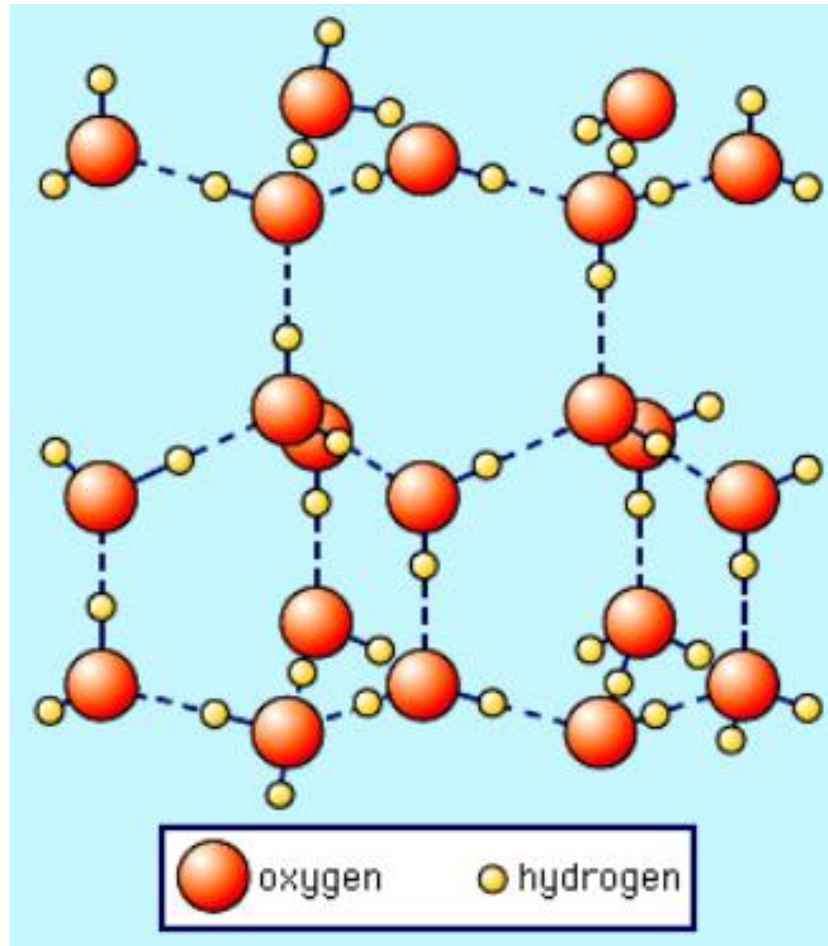
$$C_V \sim |p_c - p|^{-\alpha}.$$

连续相变
临界行为和普适性

看点2：Pauling剩余熵

In ice I_h, the oxygens form a periodic lattice isomorphic to the centre of the tetrahedra in the pyrochlore structure.





O–O 键长2.75Å, O–H键长0.96Å

在聚集体中，水分子会和多达 4 个其它水分子通过**氢键**相结合。

伯纳尔-福勒“冰法则”

https://glossarytest.ametsoc.net/wiki/Bernal-fowler_rules

看点2：Pauling剩余熵

The disordered arrangements of hydrogens produce an extensive amount of ice-ruled configurations Ω.

In 1935, Pauling calculated that $\Omega = (2)^{2N}\left(\frac{6}{16}\right)^{N} = \left(\frac{3}{2}\right)^{N}$

L. Pauling, J. Am. Chem. Soc. 57, 2680 (1935)

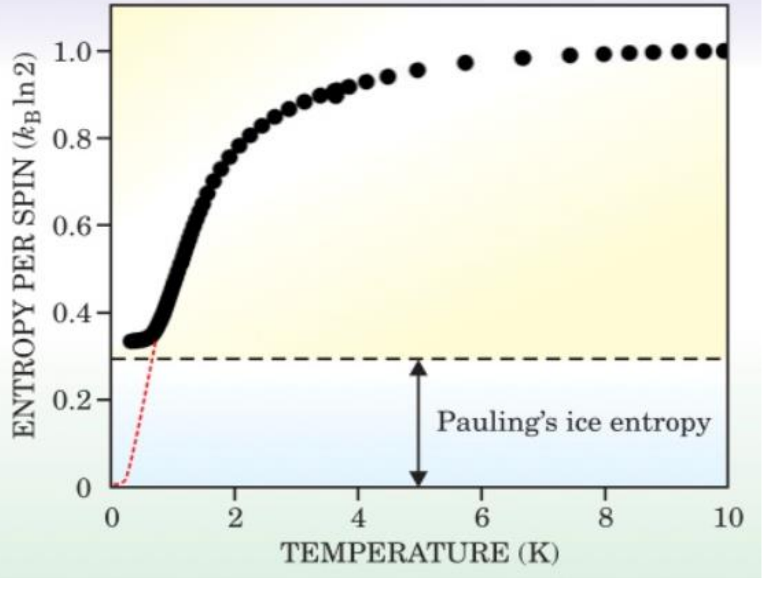
In 1966, Nagle correlated the value of *w* from 3/2 to 1.5069.

J. F. Nagle, J. Math. Phys., 7,1484-91 (1966)

The number of configurations Ω determines the Pauling residual entropy *S*:

$$S = k_B \ln w = 3.41\ \mathrm{J/(mol \cdot K)}$$

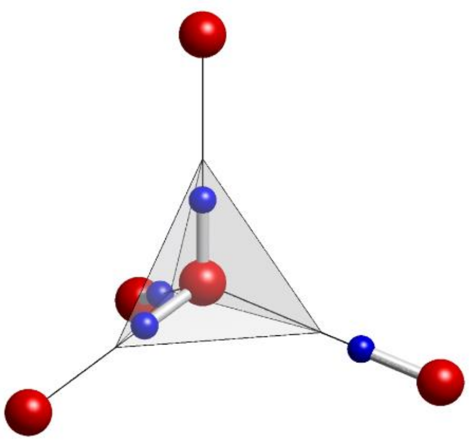
HINT: from water ice to spin ice

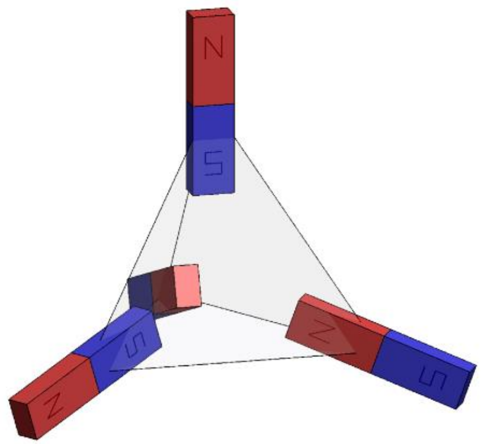


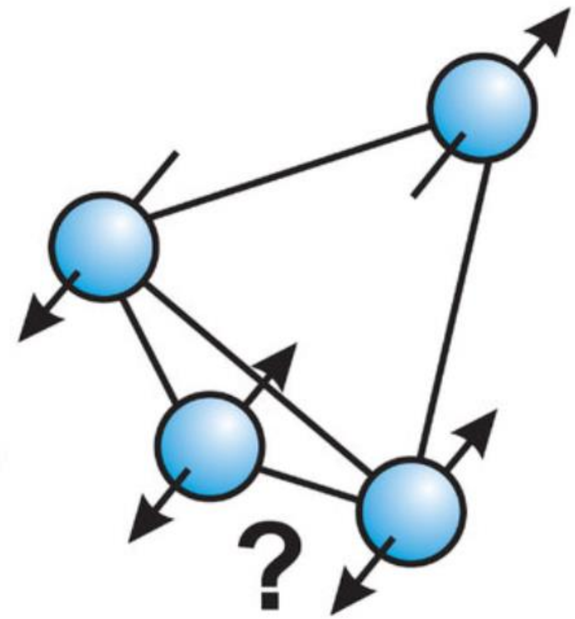
看点2：Pauling剩余熵

from water ice to spin ice

几何阻挫！

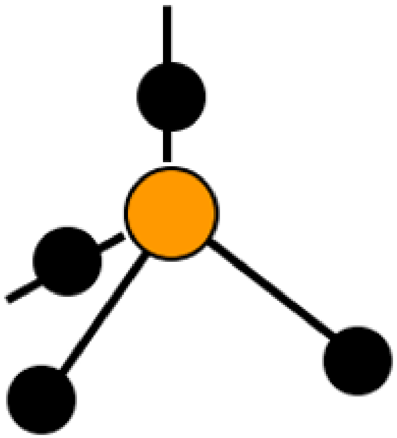


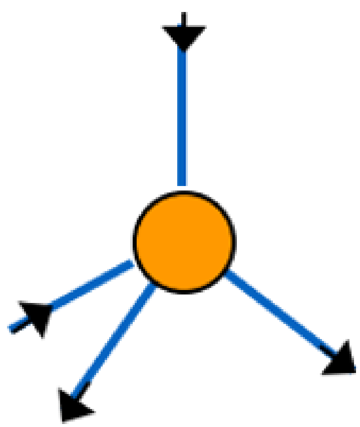




water ice

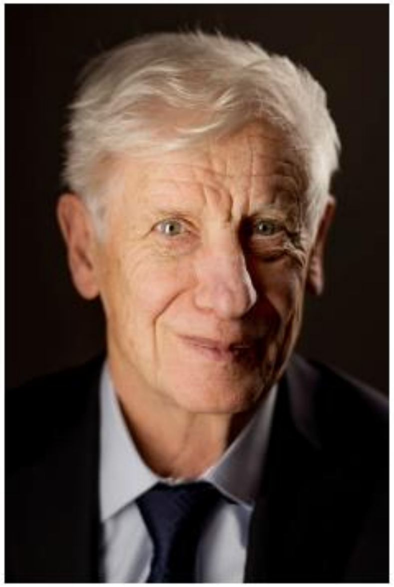
spin ice





two-in-two-out ice rule

2016年诺贝尔物理学奖



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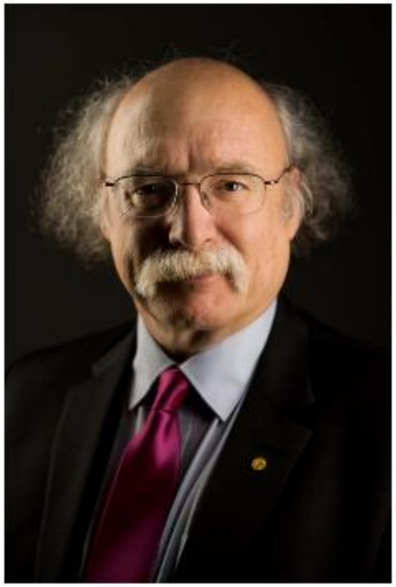
David J. Thouless

Prize share: 1/2



© Nobel Media AB. Photo: A. Mahmoud

F. Duncan M. Haldane

Prize share: 1/4

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J. Michael Kosterlitz

Prize share: 1/4

The Nobel Prize in Physics 2016 was awarded with one half to David J. Thouless, and the other half to F. Duncan M. Haldane and J. Michael Kosterlitz "*for theoretical discoveries of topological phase transitions and topological phases of matter*".

2017年APS巴克利奖

Alexei Kitaev
California Institute of Technology

Xiao-Gang Wen
Massachusetts Institute of Technology

The APS's 2017 Oliver E. Buckley Condensed Matter Prize was awarded to Alexei Kitaev and Xiao-Gang Wen “"*for contributing to the understanding of topological order and its consequences in a broad range of physical systems, including the fractional quantum Hall effect, frustrated magnets, and topological states protected by symmetry*”.

Outline

- 朗道相变理论和新突破
  - Ising模型中的相变
  - Kosterlitz-Thouless相变和去禁闭量子临界点
  - Luttinger液体和Haldane相
- 量子自旋液体和自旋轨道耦合型材料
  - 量子自旋液体简介
  - 三角晶格上的量子材料
  - 蜂窝晶格上的量子材料
- Kitaev-Γ模型中的物理
  - 自旋S=1/2和1的Kitaev-Γ自旋链
  - 自旋S=1的Kitaev-Γ模型

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History of Ising model

Wilhelm Lenz (1920)

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j$$

Wilhelm Lenz (1888.02—1957.04)

Ernst Ising (1900.05—1998.05)

Ernst Ising (1925) E. Ising, *Z. Phys* **31**, 253–258 (1925)

- A linear chain of two-state spins cannot undergo a phase transition at finite temperature.
- Ising purportedly showed that his model can not exhibit a phase transition in two and three dimensions, either.

The Pierls arguments

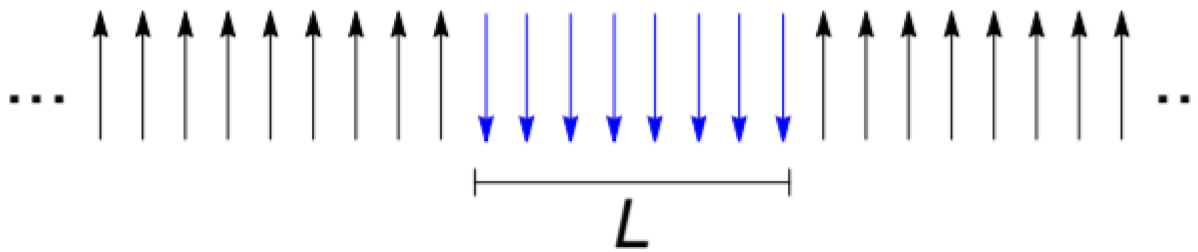
$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j$$

R. Peierls, On Ising's model of ferromagnetism. (1936).

domain wall in 1D

$$E = E_0 + 4J$$

$$S = \ln \Omega \sim \ln L$$



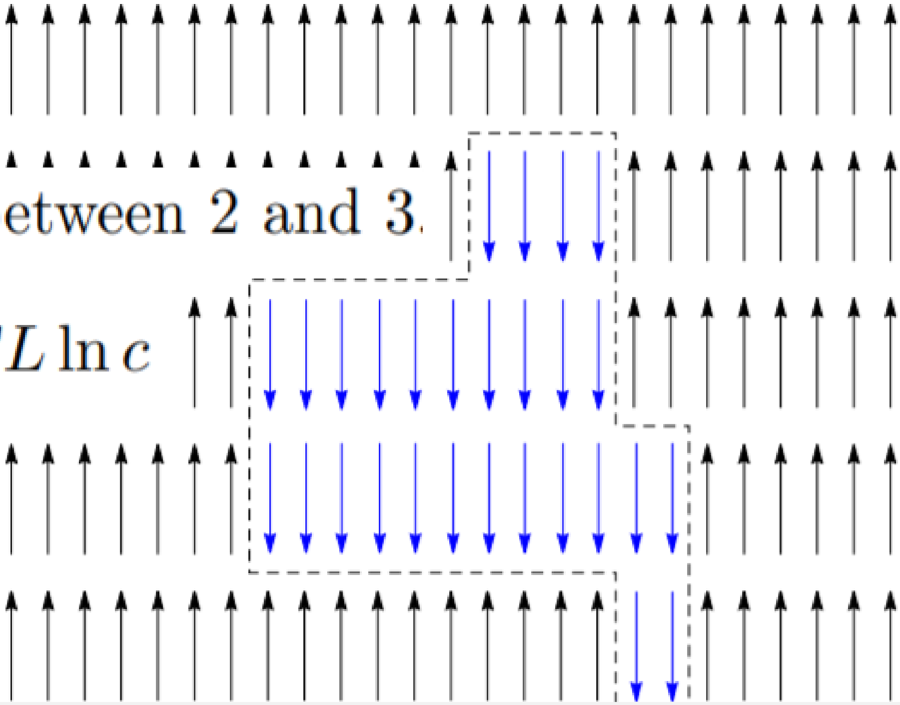
$$F = U - TS = (E_0 + 4J) - T \ln L$$ ➔ Tc=0

The Pierls arguments

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j$$

R. Peierls, On Ising's model of ferromagnetism. (1936).

domain wall in 2D



$$E = E_0 + 2JL$$

$\Omega \sim c^L$ where c is a number between 2 and 3.

$$F = U - TS \simeq E_0 + 2JL - TL \ln c$$

$$T > \frac{2J}{\ln c}$$

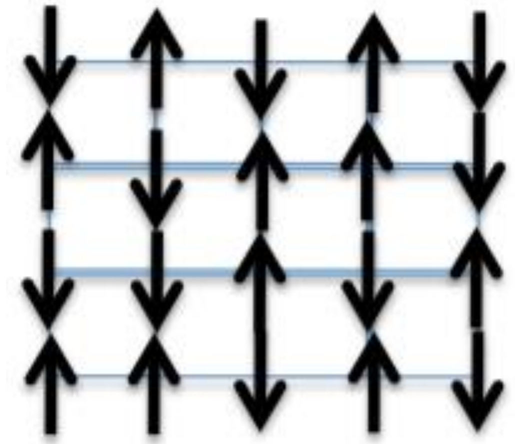
Here, it is more advantageous (from a free energy point of view) to have the system dividing up into an infinite number of domains.

Magnetism: The Ising Model

Rules for the Ising Model:

$$\sigma = +1(\uparrow), -1(\downarrow)$$

Spins can be only in two states:



$$N = N_{up} + N_{down},\ m = \frac{N_{up} - N_{down}}{N}.$$

- **No. of spin configuration**: $\Omega = \binom{N}{N_{up}} = \binom{N}{N(1+m)/2}$

- **Thermal entropy (per site)**:

$$s = \frac{S}{N} = \frac{1}{N}\ln\Omega \approx \ln 2 - \frac{(1+m)\ln(1+m)}{2} - \frac{(1-m)\ln(1-m)}{2}$$

- **energy (per site)**: $e = \frac{E}{N} \approx -\frac{J}{N}\sum_i m^2 = -\frac{1}{2}Jzm^2$

According to the Bragg-Williams theory, the free energy per site

$$f(T,m) = e - Ts$$

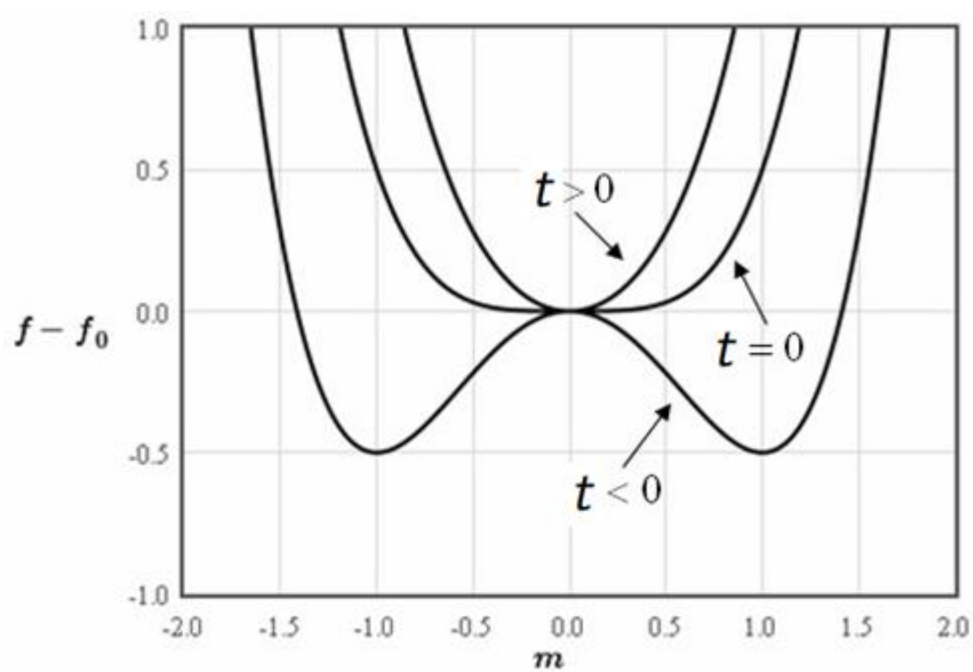
$$f(T,m) = -\frac{1}{2}Jzm^2 + \frac{1}{2}T[(1+m)\ln(1+m) + (1-m)\ln(1-m)] - T\ln 2.$$

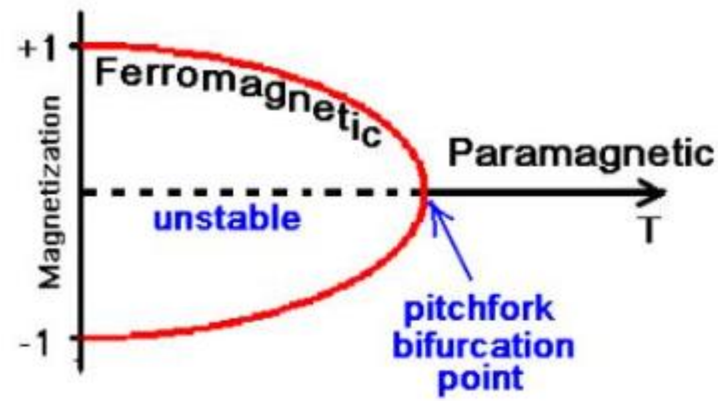
Expanding for small m, $(1+x)\log(1+x)+(1-x)\log(1-x)\approx x^2+\frac{x^4}{6}+\mathcal{O}(x^5)$

Bragg-Williams free energy per site

$$f(T,m)=\frac{F(T,m)}{N}=\frac{U-TS}{N}\simeq -T\ln 2+\frac{1}{2}(T-T_c)m^2+\frac{1}{12}Tm^4,\quad T_c=\frac{Jz}{k_B}$$

$t=(T-T_c)/T_c$





Critical exponents

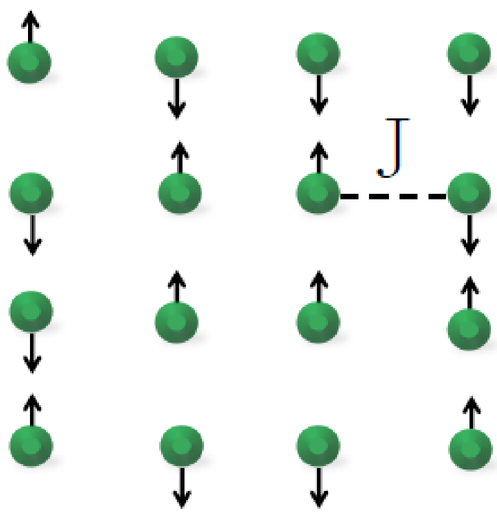
- **specific heat:** $C \propto |t|^{-\alpha}$
- **magnetization:** $m \propto |t|^{-\beta}$
- **magnetic susceptibility:** $\chi \propto |t|^{-\gamma}$
- **correlation length:** $\xi \propto |t|^{-\nu}$

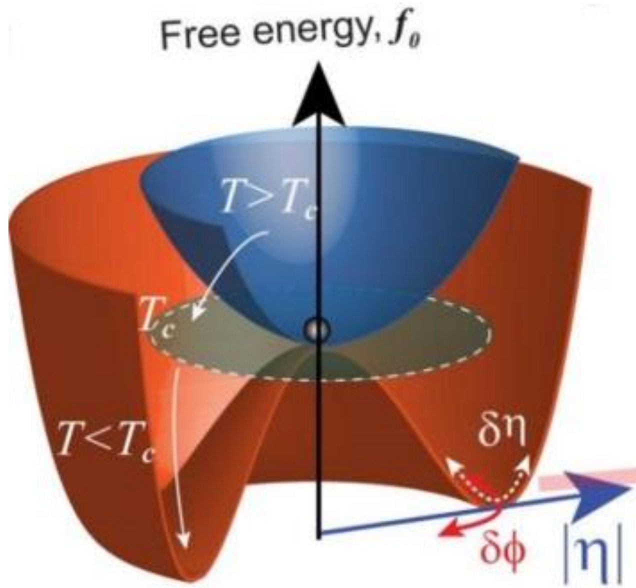
These exponents display criticality universality. This explains the success of the Ising model in providing a quantitative description of real magnets.

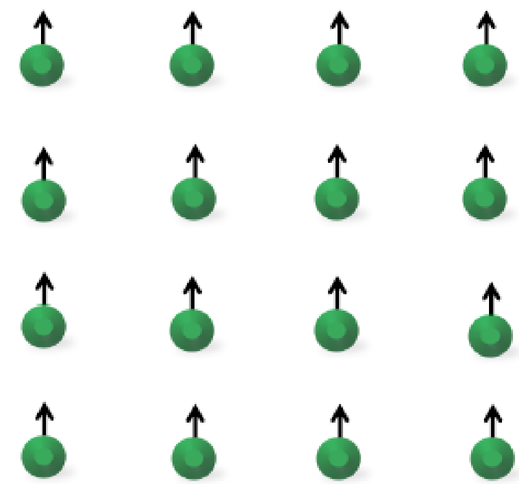
对于二维Ising模型： $C \approx -Nk\frac{2}{\pi}\left(\frac{2J}{kT_c}\right)^2 \ln\left|1-\frac{T}{T_c}\right|$

$$m = \begin{cases} \left[1-\left(\sinh\left(\ln(1+\sqrt{2})\frac{T_c}{T}\right)\right)^{-4}\right]^{1/8}, & T < T_c \\ 0, & T \geq T_c \end{cases}$$

序参量和对称性自发破缺



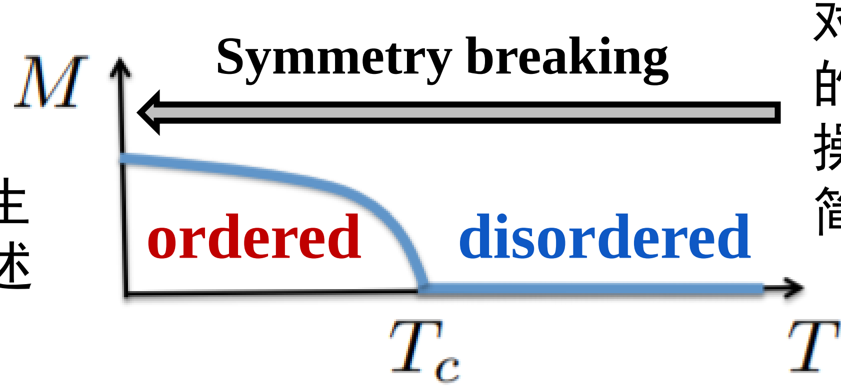




$T > T_c$，$\langle S_i \rangle = 0$

$T < T_c$，$\langle S_i \rangle \neq 0$

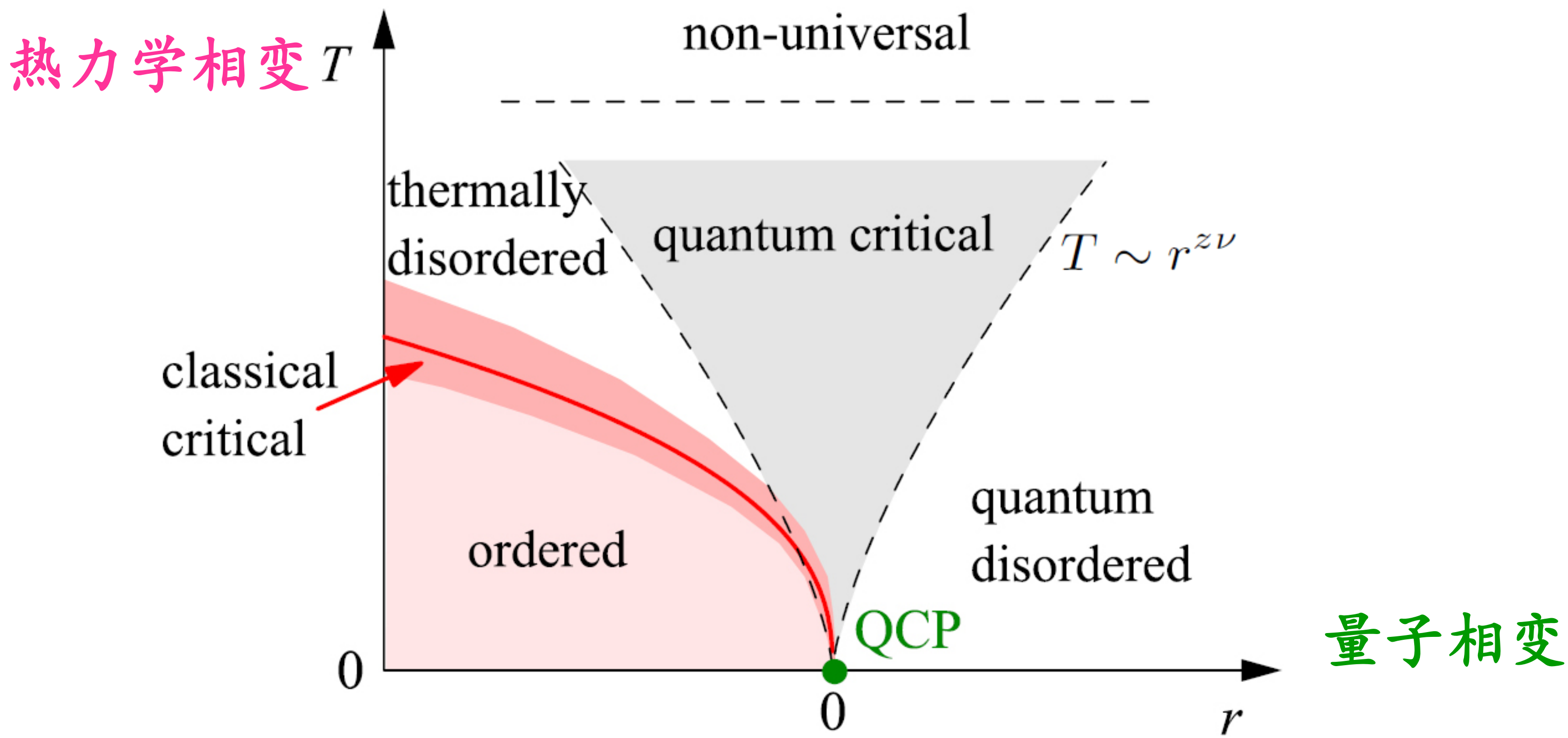
Order Parameter



序参量：描述相变发生时的特征量，也是描述有序态的物理量。

对称性自发破缺：系统的基态不满足某种对称操作，因而具有一定的简并。

Landau's paradigm：有序-无序相变



在凝聚态物理学发展历程中，朗道—金兹堡相变理论奠定了人们对物质形态和有序相及其相变的认识基础，在结合了威尔逊重正化群理论后，形成了朗道—金兹堡—威尔逊范式，并成为整个现代物理学宏伟大厦的重要基石。

张广铭和朱国毅，物理，50(9), 569-582 (2021)

Beyond Landau's paradigm：拓扑相变

❖ **Topological phase transition:无序-无序相变**

The Mermin-Wagner Theorem

In one and two dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions.

Consider a FM Heisenberg model with nearest-neighbor interaction

$$H=-J\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j+\frac{g\mu_B}{\hbar}B_z\sum_i S_i^z \quad \text{with} \quad J>0 \quad \text{and} \quad B_z\to 0^+$$

The spontaneous magnetization at $T = 0$ will be reduced by the excitation of magnons for $T > 0$, i.e.,

$$\Delta M_s(T)=M_S(0)-M_S(T)\propto\int_0^\infty \frac{D(E)}{e^{\frac{E}{k_BT}}-1}\mathrm{d}E$$

$D(E)$: 态密度

Mermin-Wagner theorem

The density of states can be calculated from the magnon dispersion relation:

$$D(E) \propto \int_{S(E)} \frac{\mathrm{d}s}{\left|\frac{\partial}{\partial k}E(k)\right|} \quad \Rightarrow \quad D(E) \propto \frac{E^{\frac{d-1}{2}}}{\sqrt{E}} = E^{\frac{d-2}{2}}$$

$$S(E) \propto k^{d-1} \propto E^{\frac{d-1}{2}} \quad \text{and} \quad \left|\frac{\partial}{\partial k}E(k)\right| \propto \frac{1}{\sqrt{E}}$$

The reduced spontaneous magnetization:

$$\Delta M_s(T) \propto \int_0^\infty \frac{E^{\frac{d-2}{2}}}{\mathrm{e}^{\frac{E}{k_B T}} - 1}\mathrm{d}E \propto T^{\frac{d}{2}} \int_0^\infty \frac{x^{\frac{d-2}{2}}}{\mathrm{e}^x - 1}\mathrm{d}x = T^{\frac{d}{2}}\zeta\left(\frac{d}{2}\right)\Gamma\left(\frac{d}{2}\right)$$

There is no spontaneous magnetization for $T > 0$ and $d \leq 2$!

Kosterlitz-Thouless transition

Two-dimensional XY model

$$H = -\frac{1}{2}\sum_{r,r'} J(r-r')\mathbf{S}(r)\cdot\mathbf{S}(r') = -\frac{1}{2}\sum_{r,r'} J(r-r')\cos(\theta_r - \theta_{r'})$$

- **reduced Hamiltonian**

$$\mathcal{H} \equiv -\beta H = K \sum_{<i,j>} \cos(\theta_i - \theta_j)$$

where $\beta = 1/k_B T$ and $K = \beta J$

- **effective Hamiltonian**

$$\mathcal{H} = E_0 - \frac{K}{2}\int d^2x\,|\nabla\theta(x)|^2$$

where $E_0 = 2KL^2/a^2$

低温下的自旋-自旋关联函数

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = \mathrm{Re}\langle e^{i(\theta(\vec{r}_i)-\theta(\vec{r}_j))}\rangle = \frac{1}{|\vec{r}_i - \vec{r}_j|^{\frac{T}{2\pi J}}}$$

代数型衰减

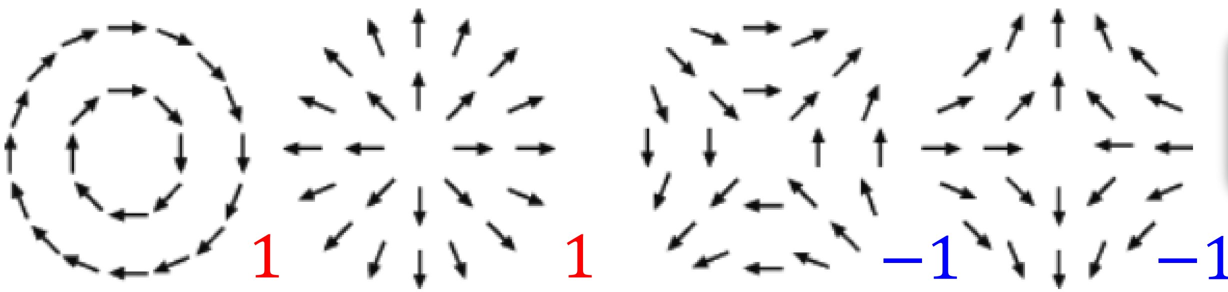
高温下的自旋-自旋关联函数

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \propto K^{|\vec{r}_i - \vec{r}_j|} \propto e^{-(\vec{r}_i - \vec{r}_j)/\left(\frac{1}{\ln(T/J)}\right)}$$

指数型衰减

Kosterlitz-Thouless transition

- **The periodicity of spins allows topological vortex configurations.**



$$\oint d\vec{l} \cdot \nabla\theta(\vec{r}) = 2\pi n_V$$

- **Spontaneous vortex formation**

$$U = \frac{J}{2}\int d^2r\,(\nabla\theta(\vec{r}))^2 = J\pi\int_a^L \frac{dr}{r} = J\pi\ln\frac{L}{a}$$

$$S = k_B\ln\Omega = k_B\ln\left(\frac{L^2}{a^2}\right) = 2k_B\ln\frac{L}{a}$$

$$F = E - TS = (\pi J - 2k_BT)\ln\frac{L}{a}$$

$$\lim_{L\to\infty}\Delta F = \begin{cases} -\infty & \text{if } T > \frac{\pi J}{2k_B} \\ +\infty & \text{if } T < \frac{\pi J}{2k_B}. \end{cases}$$

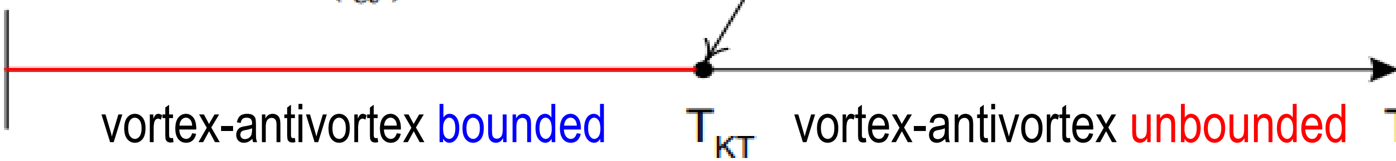
涡旋的出现使得体系的自旋从低温时的准长程序变成高温时的完全无序。因此，KT相变本质上是拓扑缺陷（即涡旋）诱导的相变。

Kosterlitz-Thouless transition

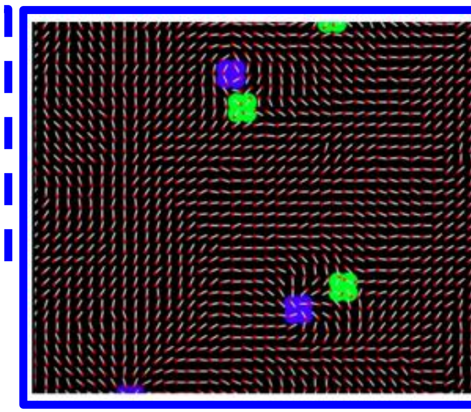
$$G(r) \sim \left(\frac{r}{a}\right)^{-\eta(T)}$$

Vortex unbinding

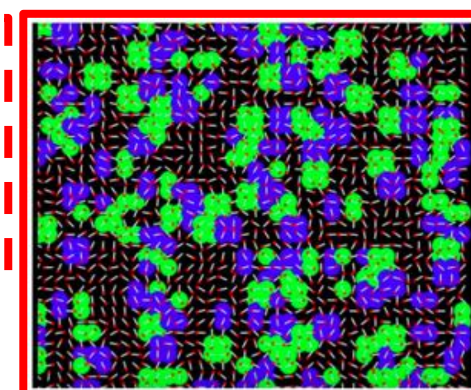
$$G(r) \sim e^{-\frac{r}{\xi(T)}}, \quad \xi(T) \sim e^{\frac{\text{const.}}{\sqrt{T-T_{\text{KT}}}}}$$



Below T_{KT}, the vortices and anti-vortices bound in pairs by a logarithmic confining potential, and their correlation function decays algebraically.



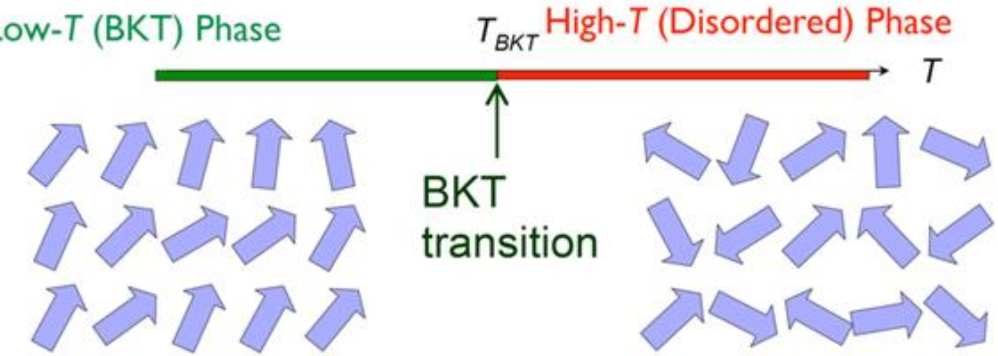
Above T_{KT}, the vortices proliferate and their correlation function decays exponentially, and the correlation length diverges extremely rapidly near the critical point.



Kosterlitz-Thouless transition

$$\langle \vec{s}_i \cdot \vec{s}_j \rangle \propto \left(\frac{1}{r}\right)^{\eta}$$

power-law decay



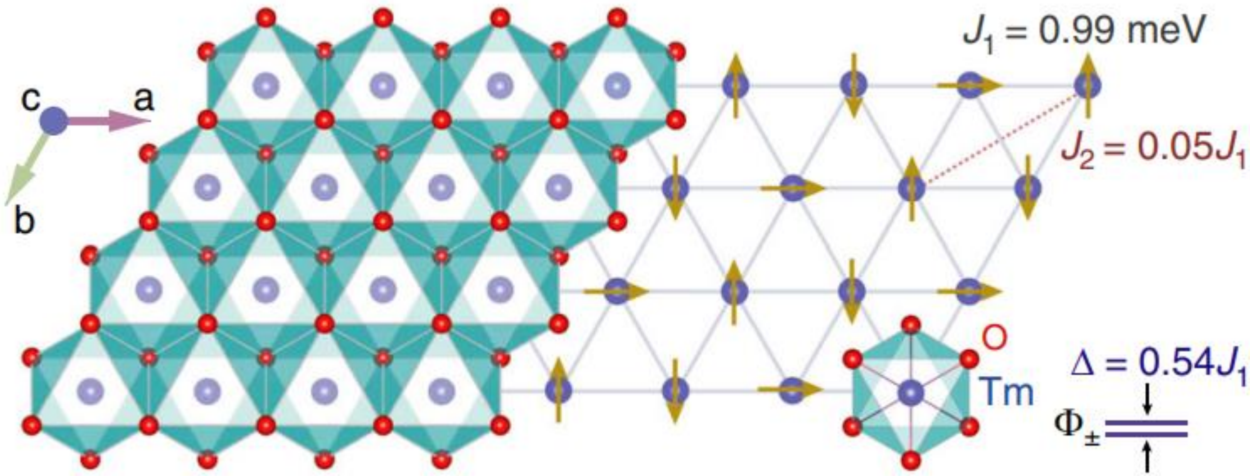
$$\langle \vec{s}_i \cdot \vec{s}_j \rangle \propto \exp\left(-\frac{r}{\xi}\right)$$

exponential decay

- No local order parameter
- No spontaneously symmetry breaking
- Phase transition caused by topological excitations
- Termed Infinite order phase transition (in the sense that no discontinuity in any order derivative of free energy)

- A phase transition that is beyond Landau paradigm
- Topology is an important concept in modern condensed matter physics.

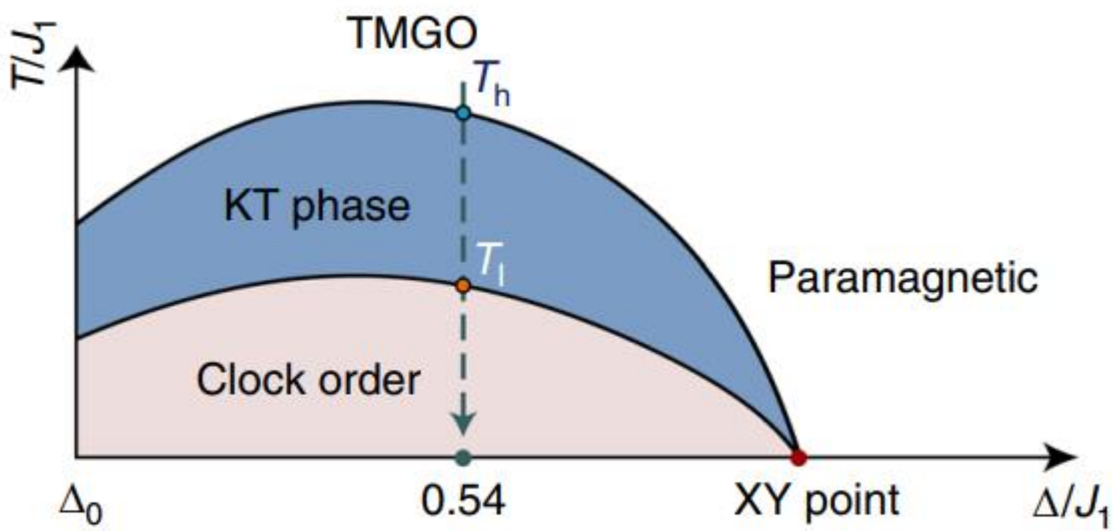
$TmMgGaO_4$: Realization of KT transition

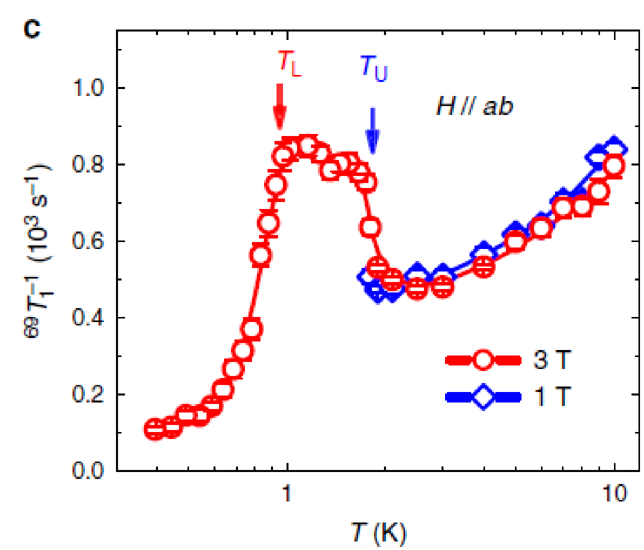


H. Li, et al., NC (2020)
李伟课题组

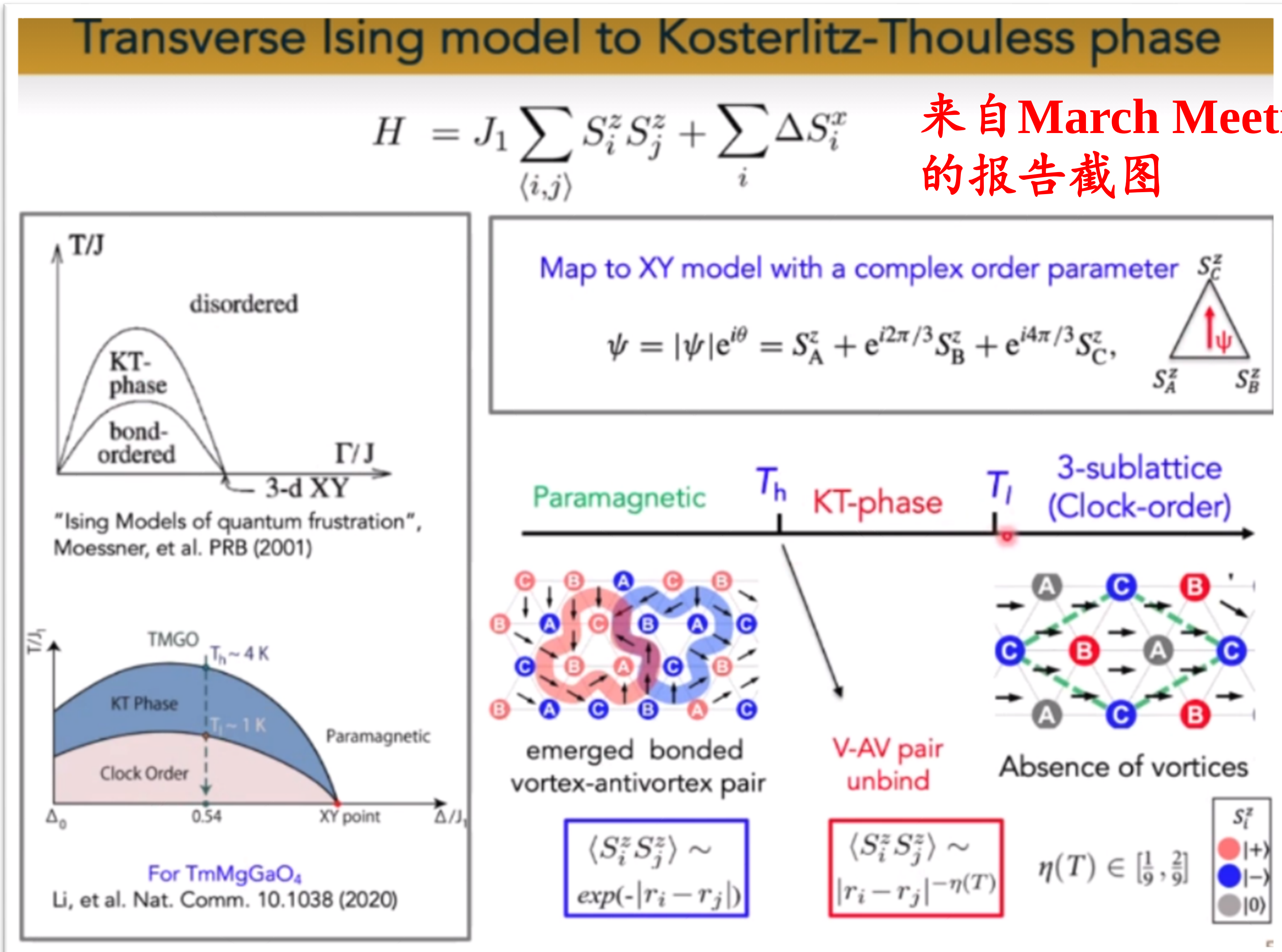
Z. Hu, et al., NC (2020)
于伟强课题组

$$H_{\mathrm{TLI}} = J_1 \sum_{\langle i,j \rangle} S_i^z S_j^z + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^z S_j^z - \sum_i (\Delta S_i^x + h\, g_{\parallel} \mu_B\, S_i^z),$$





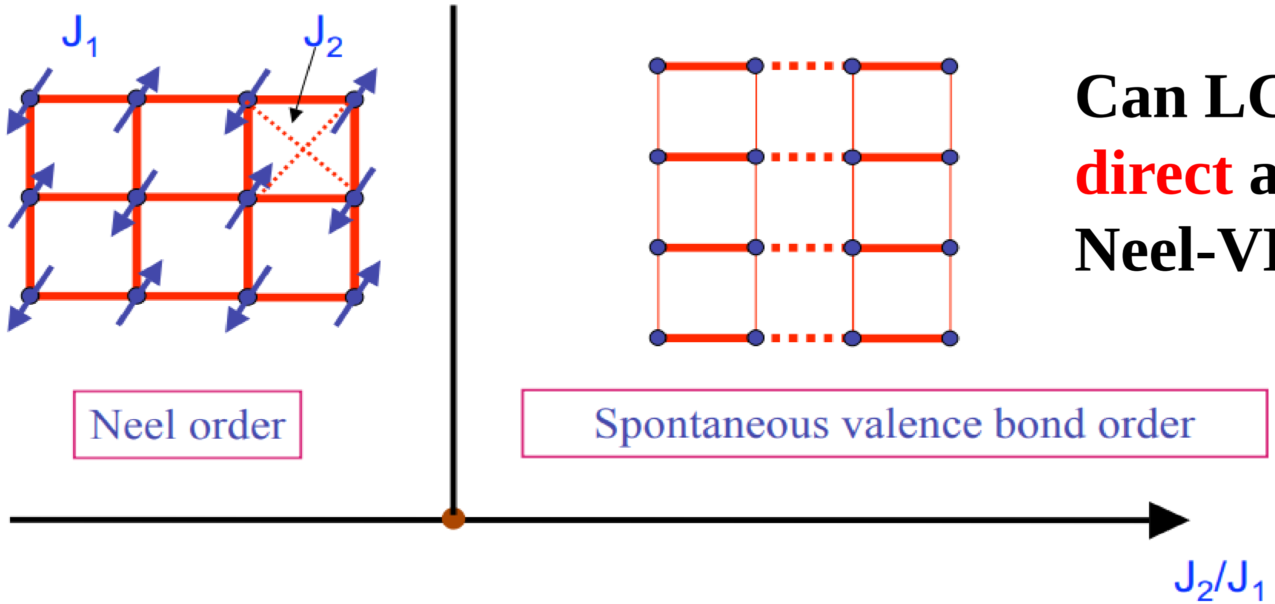
$TmMgGaO_4$: Realization of KT transition



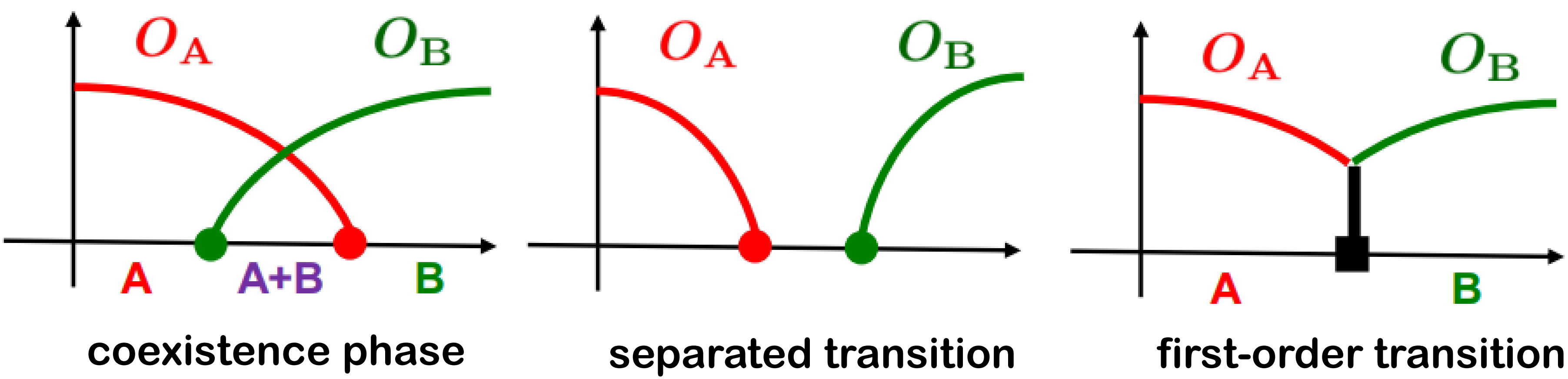
来自March Meeting
的报告截图

Beyond Landau's paradigm：去禁闭量子临界点

- Deconfined quantum criticality:有序-有序相变



Can LGW describe a **direct** and **continuous** Neel-VBS transition?



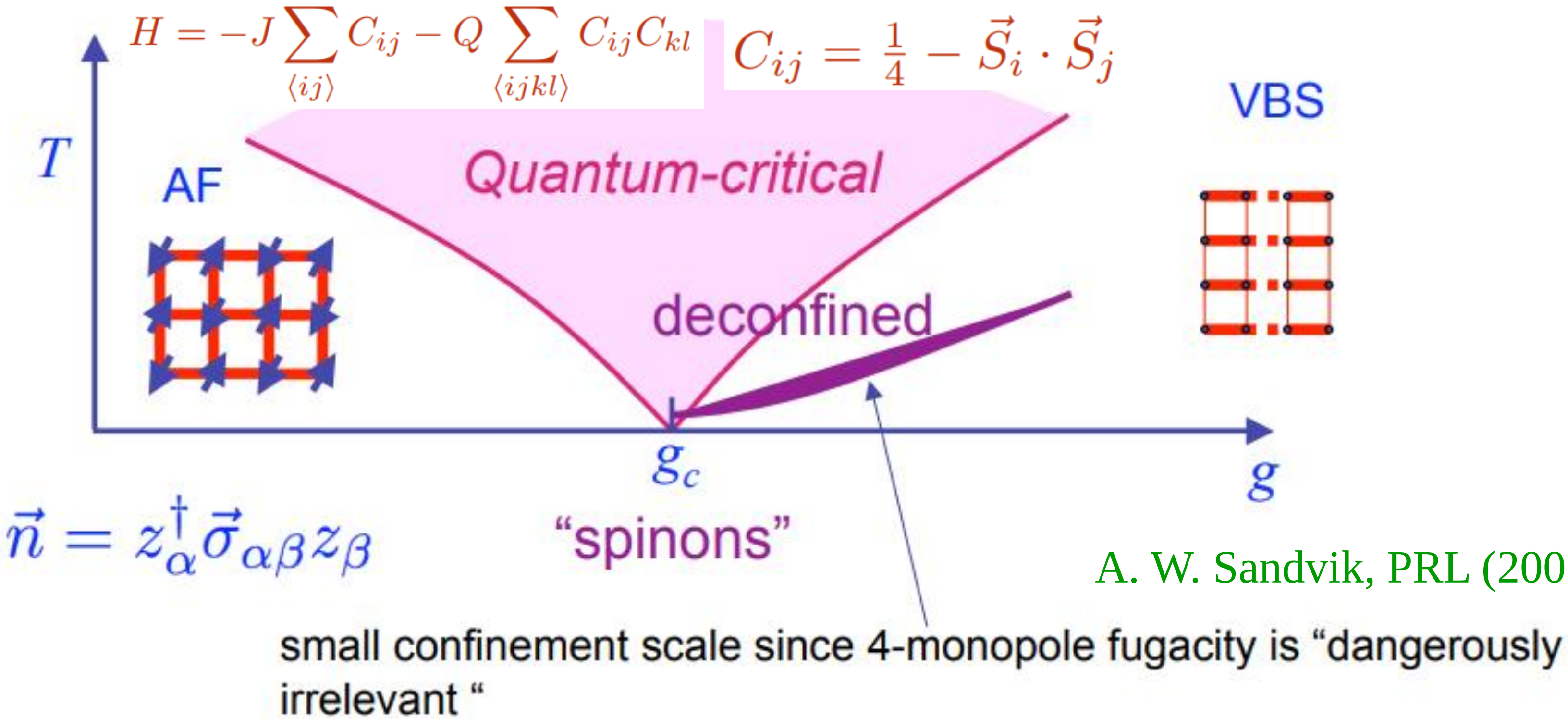
Beyond Landau's paradigm：去禁闭量子临界点

❖ **Deconfined quantum criticality:有序-有序相变**

Deconfined Quantum Critical Points

T. SENTHIL, ASHVIN VISHWANATH, LEON BALENTS, SUBIR SACHDEV, AND MATTHEW P. A. FISHER Authors Info & Affiliations

SCIENCE • 5 Mar 2004 • Vol 303, Issue 5663 • pp. 1490-1494 • DOI: 10.1126/science.1091806



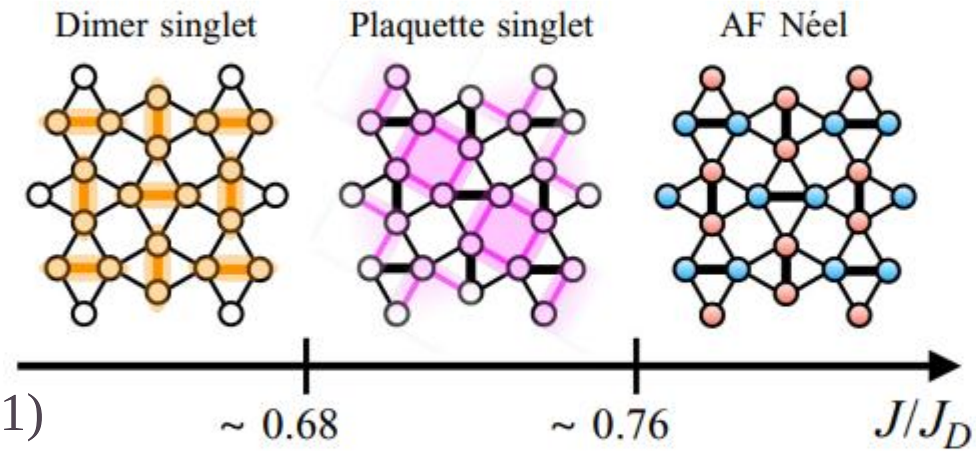
A. W. Sandvik, PRL (2007)

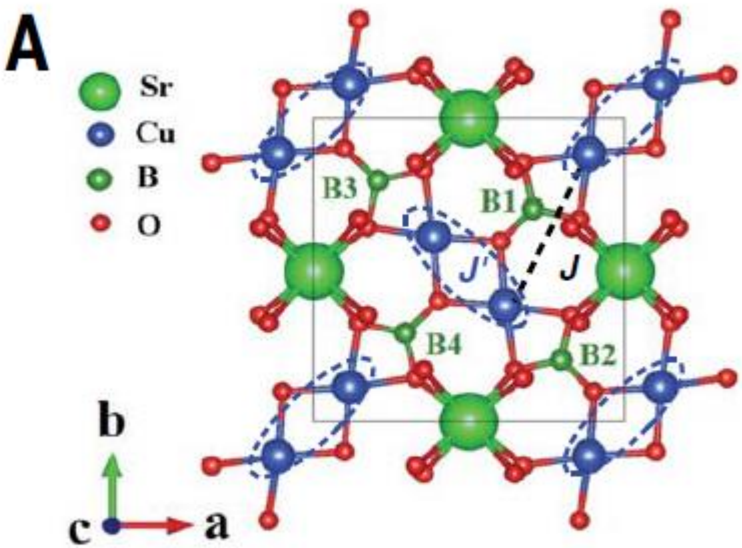
$SrCu_2(BO_3)_2$: Realization of DQCP

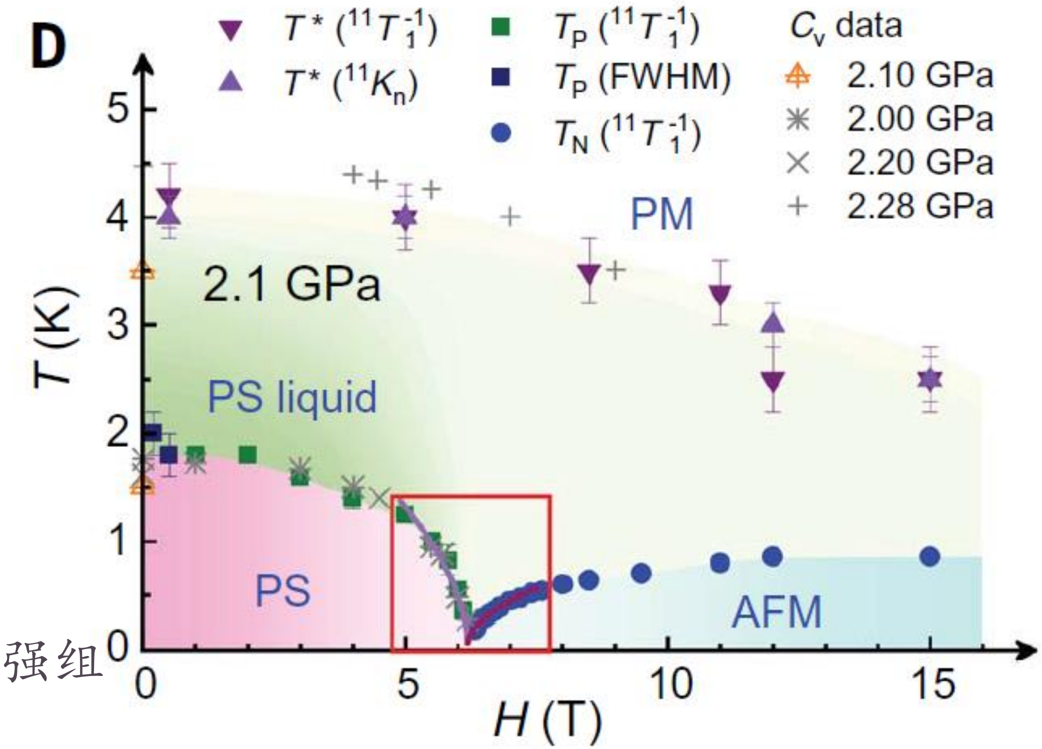
Shastry-Sutherland model

$$\mathcal{H} = J_D \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j.$$

Shastry & Sutherland Physica B+C(1981)







Y. Cui, et al., Science (2023) 于伟强组

Spinon excitation and Luttinger liquid

Heisenberg spin chain $\mathcal{H} = J\sum_j \vec{S}_j \cdot \vec{S}_{j+1}$

- **for spin-1/2 case**: the ground state is gapless with an algebraical decay of spin-spin correlation function (**quasi-long-range** order).

Lieb-Schultz-Mattis (LSM) theorem

If a quantum spin system defined on a lattice has odd number of spin-1/2 per unit cell, then any local spin Hamiltonian which preserves the spin and translation symmetry cannot have a featureless (gapped and nondegenerate) ground state.

Bethe ansatz

- $e_g^{\mathrm{LL}} = 1/4 - \ln 2 = -0.44314718\cdots$

H. A. Bethe (1931); L. Hulthen (1938)

- $\langle S_0 \cdot S_n \rangle \propto (-1)^n \frac{\sqrt{\ln n}}{n}$

Johnson etal., PRA 8, 2526 (1973)

Spinon excitation and Luttinger liquid

Heisenberg spin chain

$$\mathcal{H} = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$$

- **for spin-1/2 case**: the ground state is gapless with an algebraical decay of spin-spin correlation function (**quasi-long-range** order).

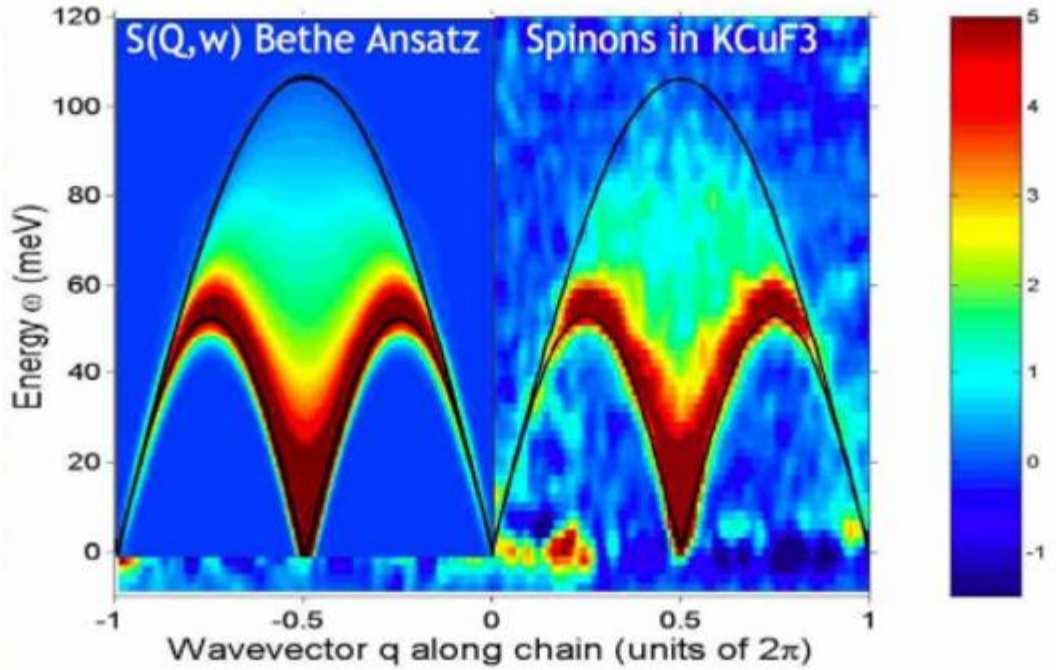
Bethe ansatz

upper bound:

$$\omega_U(q) = \pi J \sin\left(\frac{1}{2}q\right)$$

lower bound:

$$\omega_L(q) = \frac{\pi}{2} J \sin(q)$$



→ Continuous spectrum implies that the ground state is a spin liquid with the spinon as its excitation.

Spinon excitation and Luttinger liquid

Heisenberg spin chain

$$\mathcal{H} = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$$

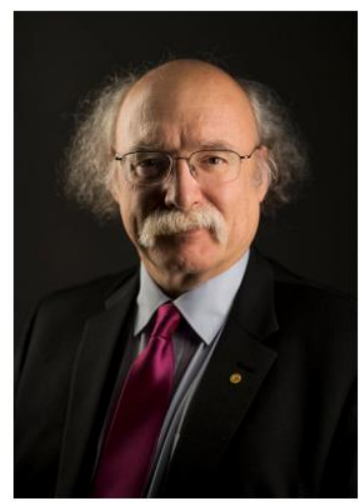
- **for spin-1 case**: the ground state is gapped with an exponential decay of spin-spin correlation function (**short-range** order).

F. D. M. Haldane,. PRL 50, 1153 (1983)

The Nobel Prize in Physics 2016
David J. Thouless, F. Duncan M. Haldane, J. Michael Kosterlitz

Share this: 61

F. Duncan M. Haldane - Facts



F. Duncan M. Haldane

Born: 14 September 1951, London, United Kingdom

Affiliation at the time of the award: Princeton University, Princeton, NJ, USA

Prize motivation: "for theoretical discoveries of topological phase transitions and topological phases of matter"

Prize share: 1/4

Haldane conjecture

- **For** $S = \frac{1}{2}, \frac{3}{2}, \frac{5}{3}, \cdots$, **the ground state is gapless.**

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \propto \left(\frac{1}{r}\right)^{\eta}$$

similar to the **low-*T*** phase of 2D XY model

- **For** $S = 1, 2, 3, \cdots$, **the ground state is gapped.**

$$\langle \vec{S}_i \cdot \vec{S}_j \rangle \propto \exp\left(-\frac{r}{\xi}\right)$$

similar to the **high-*T*** phase of 2D XY model

☆ **DMRG Calculation of Haldane Gap**

$$\Delta_{\text{Hald}} \propto \hbar c/\xi = JSe^{-\pi S}.$$

arXiv:1906.12207

$$\Delta(S=1) \simeq 0.41050(2)$$

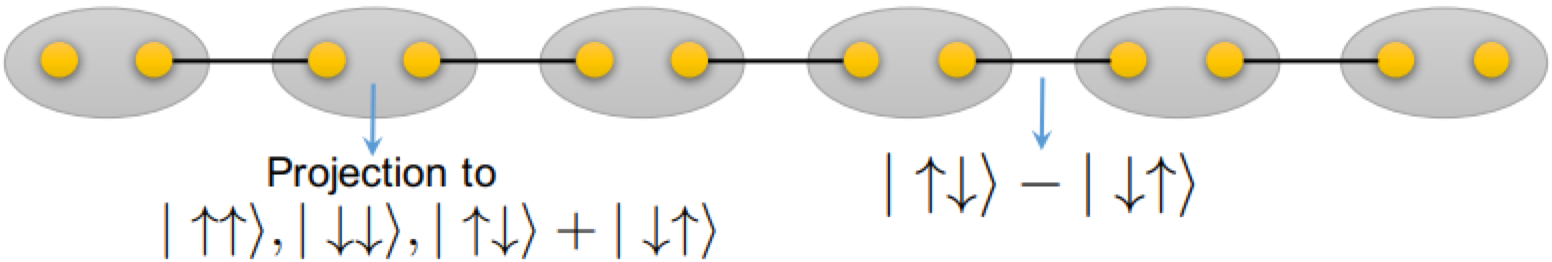
S. R. White & D. A. Huse, PRB (1993)

$$\Delta(S=2) \simeq 0.0876(13)$$

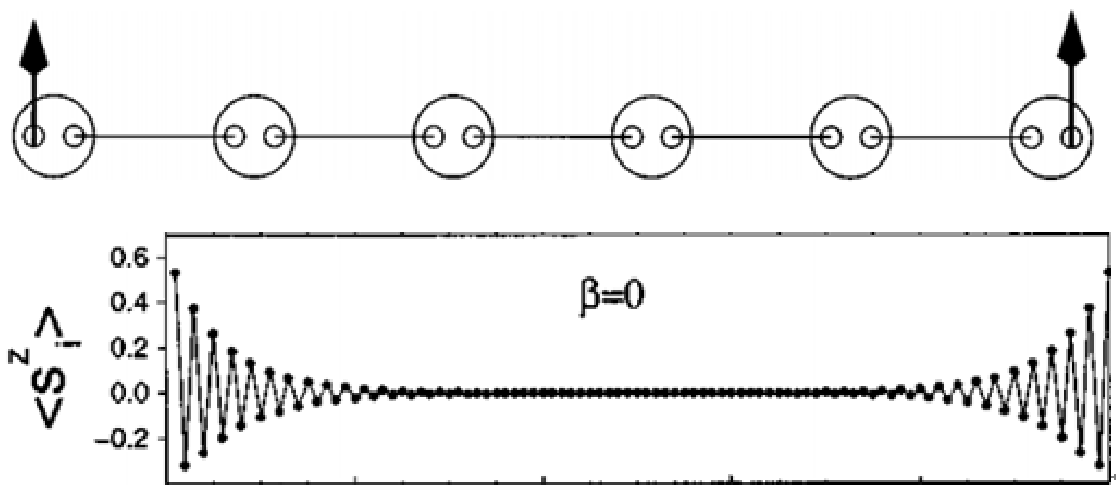
X. Wang, S. Qin, and L. Yu, PRB (1999)

edge states and symmetry fractionalization

- **Spin-1/2 edge states**



- Spin singles are formed between nearest-neighbor sites.
- There are two isolated spin 1/2's at the ends of an **open** chain, giving rise to a four-fold ground-state degeneracy.



Nonlocal string order parameter

- **Diluted AFM order**

$$\uparrow 0\,0\,0 \downarrow 0 \uparrow 0\,0 \downarrow 0 \uparrow 0\,0\,0 \downarrow 0 \uparrow 0\,0\,0\,0 \downarrow$$

$$\uparrow \quad \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \quad \downarrow$$

- **Hidden string order parameter**

M. den Nijs & K. Rommelse, PRB 40, 4709 (1989)

$$\mathcal{O}^{\alpha}_{\mathrm{str}} = -\lim_{|i-j|\to\infty} \left\langle S^{\alpha}_{i} e^{i\pi \sum_{l=i+1}^{j-1} S^{\alpha}_{l}} S^{\alpha}_{j} \right\rangle, \qquad \alpha = x, y, z.$$

$$\begin{aligned}|S{=}1\ \mathrm{VBS}\rangle &= |\cdots 00000000 \cdots\rangle + \cdots + |\cdots + 000000 - \cdots\rangle \\ &+ |\cdots 0 + 000 - 00 \cdots\rangle + |\cdots - 0 + 00 - 0 + \cdots\rangle \\ &+ |\cdots + - 0 + 0 - 0 + \cdots\rangle + \cdots \\ &+ |\cdots + - + - + - + - \cdots\rangle\end{aligned}$$

Outline

❑ 朗道相变理论和新突破

- ➢ Ising模型中的相变
- ➢ Kosterlitz-Thouless相变和去禁闭量子临界点
- ➢ Luttinger液体和Haldane相

❑ 量子自旋液体和自旋轨道耦合型材料

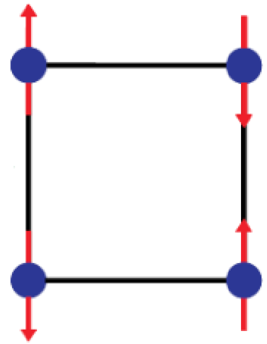
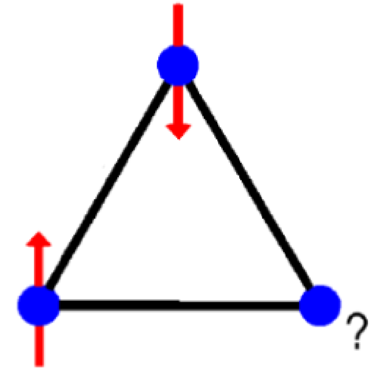
- ➢ 量子自旋液体简介
- ➢ 三角晶格上的量子材料
- ➢ 蜂窝晶格上的量子材料

❑ Kitaev-Γ模型中的物理

- ➢ 自旋S=1/2和1的Kitaev-Γ自旋链
- ➢ 自旋S=1的Kitaev-Γ模型

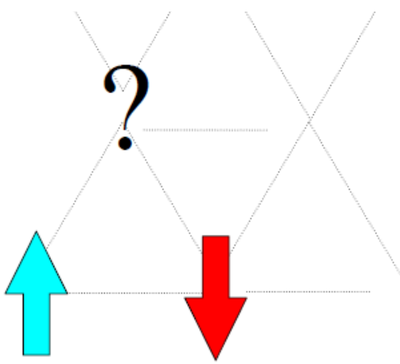
Triangular Ising antiferromagnet

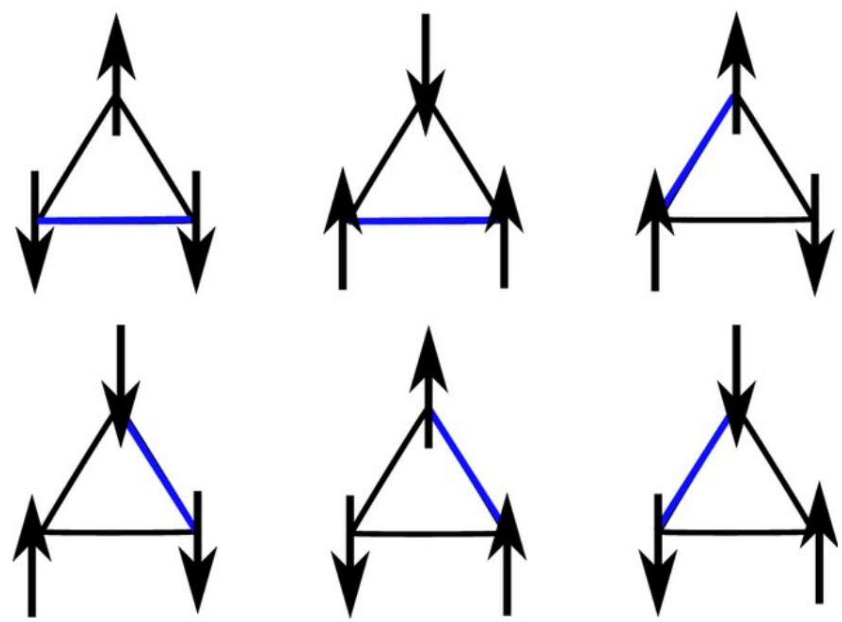
frustrated
vs
un-frustrated

Geometrical Frustration: The geometry of the lattice precludes the *simultaneous* minimization of all interactions.

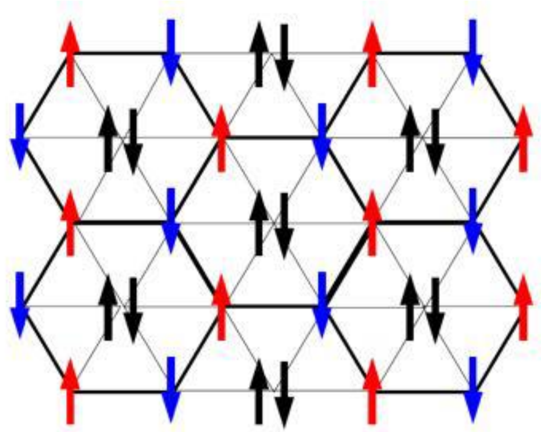
$$H = -J \sum_{\langle i,j \rangle} S_i S_j$$





Triangular Ising antiferromagnet

- **Extensive ground-state degeneracy**



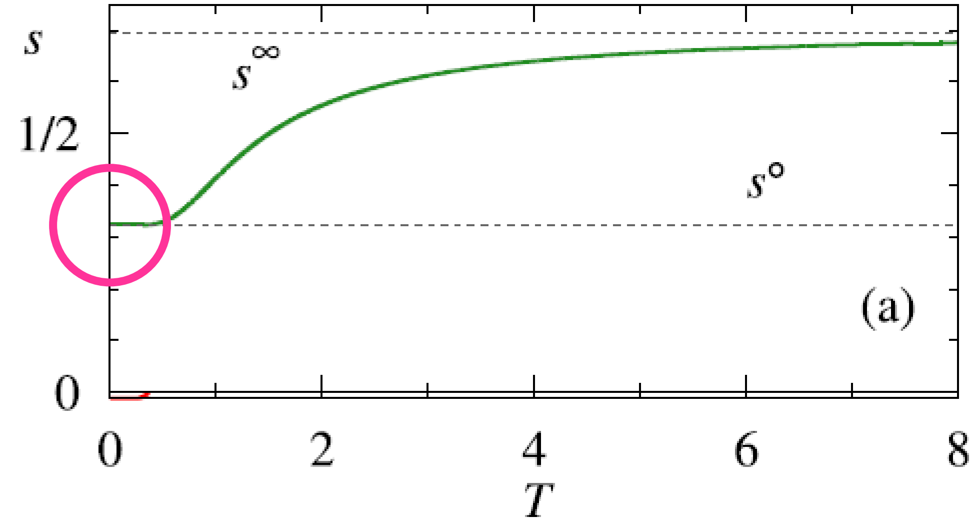
at least $2^{N/3}$ ground-state degeneracy.

residue entropy $s > \ln 2/3 \approx 0.210$.

- **Residue entropy**

$$s^\circ = \frac{2}{\pi} \int_0^{\pi/3} \ln(2\cos\alpha)\, d\alpha \approx 0.323\,066.$$

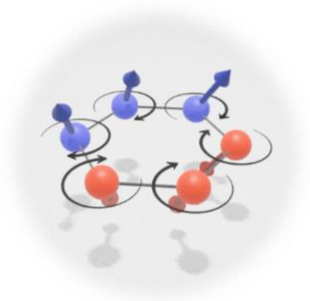
G. H. Wannier, Phys. Rev. 79, 357 (1950)

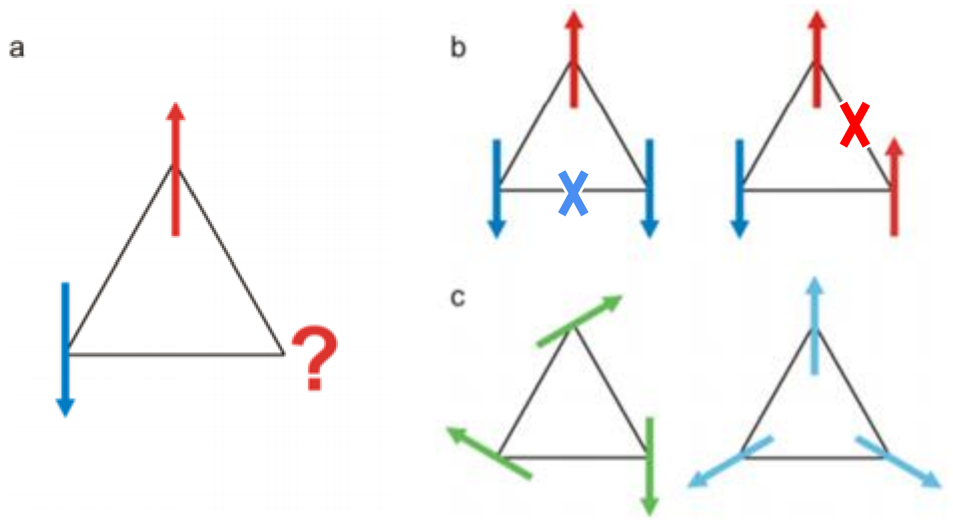


Triangular Heisenberg antiferromagnet

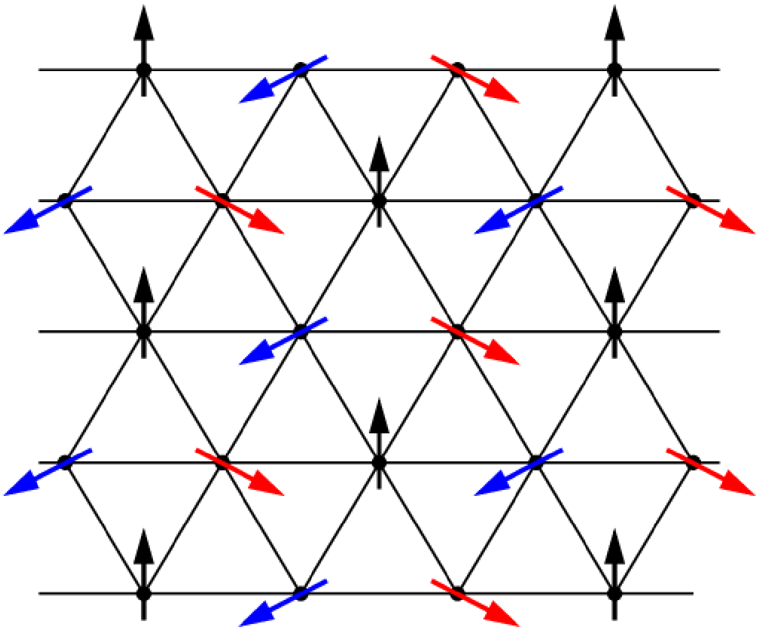
- Spin-1/2 Heisenberg antiferromagnet

$$H = J \sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \cdots$$



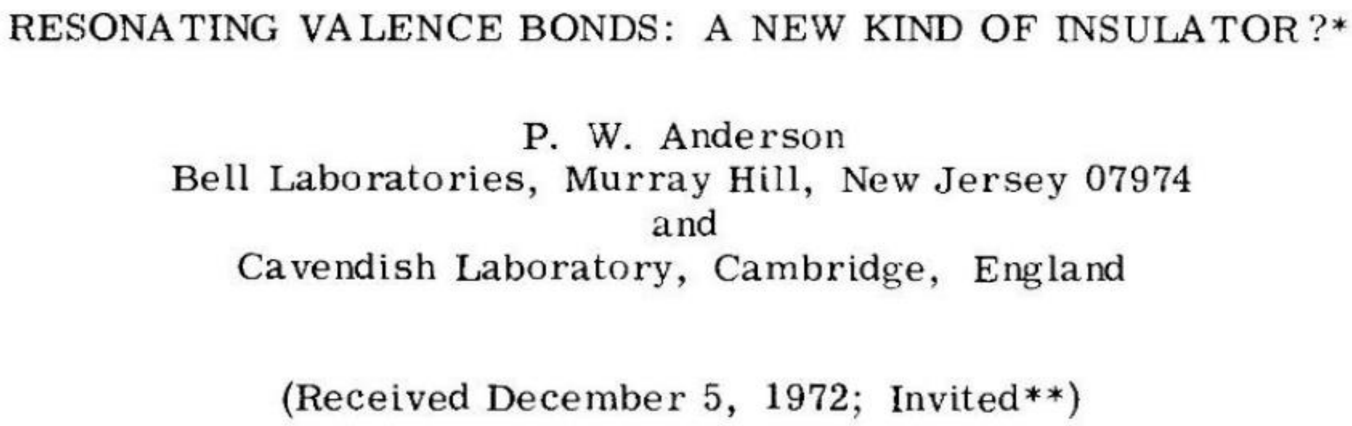


geometrical frustration



three-sublattice 120° order

Triangular Heisenberg antiferromagnet

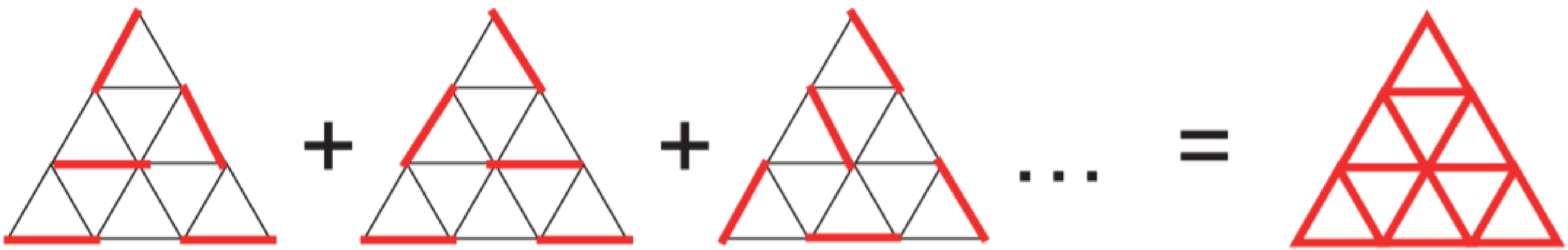

RESONATING VALENCE BONDS: A NEW KIND OF INSULATOR?*

P. W. Anderson
Bell Laboratories, Murray Hill, New Jersey 07974
and
Cavendish Laboratory, Cambridge, England

(Received December 5, 1972; Invited**)

Anderson's proposal: **Anderson, Mater. Res. Bull. 8, 153 (1973)**

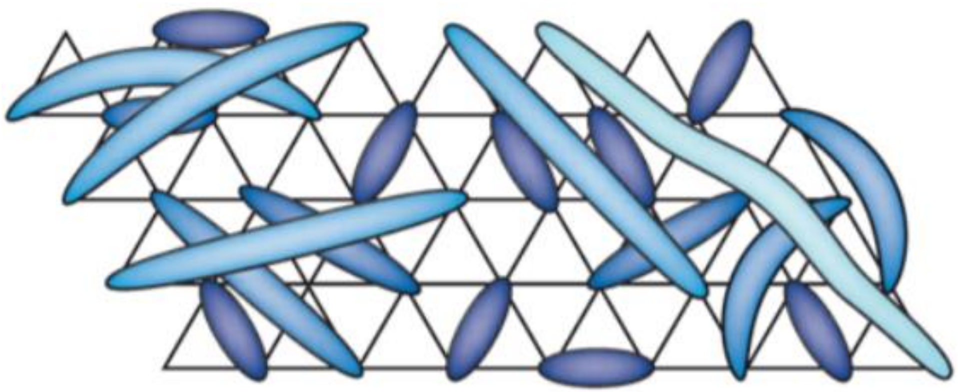
a short-range Resonating-Valence Bond (**RVB**) state



Linear superposition of infinite No. of VB configurations

Quantum Spin Liquid

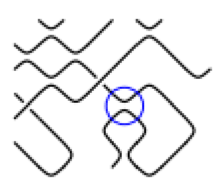
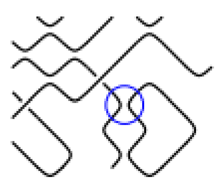
QSL is a nonmagnetic state with **long-range entanglement**



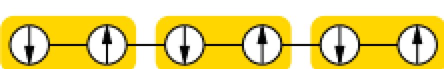
+ ...

Xiao-Gang Wen

(cannot be written as a product state of short-range-entangled blocks)

$$|\Psi_{\mathrm{RVB}}\rangle \sim |\Psi_{\mathrm{loop/string}}\rangle = \Big|$$  $$\Big\rangle + \Big|$$  $$\Big\rangle + \cdots$$

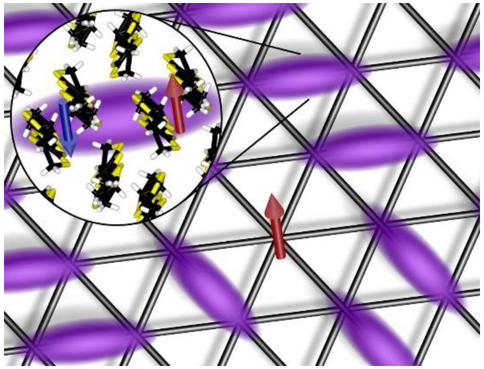
no local unitaries

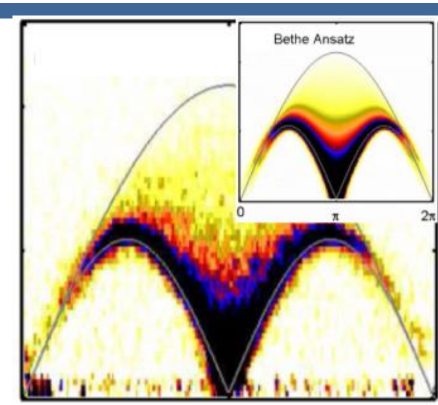


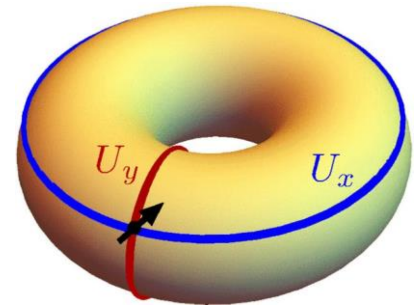
$$= (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle) \otimes (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle) \otimes \ldots$$

Product state of short-range entangled blocks

Quantum Spin Liquid





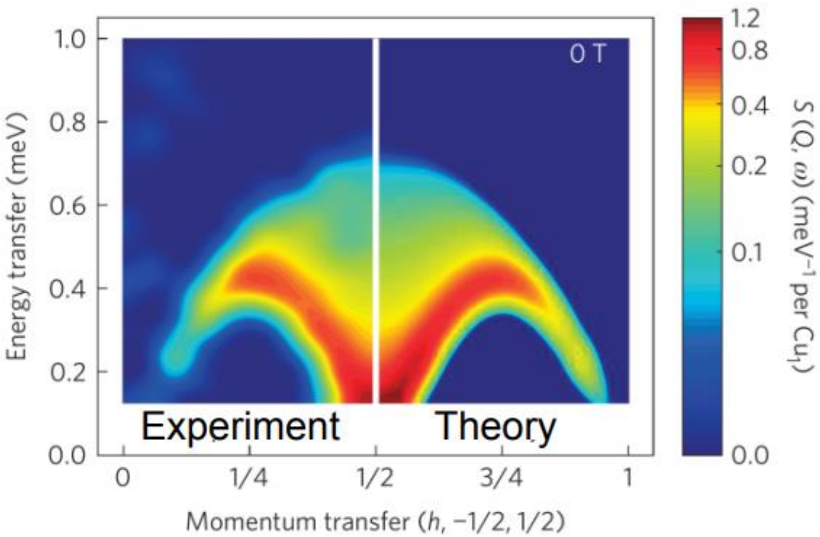


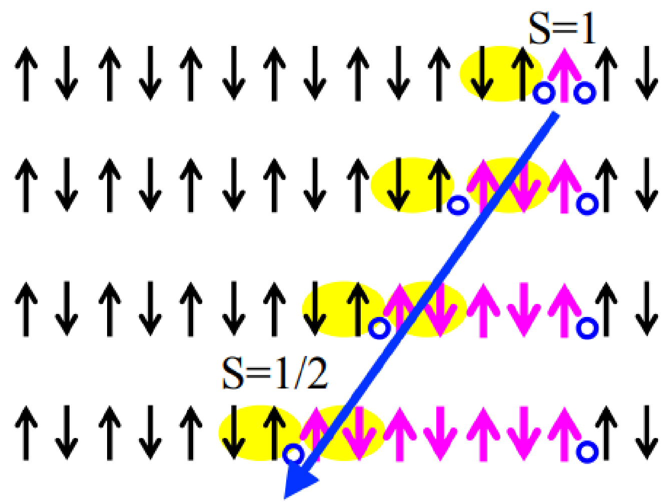
fractionalized excitations
spinon, vison, etc

continuum spectrum
$S(q, \omega)$

topological degeneracy

1D example: spin-1/2 Heisenberg chain



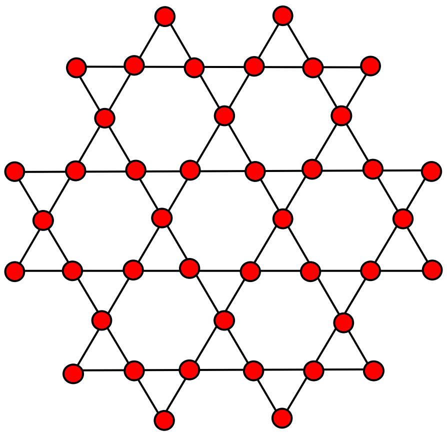


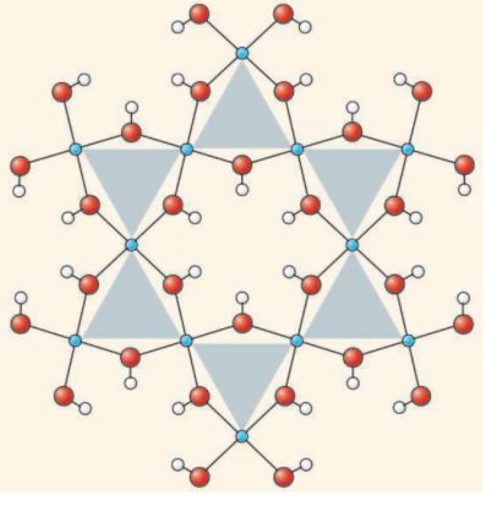
No energy cost in moving spinons far apart

几何阻挫：Kagome Lattice

Kagome Heisenberg model

$$H = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad J > 0$$





Herbertsmithite: $ZnCu_3(OH)_6Cl_2$

Shores, *et al.*, J. Am. Chem. Soc. (2005).

- **low** dimension (d = 2)
- **low** spin (S = 1/2)
- **low** coordination number (z = 4)
- **non-bipartite** nature

Kagome SL

Yan et al., Science **332**, 1173 ('11)

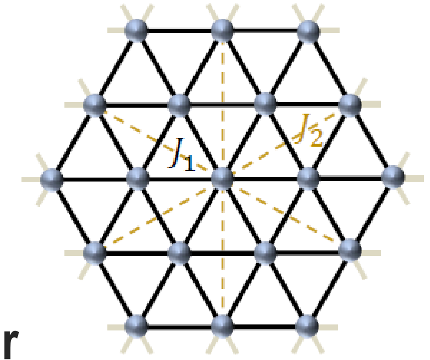
Liao et al., PRL **118**, 137202 ('17)

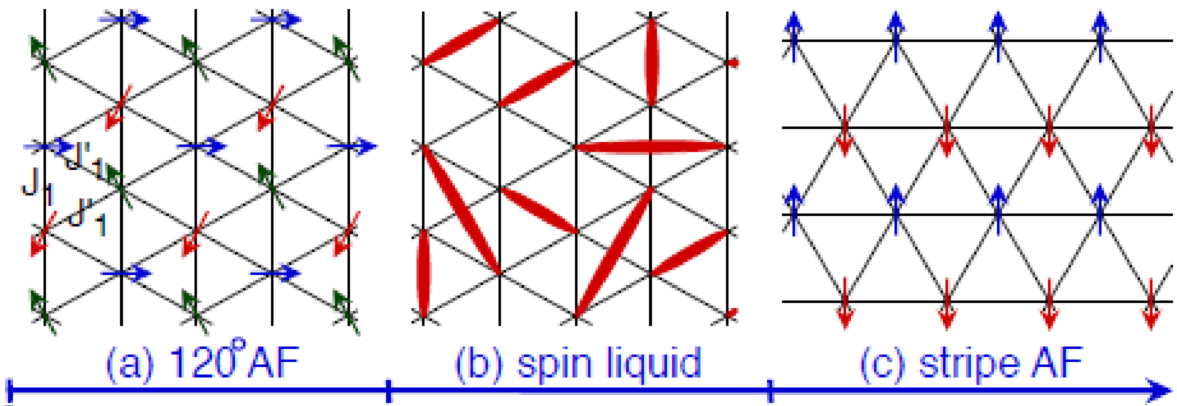
and more …

竞争相互作用：J_1-J_2模型

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} S_i S_j + J_2 \sum_{\langle\langle ij \rangle\rangle} S_i S_j$$

三角晶格





Hu, et al., PRL **123**, 207203 ('19)

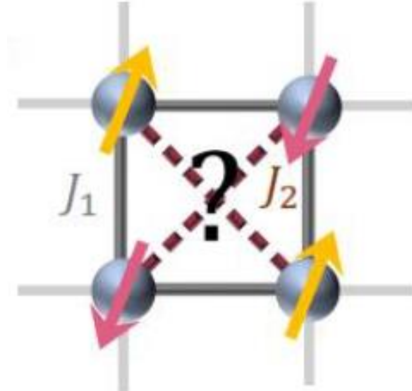
S-S Gong, et al. PRB 100, 241111(R) ('19)

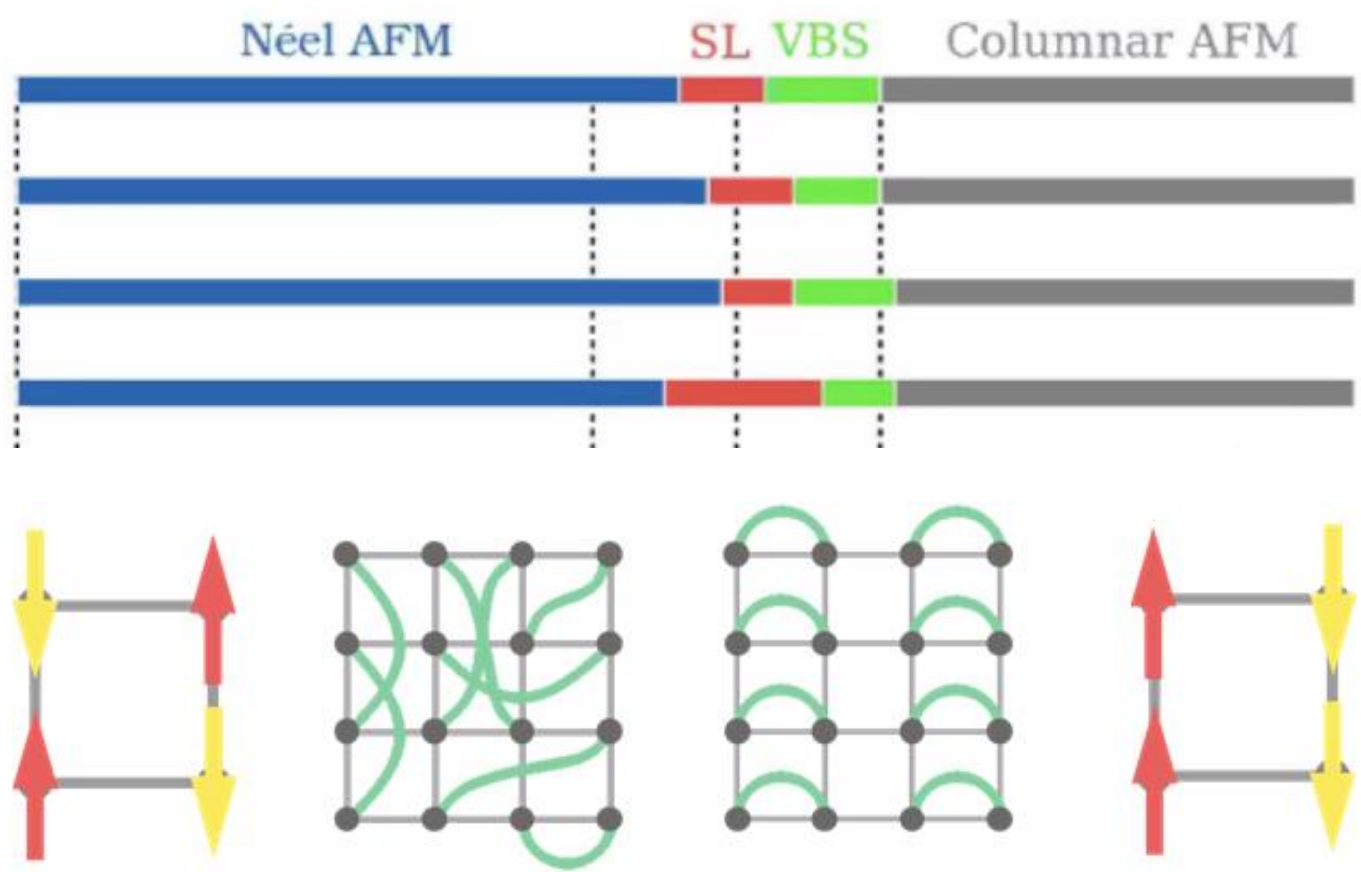
F. Ferrari and F. Becca. PRX 9, 031026 ('19), and more

竞争相互作用：J_1-J_2模型

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} S_i S_j + J_2 \sum_{\langle\langle ij \rangle\rangle} S_i S_j$$

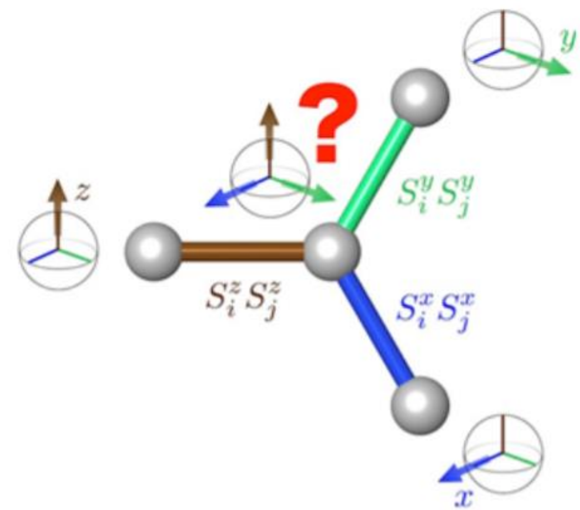
四方晶格





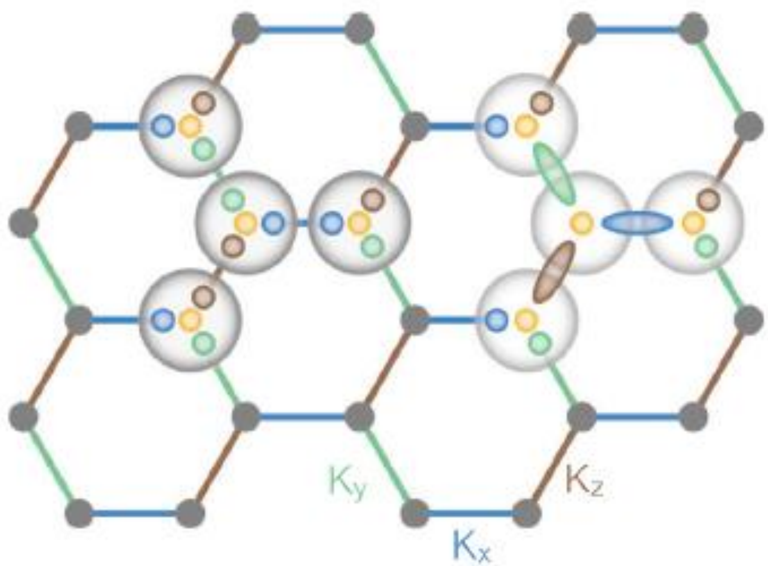
交换耦合效应：Kitaev蜂窝模型

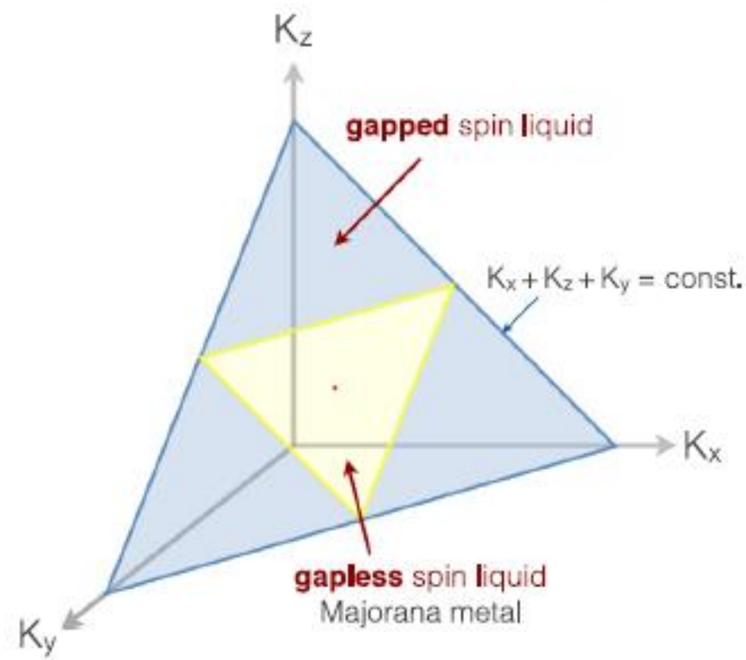
$$\mathcal{H} = -\sum_{\gamma-\text{bonds}} K_\gamma \, S_i^\gamma S_j^\gamma$$



Kitaev SL

Kitaev, Ann. Phys. **321**, 2-111 ('06)

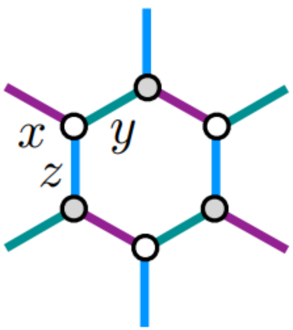


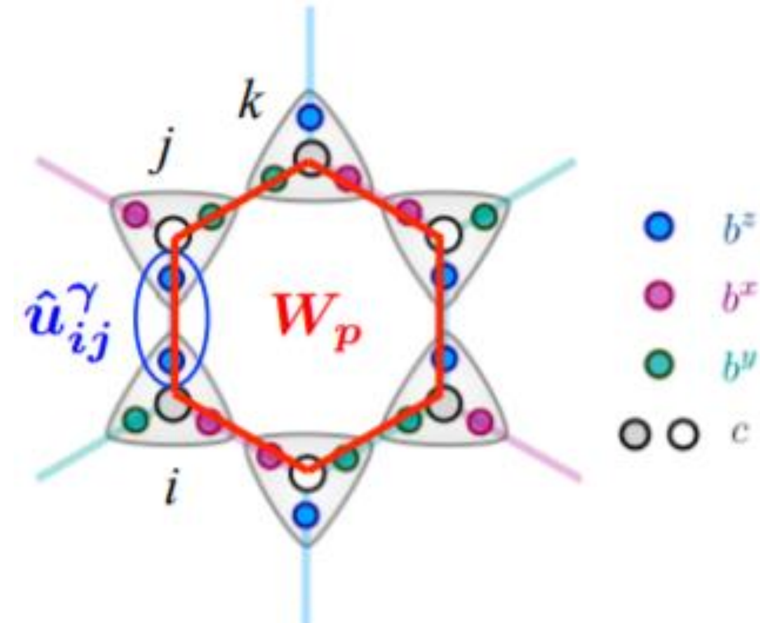


交换耦合效应：Kitaev蜂窝模型

- Kitaev model: $\mathcal{H} = \sum_{\langle ij\rangle \in \mathrm{red}} S_i^x S_j^x + \sum_{\langle ij\rangle \in \mathrm{green}} S_i^y S_j^y + \sum_{\langle ij\rangle \in \mathrm{blue}} S_i^z S_j^z$

A. Kitaev, Ann. Phys. (NY) **321**, 2-111 (2006)





Majorana fermions

$$b^x = a_\uparrow + a_\downarrow^\dagger$$
$$b^y = -i\left(a_\uparrow - a_\downarrow^\dagger\right)$$
$$b^z = a_\downarrow + a_\uparrow^\dagger$$
$$c = -i\left(a_\downarrow - a_\uparrow^\dagger\right)$$

$$\sigma^x = ib^x c$$
$$\sigma^y = ib^y c$$
$$\sigma^z = ib^z c$$

→

$$\mathcal{H} = \frac{i}{4}\sum_{i,j} J_{\gamma_{ij}} u_{ij} c_i c_j$$

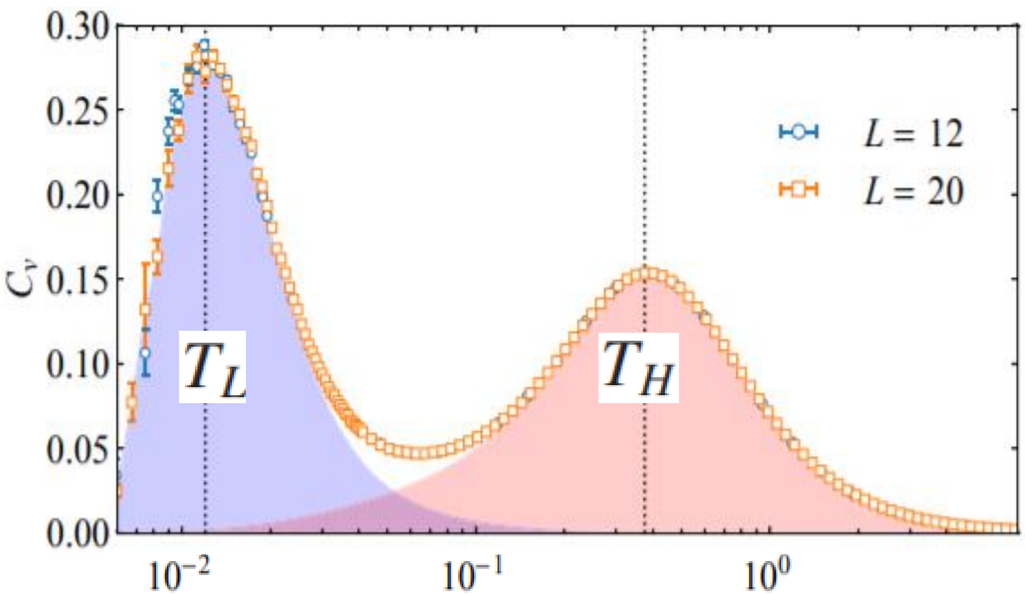
quadratic

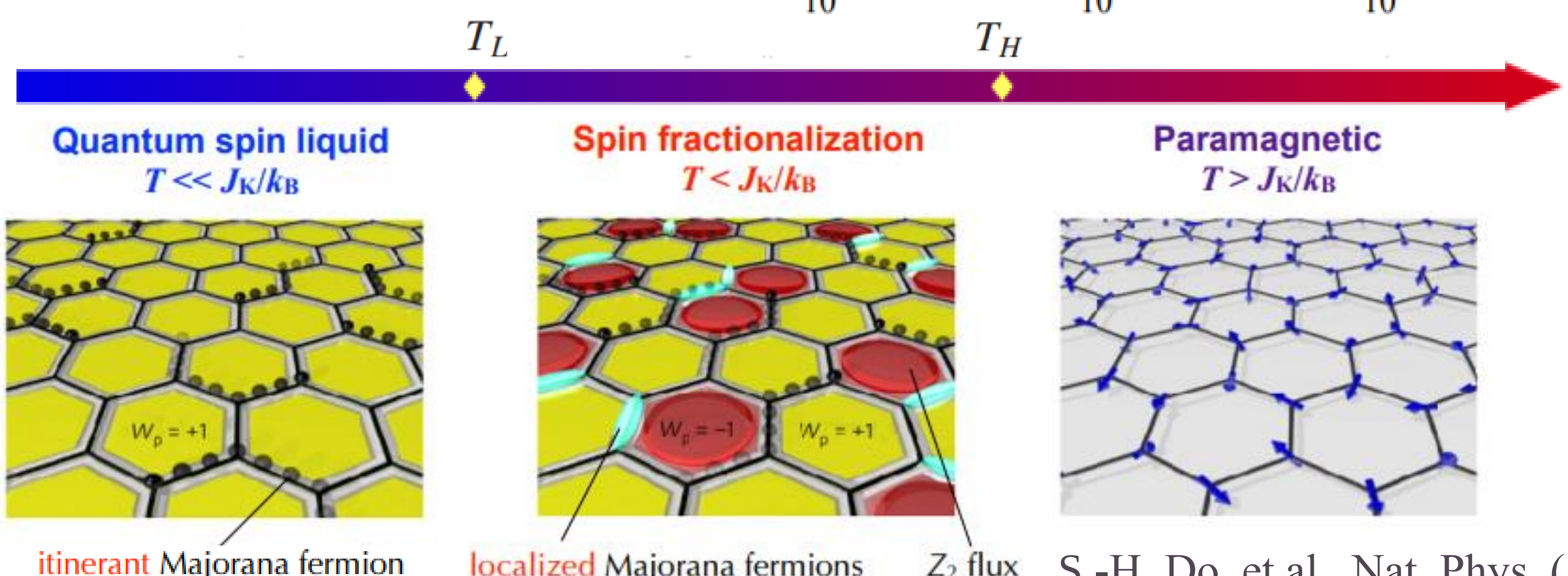
交换耦合效应：Kitaev蜂窝模型

- Spin fractionalization

S_i → c **Itinerant** Majorana fermion
S_i → b^γ **Localized** Z_2 fluxes

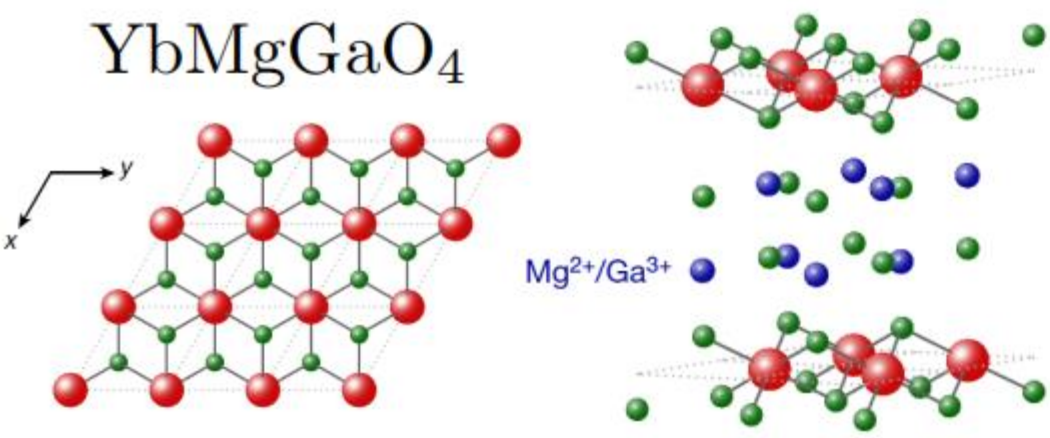
J. Knolle, *et al.*, PRL **112**, 207203 (2014)
J. Nasu, *et al.*, PRB **92**, 115122 (2015)



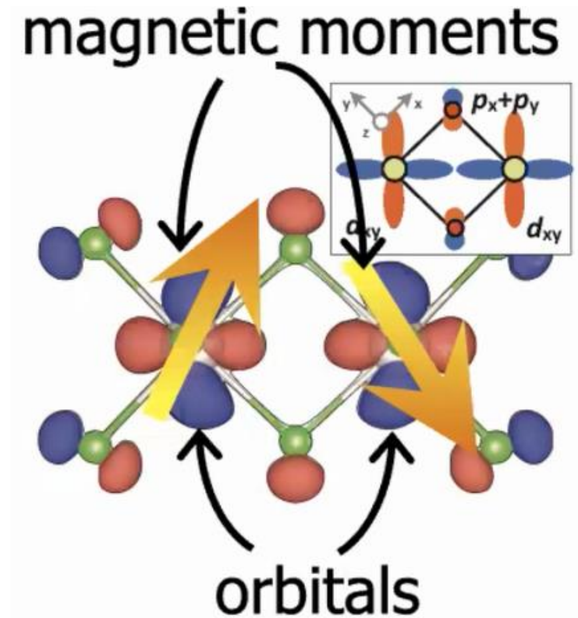


S.-H. Do, et al., Nat. Phys. ('17)

三角晶格QSL候选材料：$YbMgGaO_4$



Li et al., Scientific Reports 5, 16419 (2015).
Li et al., Phys. Rev. Lett. 115, 167203 (2015).



- rare-earth, Yb^{3+}, ***J***=*7/2*, + crystal-field splitting
- lowest doublet, effective *S*=*1/2*
- anisotropic exchanges … (compare to Heisenberg)

- octahedral environment …
- lattice symmetries ⇛ **four** terms in the exchange matrix
- mostly nearest-neighbor exchanges (***f***-electrons)

三角晶格QSL候选材料：$YbMgGaO_4$

Experimental facts

- $C_v \sim T^{2/3}$ at H=0

Li et al., Sci. Rep. 2015, Y.Xu, et al, PRL 2016, J. Paddison et al， NPhys 2017

- Constant susceptibility at T～0

Li et al., PRL 2015， Y. Shen， Nature 2016

- Constant μSR rate Li et al., PRL 2016

- Zero spin entropy: spin singlet ground state

Li et al., PRL 2015， J. Paddison et al， NPhys, 2017

- Neutron scattering: Diffusive spin excitations & Spinon Fermi surface Y. Shen, et al Nature 2016, J. Paddison et al， NPhys 2017

$\Rightarrow$ U(1) gapless quantum spin liquid

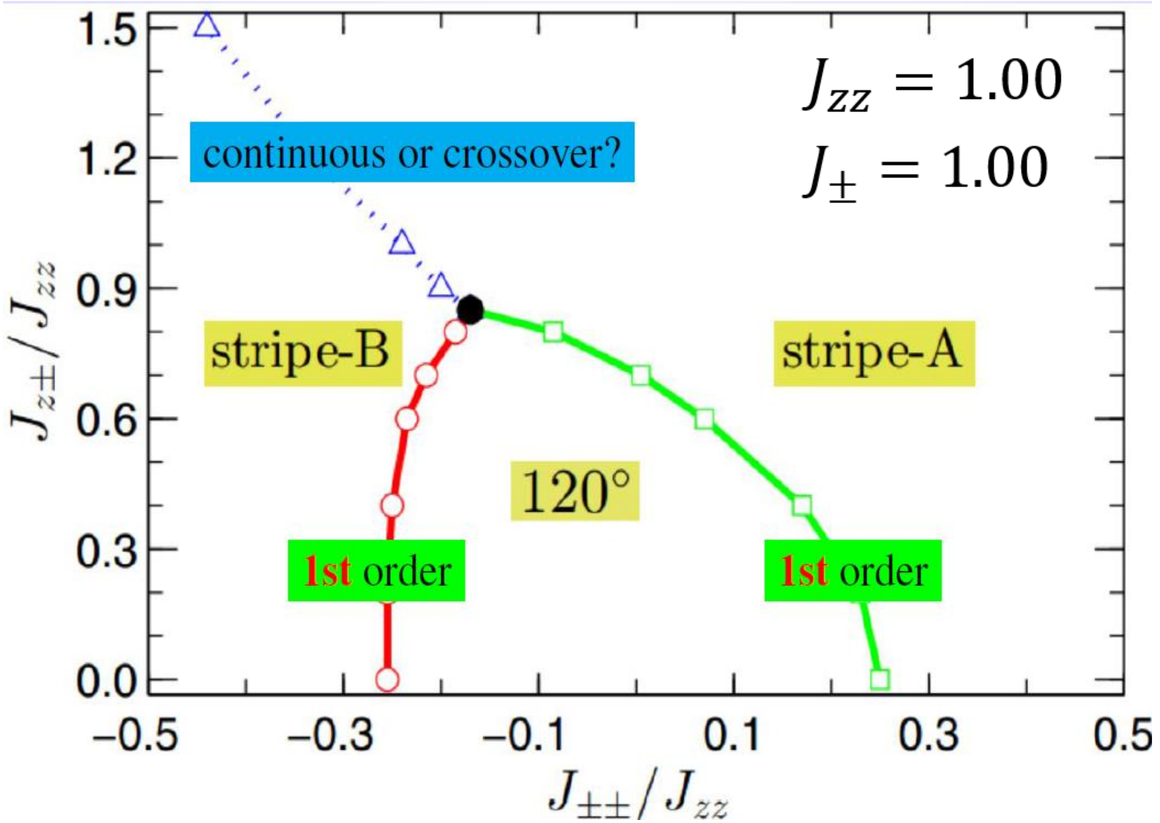
三角晶格QSL候选材料：$YbMgGaO_4$

$$\mathcal{H} = \sum_{\langle ij \rangle} \Big[\underline{J_{zz} S_i^z S_j^z + J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+)} \Longleftarrow \text{XXZ term}$$

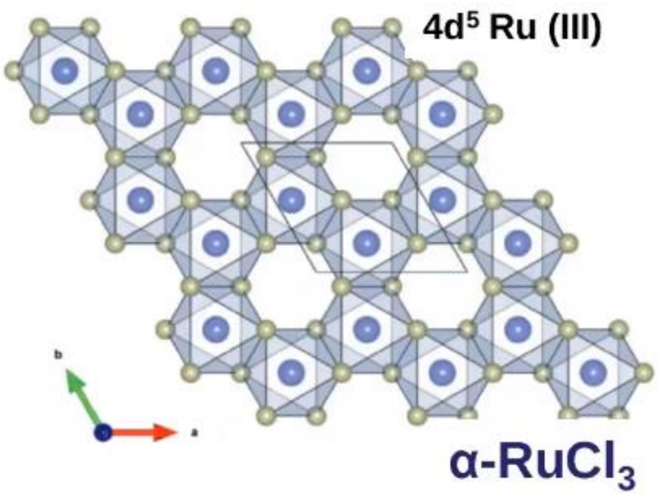
$$+ \underline{J_{\pm\pm}(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) - \frac{iJ_{z\pm}}{2}(\gamma_{ij}^* S_i^+ S_j^z - \gamma_{ij} S_i^- S_j^z + \langle i \leftrightarrow j \rangle)} \Big] \Longleftarrow \text{SOC}$$

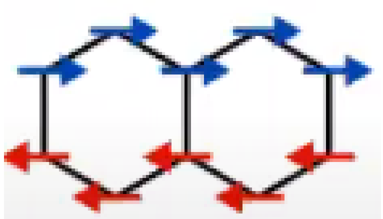
Q. Luo et al., PRB ('17)

$J_{zz} = 0.98(8)$K,
$J_{\pm} = 0.90(8)$K;
$J_{\pm\pm} = \pm 0.155(3)$K;
$J_{z\pm} = \pm 0.04(8)$K.



蜂窝晶格QSL候选材料：α-$RuCl_3$



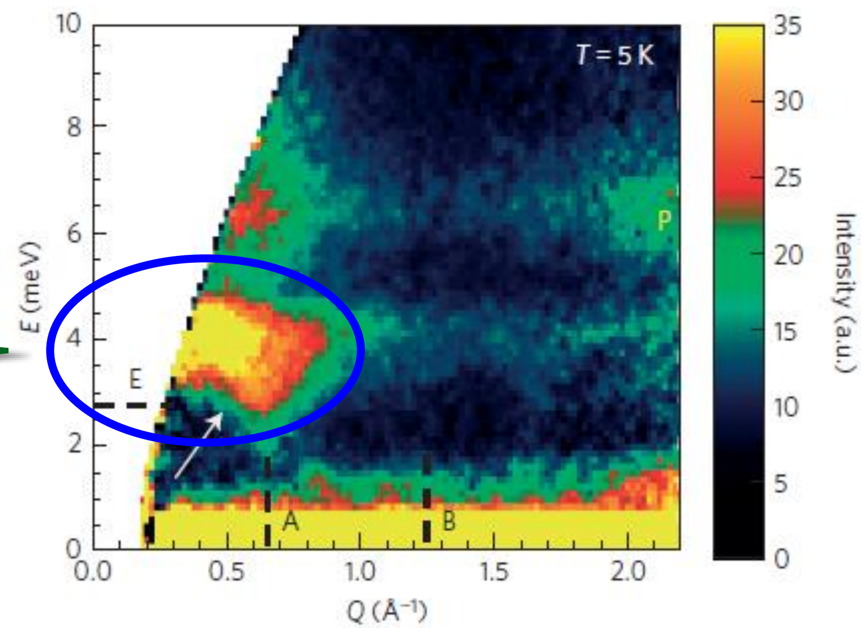


α-RuCl3: Zigzag order at T_N = 7 K

Plumb et al., PRB **90**, 041112(R) ('14)

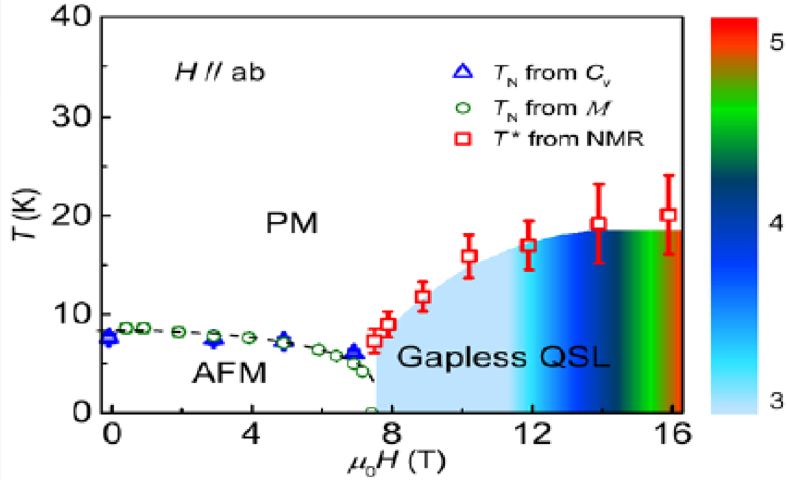
Continuum spectrum

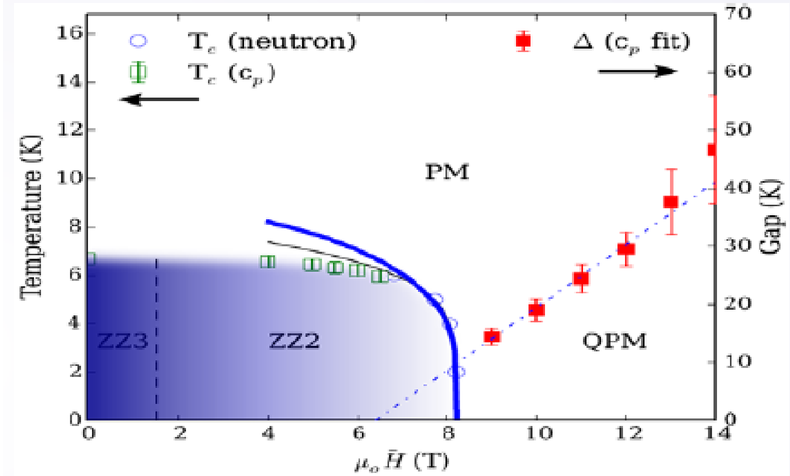
A. Banerjee et al., Nat. Phys. ('16)



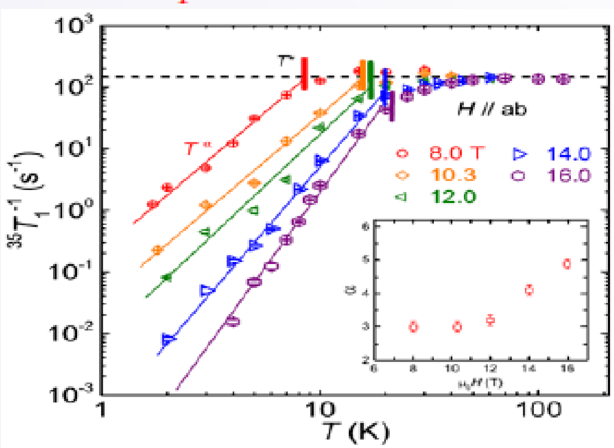
蜂窝晶格QSL候选材料：α-$RuCl_3$

- in-plane magnetic-field-induced QSL

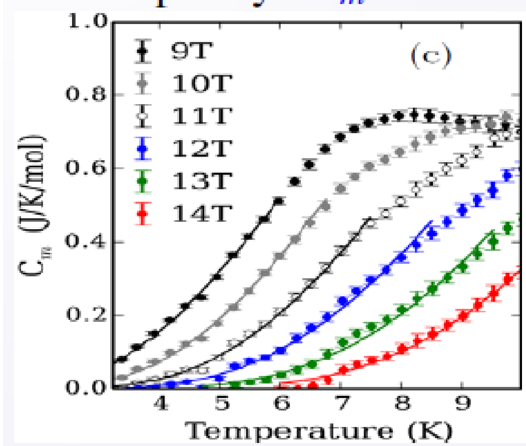




NMR: $T_1^{-1} \propto T^{\alpha}$



heat capacity: $C_m \propto e^{-\Delta/T}$

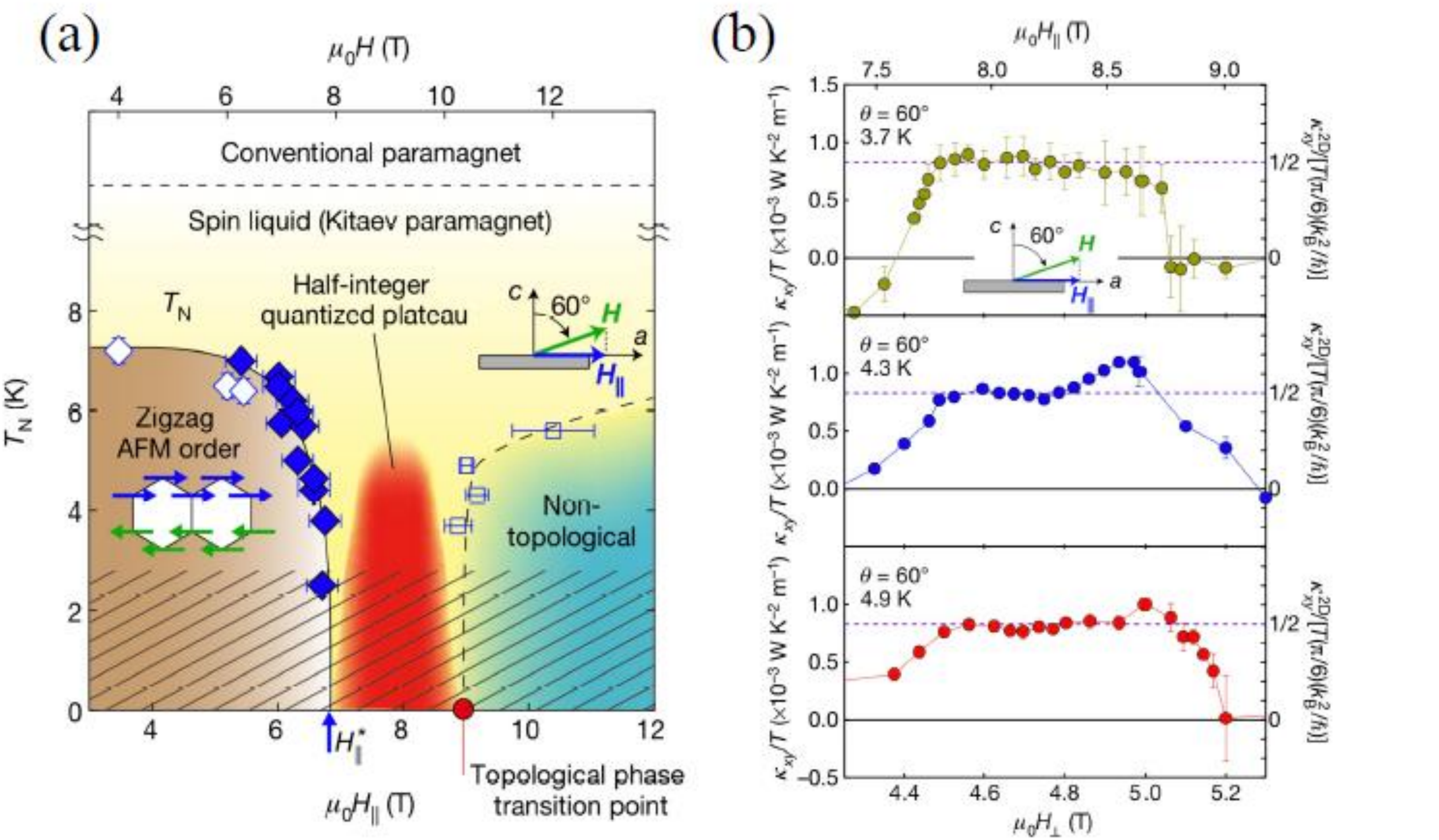


J. Zheng, et al., PRL (2017)

J. A. Sears, et al., PRB (2017)

蜂窝晶格QSL候选材料：α-RuCl3

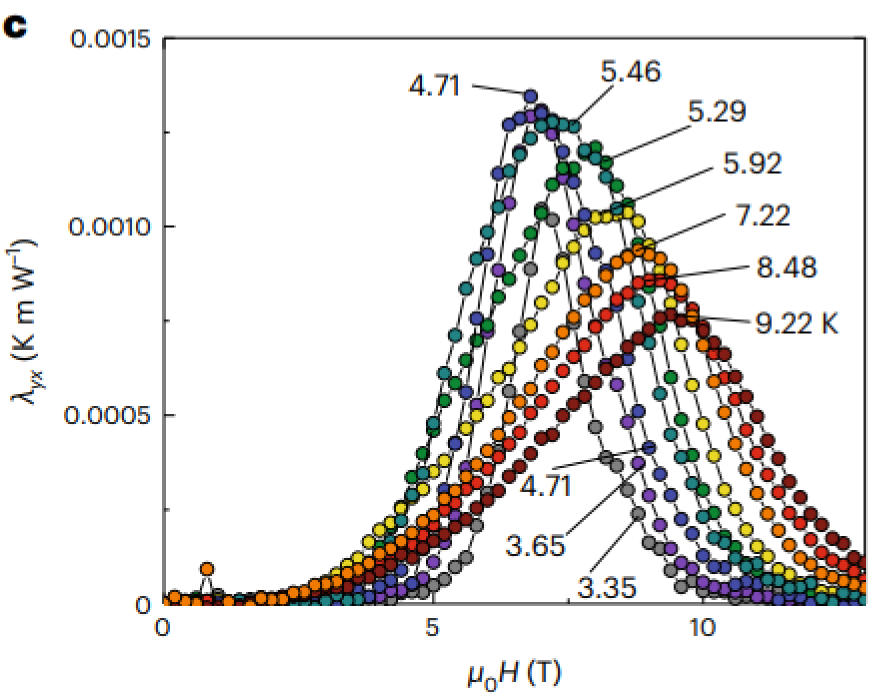
- half-integer quantized thermal Hall conductivity

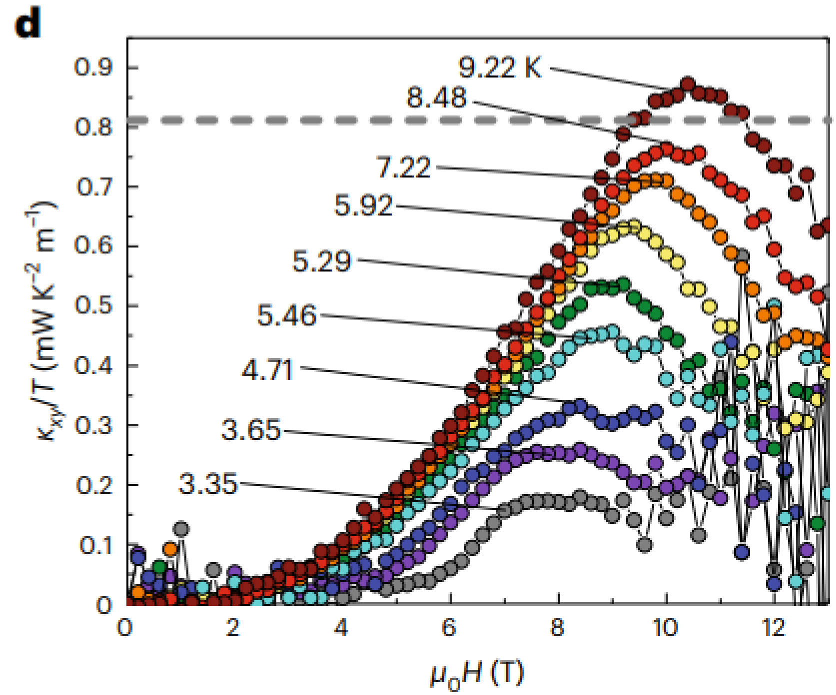


Kasahara, Y. et al. *Nature* 559, 227–231 (2018).

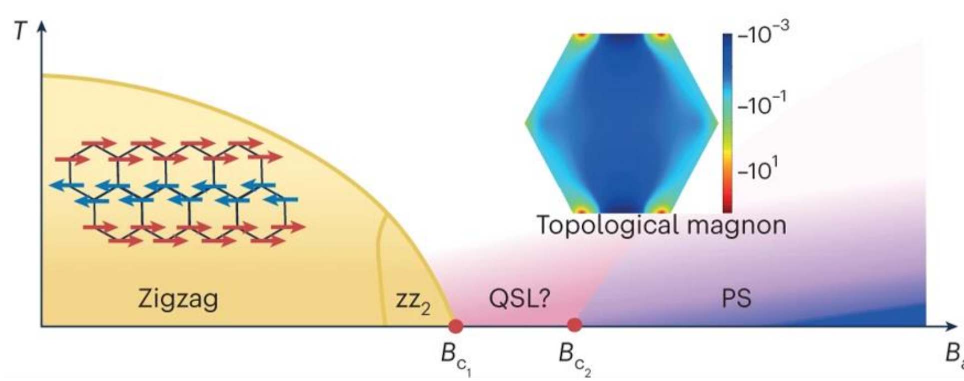
蜂窝晶格QSL候选材料：α-$RuCl_3$

- absence of quantized thermal Hall conductivity



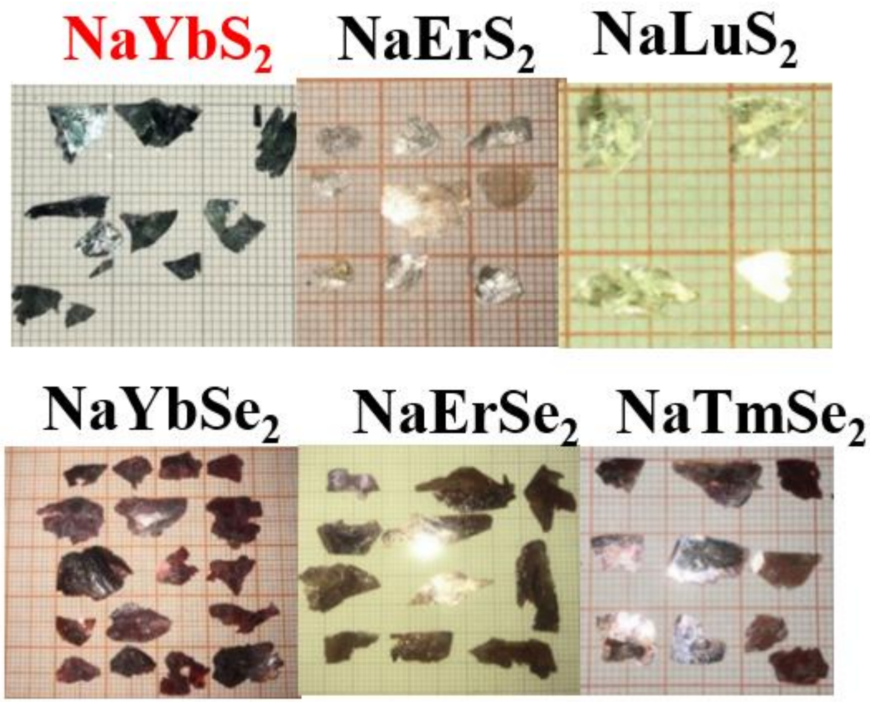


Peter Czajka, et al.
Nature Mater. 22, 36-41 (2023).



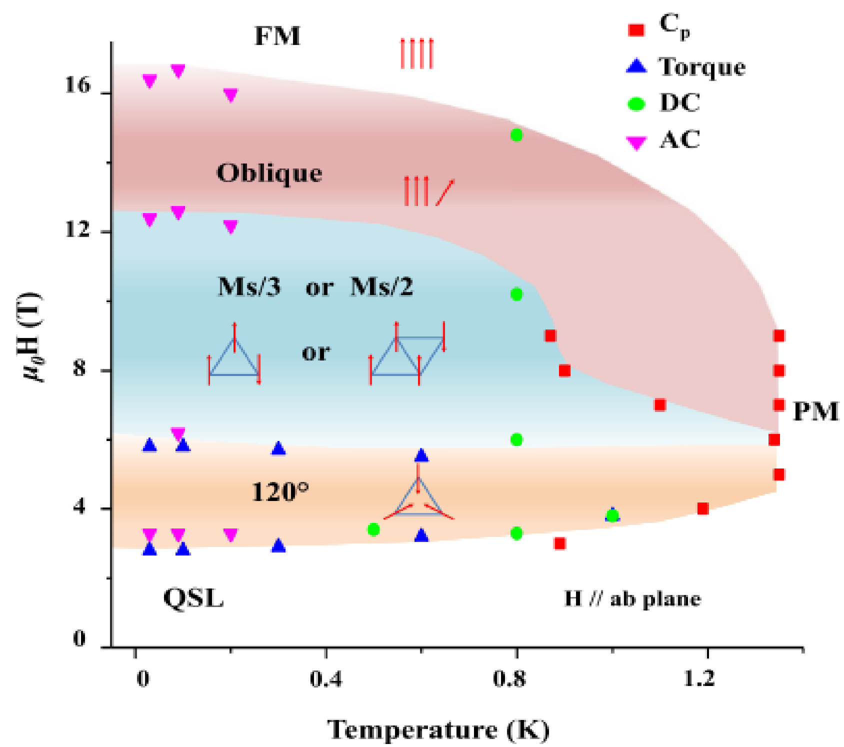
Yb基QSL候选材料

已生长出20种以上单晶



Chin. Phys. Lett. 35, 117501 (2018)

$NaYbS_2$

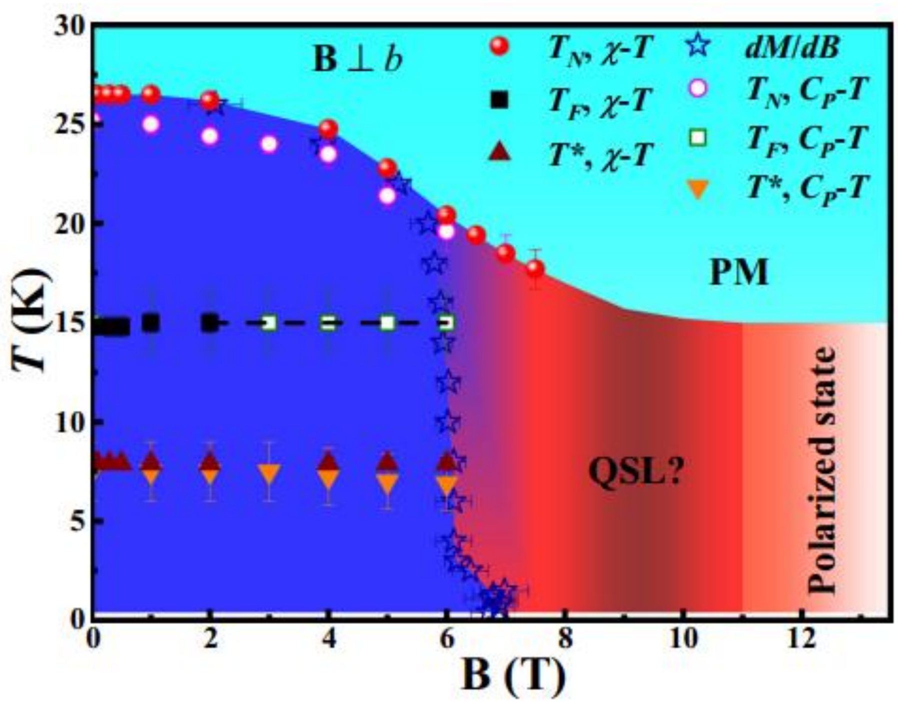


Quan. Frontiers. 1, 13 (2022)

丰富的稀土磁体，为探索QSL提供了肥沃的土壤

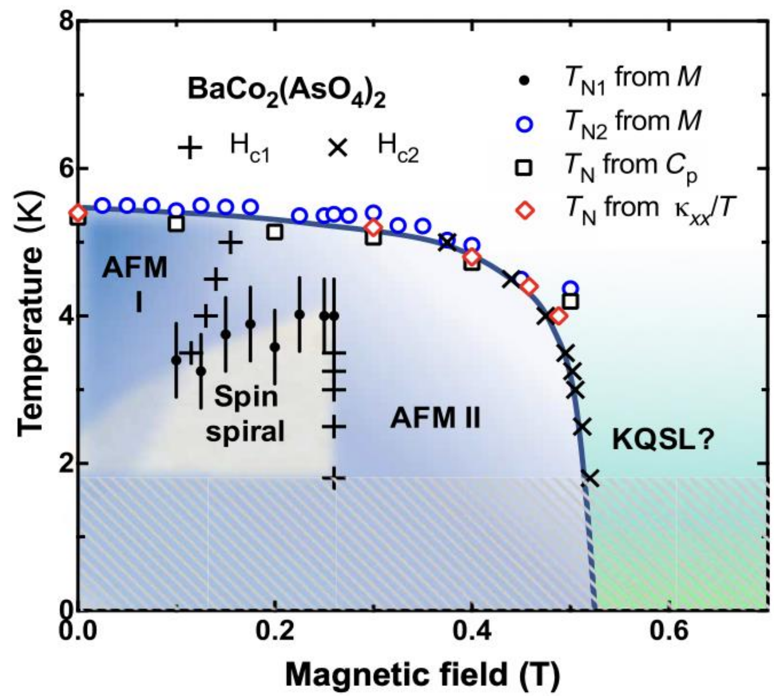
Co基Kitaev材料

$Na_2Co_2TeO_6$



Nat. Comm 12, 5559 (2021)

$BaCo_2(AsO_4)_2$



Sci. Adv. 6, 6953 (2020)

Possible evidences of QSL have been reported in several Co-based Kitaev materials.

Outline

❑ 朗道相变理论和新突破

- ➢ Ising模型中的相变
- ➢ Kosterlitz-Thouless相变和去禁闭量子临界点
- ➢ Luttinger液体和Haldane相

❑ 量子自旋液体和自旋轨道耦合型材料

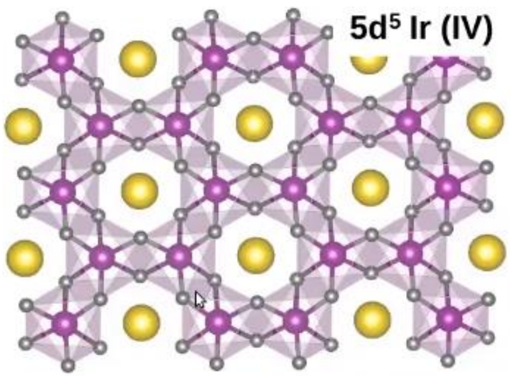
- ➢ 量子自旋液体简介
- ➢ 三角晶格上的量子材料
- ➢ 蜂窝晶格上的量子材料

❑ Kitaev-Γ模型中的物理

- ➢ 自旋S=1/2和1的Kitaev-Γ自旋链
- ➢ 自旋S=1的Kitaev-Γ模型

Kitaev materials and Kitaev-Γ model

- **non-Kitaev** interactions in Kitaev materials

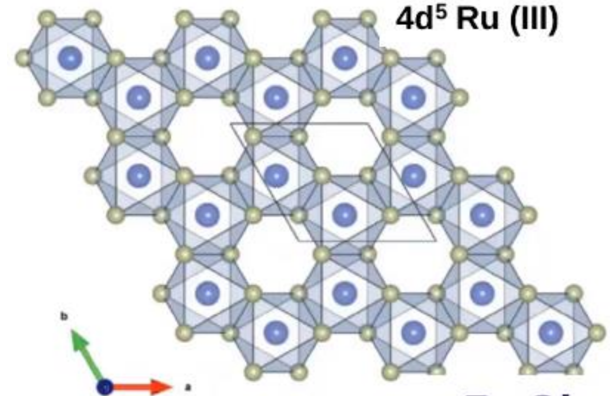


A_2IrO_3 (A = Li, Na)

zigzag order

☜ T_N = 15 K

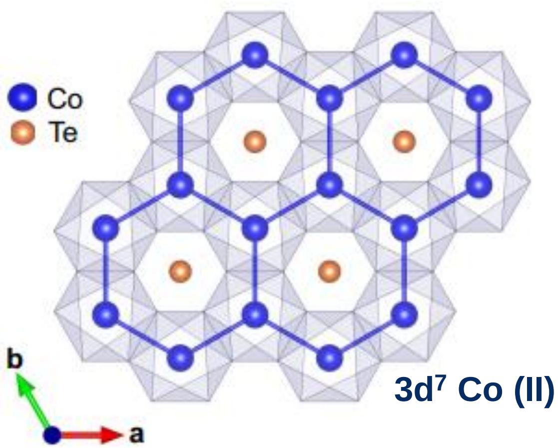
T_N = 7 K ☞



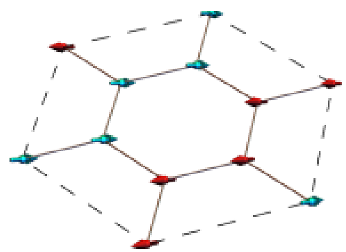
α-$RuCl_3$

Singh and Gegenwart, PRB **82**, 064412 ('10)

Plumb et al., PRB **90**, 041112(R) ('14)

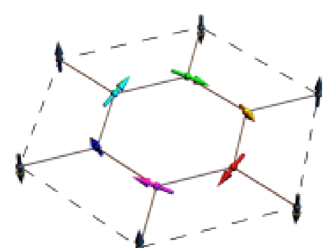


$Na_2Co_2TeO_6$



- zigzag order (4-site)

  Gaoting Lin, et al., NC (2021)



- triple-q order (8-site)

  W. Chen, et al., PRB (2021)
  W. G. F. Fruger, et al., PRL (2023)

Kitaev materials and Kitaev-Γ model

- Generic J-K-Γ model

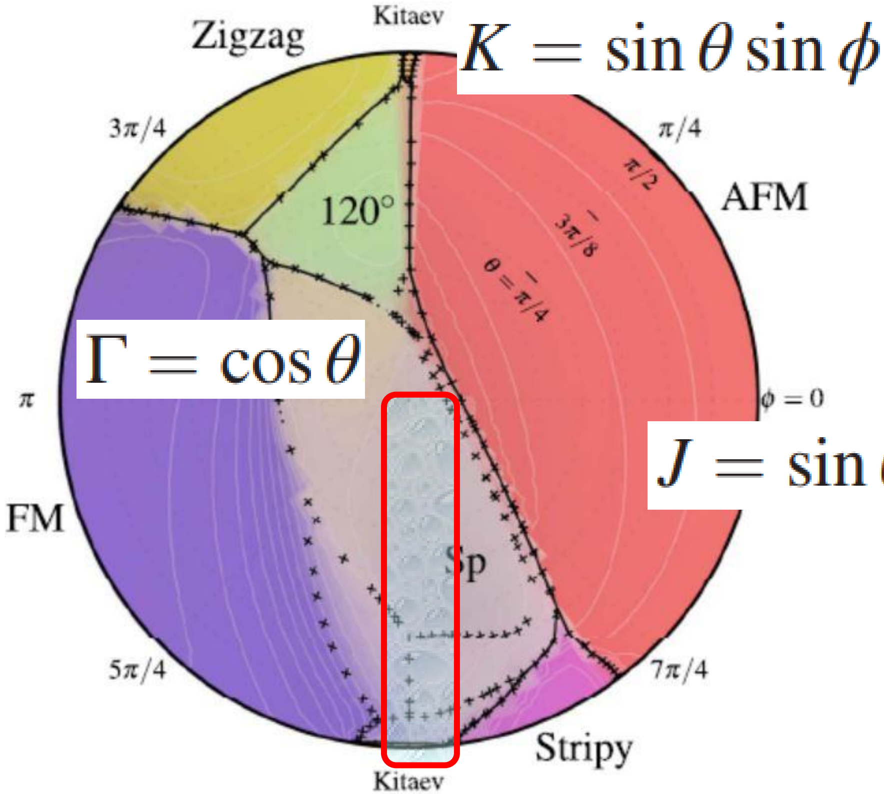
Rau, Lee, and Kee, PRL **112**, 077204 (2014)

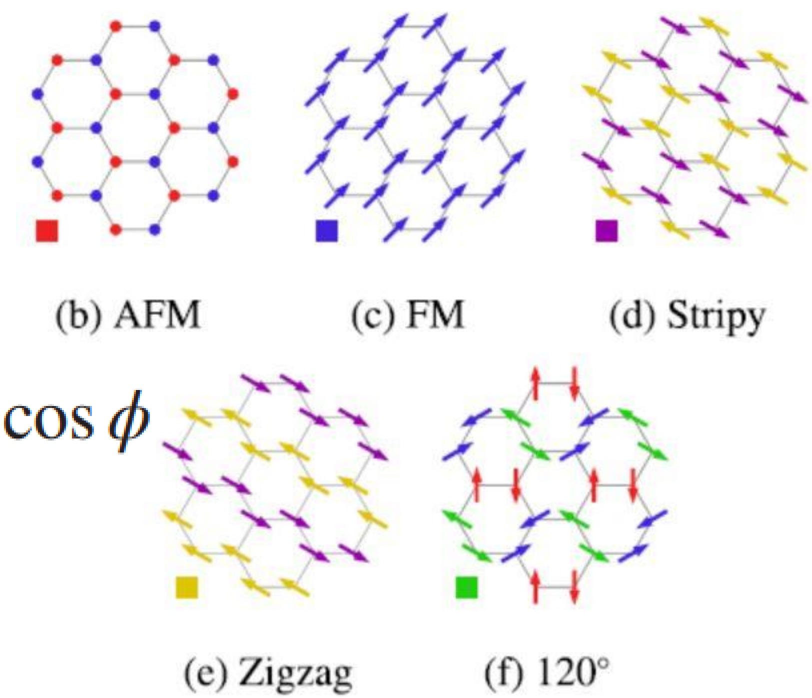
$$\mathcal{H} = \sum_{\langle ij \rangle \| \gamma} \left[J \mathbf{S}_i \cdot \mathbf{S}_j + K S_i^\gamma S_j^\gamma + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right]$$

$K = \sin\theta \sin\phi$

$\Gamma = \cos\theta$

$J = \sin\theta \cos\phi$

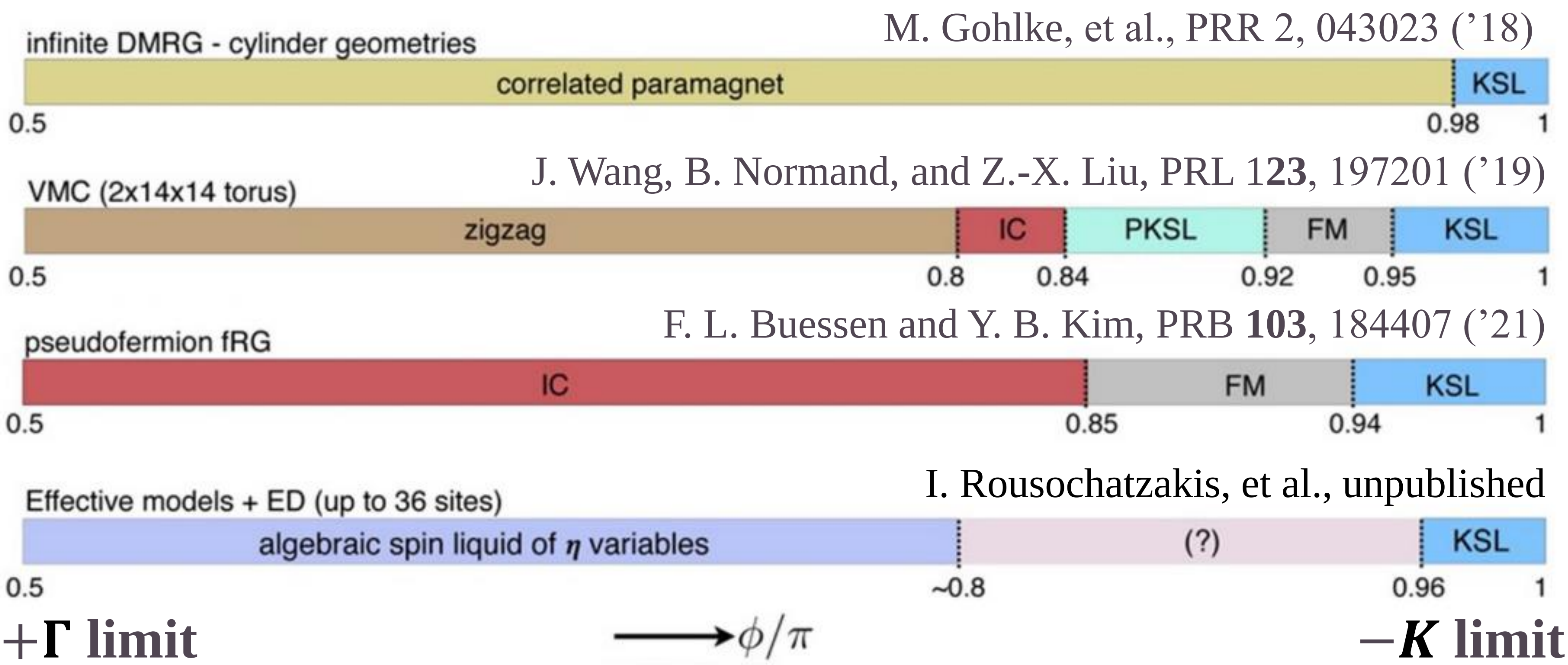




When **KΓ < 0** (e.g., K<0 & Γ >0), the model is frustrated!

Kitaev materials and Kitaev-Γ model

Debates on the spin-1/2 Kitaev-Γ model



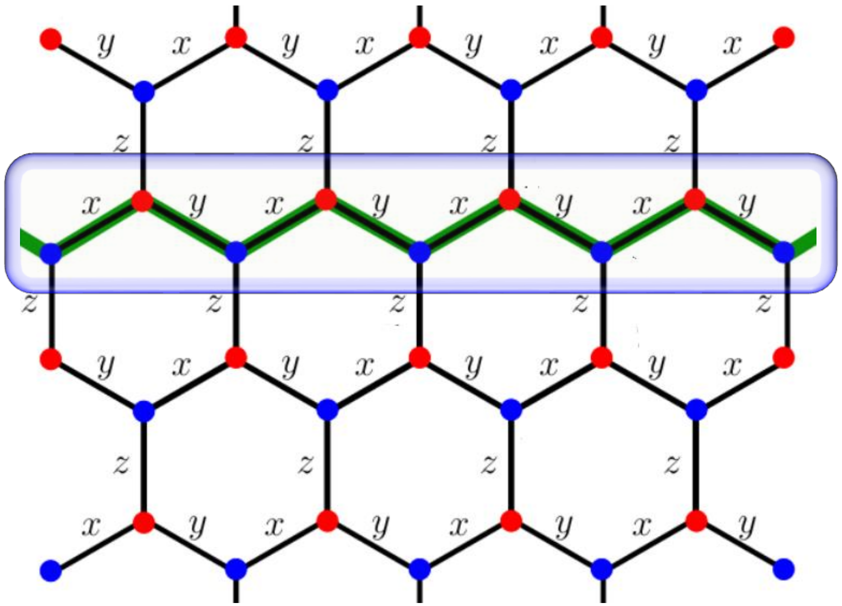
for a review, see:

Ioannis Rousochatzakis, Natalia B Perkins, **Qiang Luo**, and Hae-Young Kee*
Beyond Kitaev physics in strong spin-orbit coupled magnets,
Rep. Prog. Phys. 87, 026502 (2024).

From 2D to 1D: Reducing the complexity

2D K-Γ model

$$H = \sum_{\langle i,j\rangle \in \alpha\beta(\gamma)} \left[K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)\right]$$

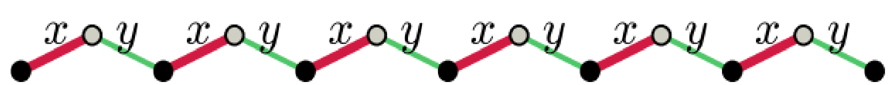


Notorious difficulty!

1D anisotropic K-Γ chain

$$\mathcal{H} = \sum_{l=1}^{L/2} g_x \mathcal{H}^{(x)}_{2l-1,2l}(\theta) + g_y \mathcal{H}^{(y)}_{2l,2l+1}(\theta)$$

$$\mathcal{H}^{(\gamma)}_{i,j}(\theta) = K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha).$$



Motivation

- insight into 2D problems
- analytical methods, e.g., CFT, bosonization, are available
- **DMRG and TMRG!**

Bond-alternating Kitaev-Γ chain

$$\mathcal{H} = \sum_{l=1}^{L/2} g_x \mathcal{H}^{(x)}_{2l-1,2l}(\theta) + g_y \mathcal{H}^{(y)}_{2l,2l+1}(\theta)$$

$$\mathcal{H}^{(\gamma)}_{i,j}(\theta) = K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)$$

$$g \equiv g_y / g_x$$

Symmetry analysis

- **Self-dual relation**

$$(S_i^x, S_i^y, S_i^z) \to (-S_i^y, -S_i^x, -S_i^z) \quad \Rightarrow \quad E(g) = gE(1/g)$$

- **Mirror symmetry**

$$(S_i^x, S_i^y, S_i^z) \to (S_i^y, -S_i^x, S_i^z) \quad \Rightarrow \quad E(K, \Gamma) = E(K, -\Gamma)$$

- **Hidden SU(2) symmetry** ⇒ SU(2) Heisenberg point

Bond-alternating Kitaev-Γ chain

Site-ordering cross decimation (U_6) rotation

$$\mathcal{H}^{(\gamma)}_{i,j}(\theta) = K S_i^\gamma S_j^\gamma + \Gamma\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right).$$

sublattice 1 : $(x, y, z) \to (\tilde{x}, \tilde{y}, \tilde{z})$,

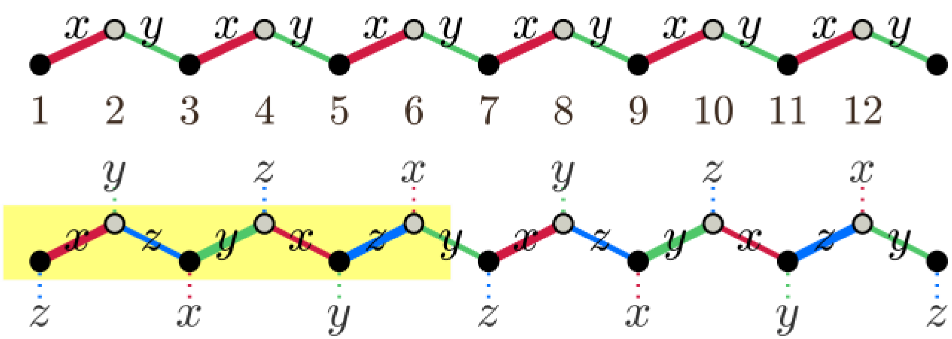
sublattice 2 : $(x, y, z) \to (-\tilde{x}, -\tilde{z}, -\tilde{y})$,

sublattice 3 : $(x, y, z) \to (\tilde{y}, \tilde{z}, \tilde{x})$,

sublattice 4 : $(x, y, z) \to (-\tilde{y}, -\tilde{x}, -\tilde{z})$,

sublattice 5 : $(x, y, z) \to (\tilde{z}, \tilde{x}, \tilde{y})$,

sublattice 6 : $(x, y, z) \to (-\tilde{z}, -\tilde{y}, -\tilde{x})$,



$$\tilde{\mathcal{H}}^{(\gamma)}_{i,j}(\theta) = -K \tilde{S}_i^\gamma \tilde{S}_j^\gamma - \Gamma\left(\tilde{S}_i^\alpha \tilde{S}_j^\alpha + \tilde{S}_i^\beta \tilde{S}_j^\beta\right)$$

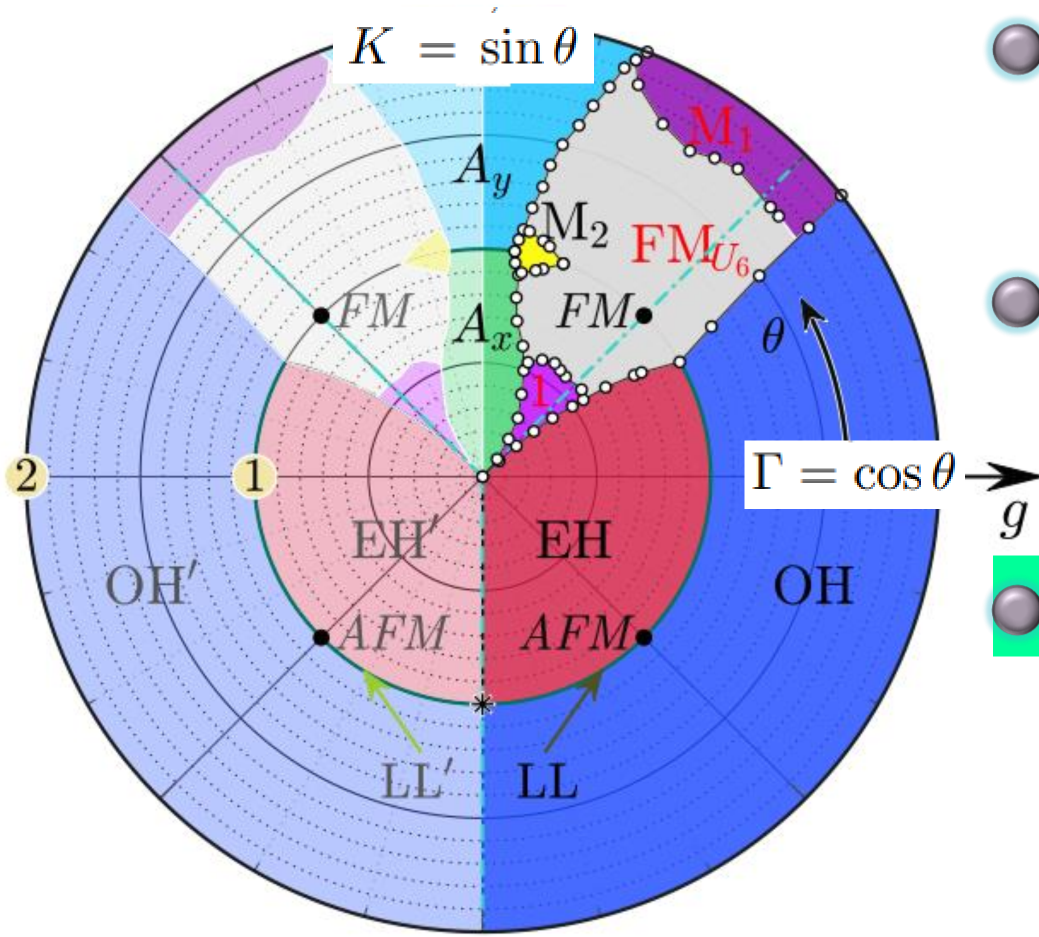
- **Hidden SU(2) symmetry**

Yang, *et al.*, PRL **124,** 147205 (20)

When **K = |Γ| > 0**, **FM** SU(2) Heisenberg point

When **K = -|Γ| < 0**, **AFM** SU(2) Heisenberg point

bond-alternating spin-1/2 K-Γ chain



Q. Luo, *et al.*, PRB **103**, 144423 (2021)

EH vs **OH**: **Even**/**Odd**-Haldane

LL: **L**uttinger **L**iquid

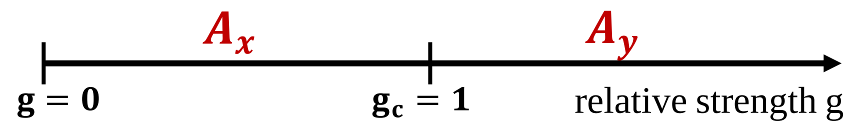
- **Four disordered states**
  EH vs OH, A_x vs A_y
  OH: a SPT phase
- **Three SSB phases**
  FM_{U6}: 6-fold degeneracy
  M1/M2: 8-fold degeneracy
- **Two topological QPTs**
  A_x—A_y transition:
  Ising university class with **c = 1/2**
  EH—OH transition:
  Gaussian university class with **c = 1**
- **One multicritical point**
  A_x—A_y and LL—LL' meet at FM Kitaev point.

Ising A_x-A_y topological phase transition

1D Kitaev spin chain

Feng, Zhang, Xiang, PRL **98**, 087204 (2007)

$$H = \sum_{j=1}^{N/2} \left(J_1 \sigma_{2j-1}^x \sigma_{2j}^x + J_2 \sigma_{2j}^y \sigma_{2j+1}^y \right)$$

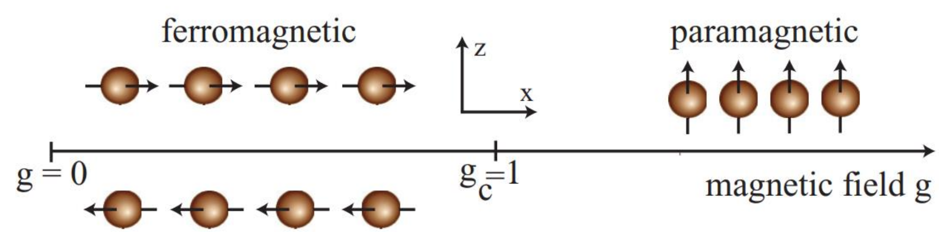


$$\sigma_j^x = \tau_{j-1}^x \tau_j^x, \qquad \sigma_j^y = \prod_{k=j}^{2N} \tau_k^y,$$

spin duality transformation

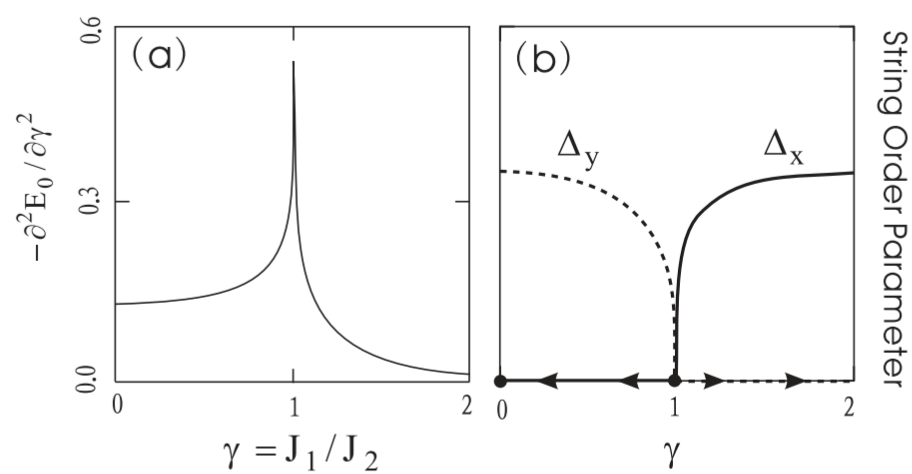
1D Ising spin chain

$$H_d = \sum_{j=1}^{N} \left(J_1 \tau_{2j-2}^x \tau_{2j}^x + J_2 \tau_{2j}^y \right).$$



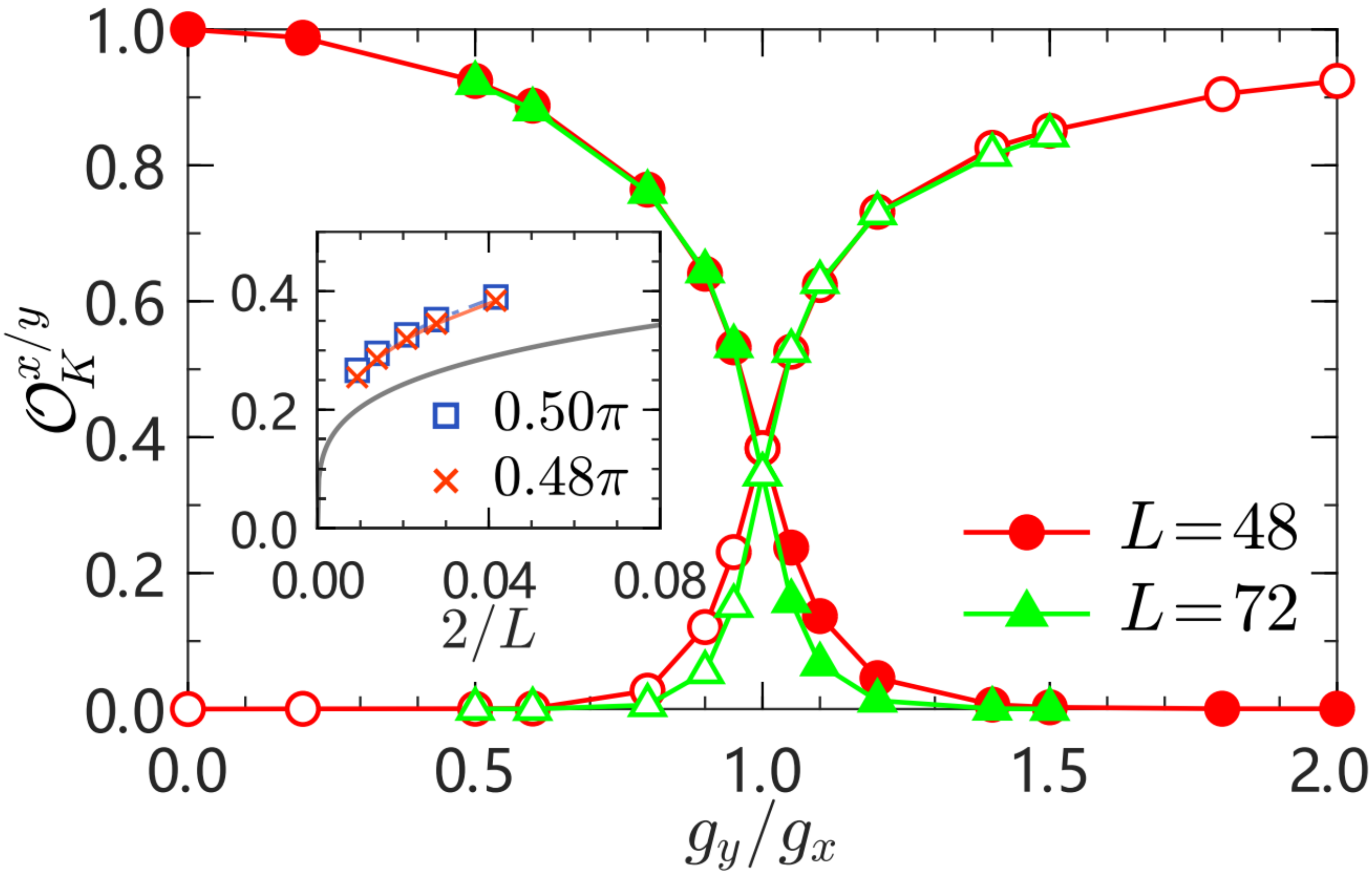
$$\mathcal{O}_K^x(2r) = \lim_{r\to\infty} \left\langle \prod_{k=1}^{2r} \sigma_k^x \right\rangle$$

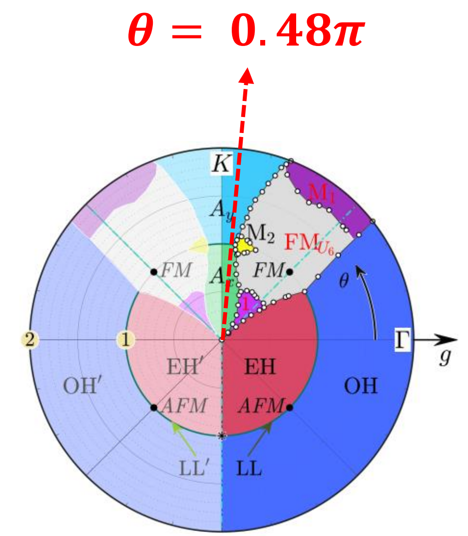
$$\mathcal{O}_K^y(2r) = \lim_{r\to\infty} \left\langle \prod_{k=2}^{2r+1} \sigma_k^y \right\rangle,$$



Ising A_x-A_y topological phase transition

- **Example at $\theta = 0.48\pi$: String order parameter**





$$\mathcal{O}_K^{x/y}(n) = e^{1/4} 2^{1/12} A^{-3} n^{-1/4}\left(1 - \frac{1}{64} n^{-2} + \cdots\right), \ A \simeq 1.2824.$$

Ising A_x-A_y topological phase transition

Example at $\theta = 0.48\pi$: Central charge

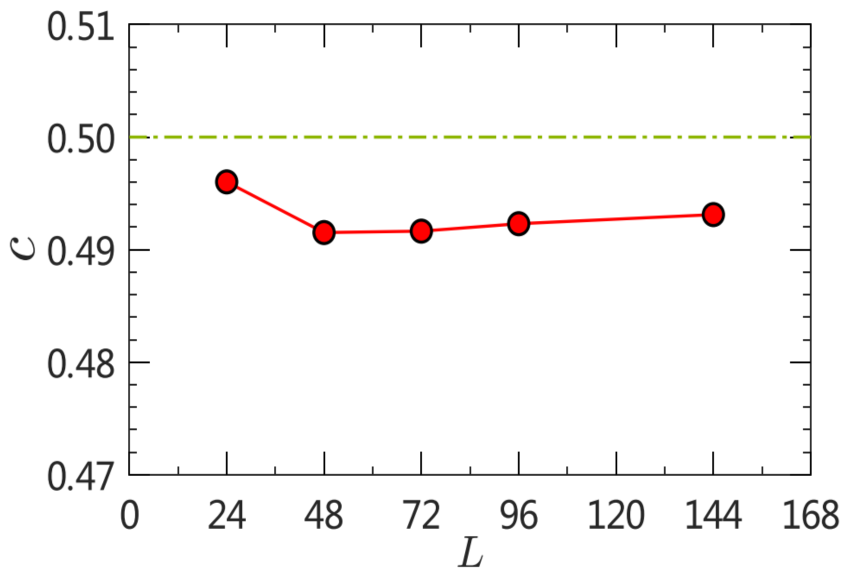
G.S. degeneracy $O(2^{N/2})$, leading to a huge entanglement entropy S:

$$S(l) = -\mathrm{tr}(\rho \ln \rho) = \frac{c}{3} \ln\left(\frac{L}{\pi} \sin\left(\frac{\pi\, l}{L}\right)\right) + c'$$

G.S. energy $E_g(L)$ obeys [PBC]:

$$E_g(L) = Le_g + \epsilon_b - \frac{\pi c}{6L} + O(L^{-2})$$

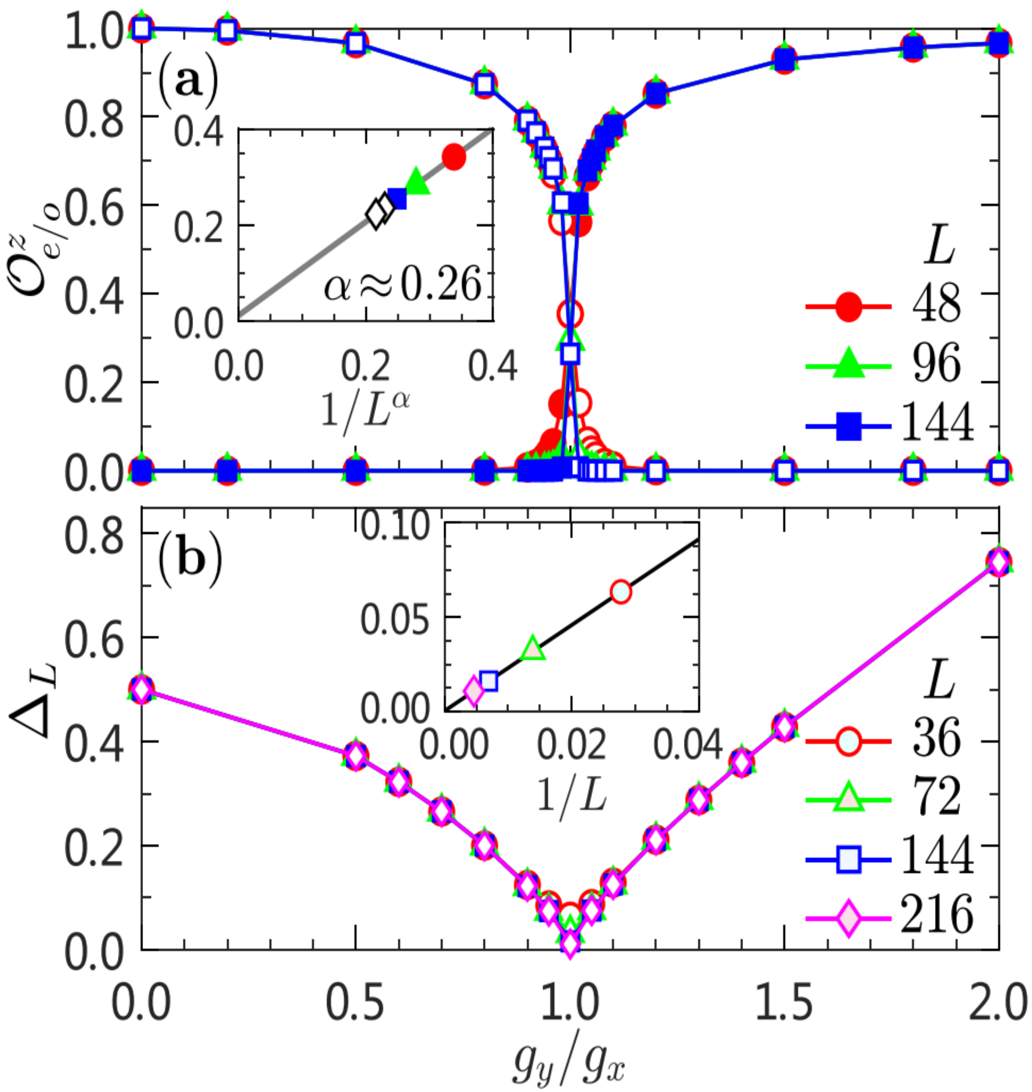
$$c_L \simeq \frac{6}{\pi}[Le_g - E_g(L)]L$$



$e_g \approx -0.1591\,092$ ($\theta = 0.48\pi$); $\qquad e_g = -\frac{1}{2\pi} \approx -0.1591\,549$ ($\theta = 0.50\pi$)

Even-Haldane—Odd-Haldane transition

Example at $\theta = 0$: String order parameters



Even Haldane: (g < 1)

$$\mathcal{O}^\alpha_e = \lim_{|j-i|\to\infty} \mathcal{O}^\alpha(2i, 2j+1),$$

Odd Haldane: (g > 1)

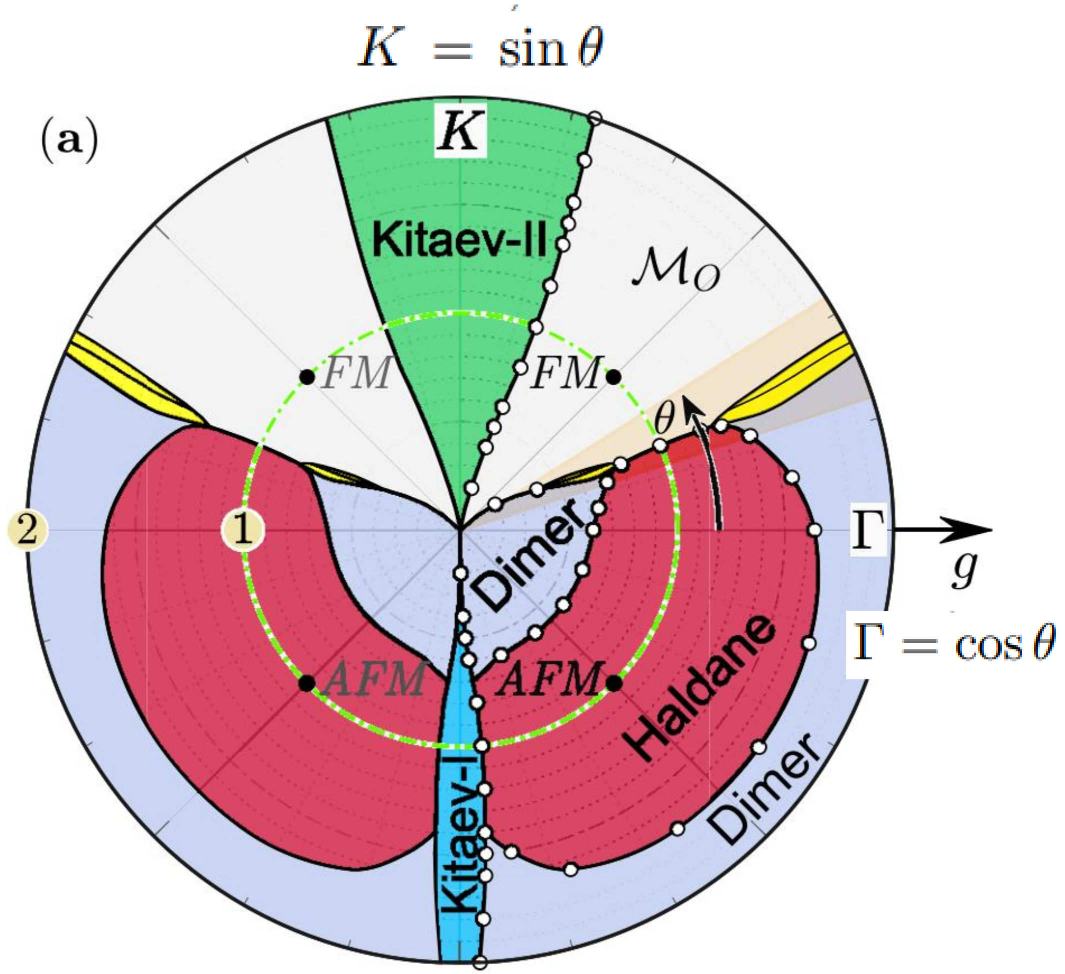
$$\mathcal{O}^\alpha_o = \lim_{|j-i|\to\infty} \mathcal{O}^\alpha(2i-1, 2j),$$

$$\mathcal{O}^\alpha(p,q) = -4\left\langle \tilde{S}^\alpha_p \left(\prod_{p<r<q} e^{i\pi \tilde{S}^\alpha_r}\right) \tilde{S}^\alpha_q \right\rangle.$$

when g = 1, $\mathcal{O} \simeq L^{-1/4}$

Bortz, *et al.*, J. Phys. A **40**, 4253 (07)

bond-alternating spin-1 K-Γ chain



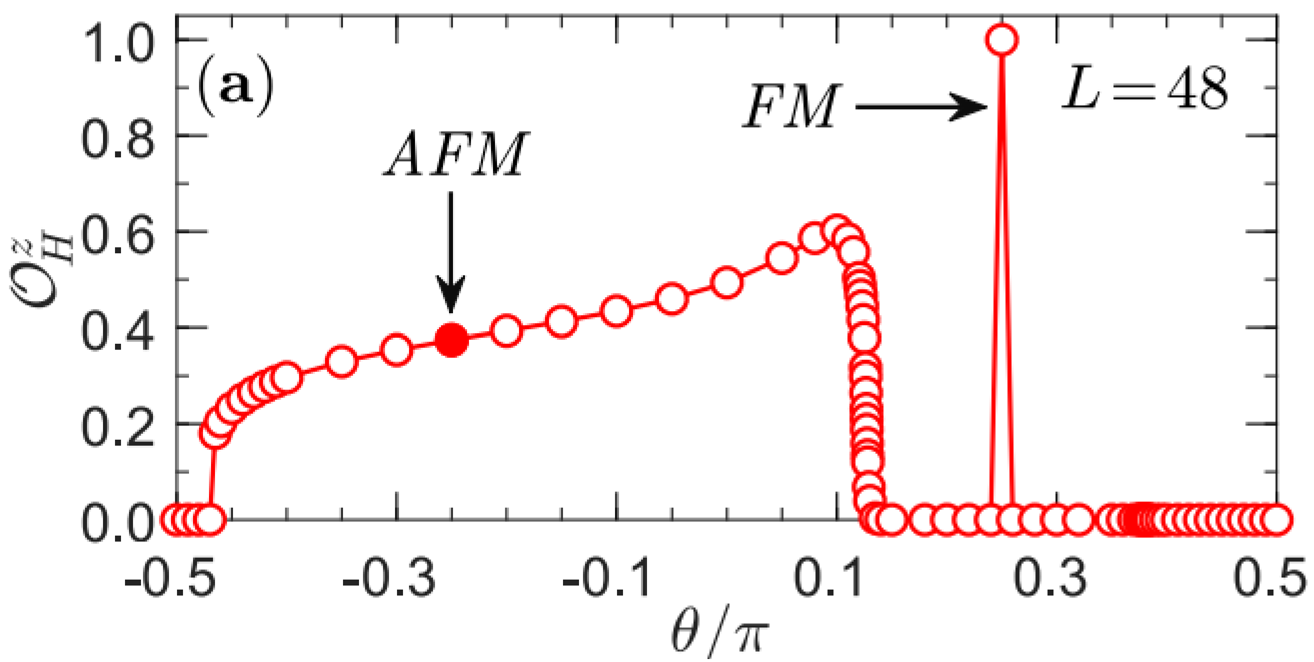
Q. Luo, S. Hu, and H.-Y. Kee, PRR **3**, 033048 (2021)

Haldane phase vs Kitaev phase

Haldane phase: SOP and edge states

String Order Parameter

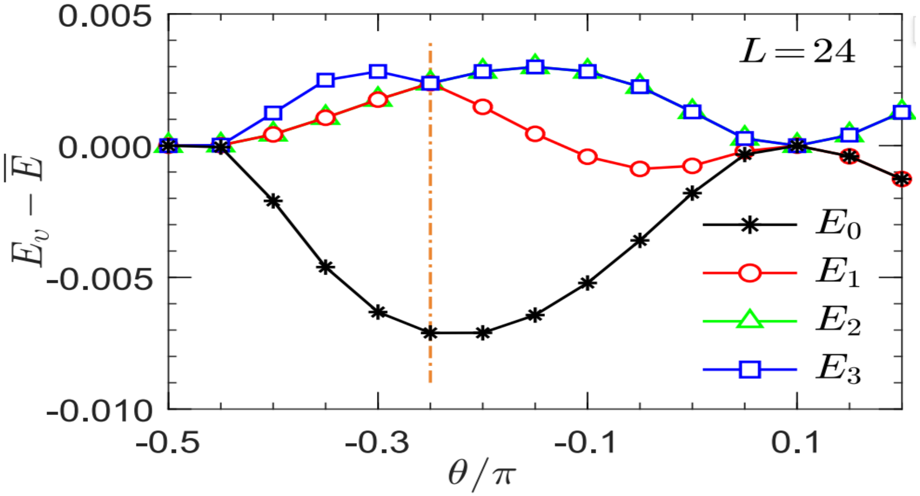
$$\mathcal{O}_H^z = -\lim_{|q-p|\to\infty}\left\langle \tilde{S}_p^z \left(\prod_{p<r<q} e^{i\pi \tilde{S}_r^z}\right)\tilde{S}_q^z \right\rangle$$



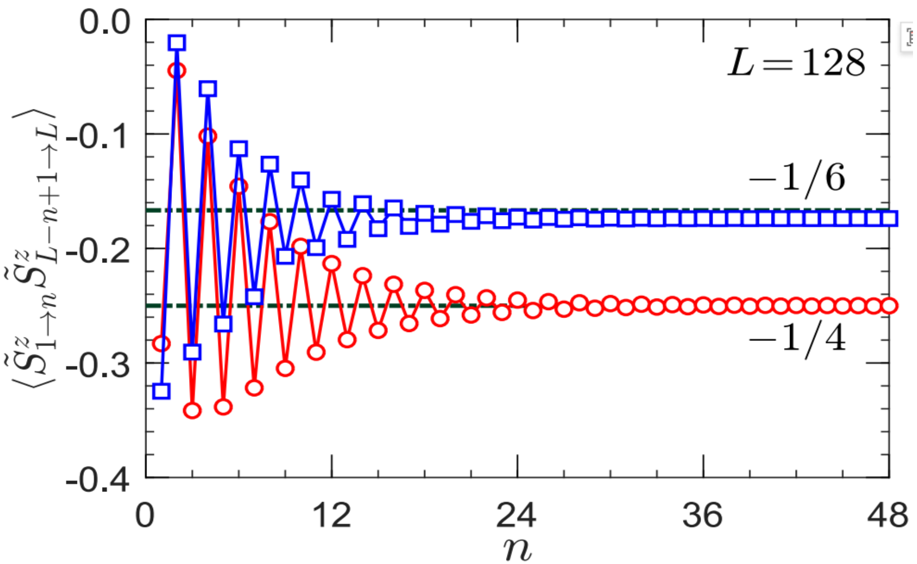
- ❑ when $\theta = -\frac{\pi}{4}$ (i.e., AFM **Heisenberg chain**), $O_H^z \approx 0.3743$;
- ❑ when $\theta = 0$ (i.e., **Γ chain**), $O_H^z \approx 0.4935$.

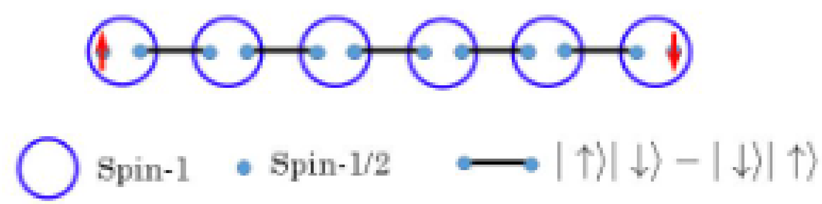
Haldane phase: SOP and edge states

G.S. degeneracy and Edge states



- ❑ when $\theta < -\pi/4$, it has "**1 + 2 + 1**" structure.
- ❑ when $\theta > -\pi/4$, it has "**1 + 1 + 2**" structure.



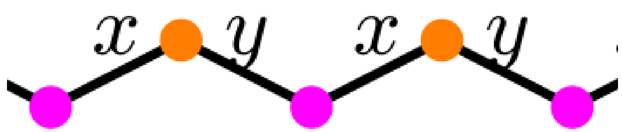


$$C_n^z = \langle \tilde{S}^z_{1\to n} \tilde{S}^z_{L-n+1\to L} \rangle$$

Liu, Zhou, Tu *et al.*, PRB **85**, 195144 (12)

Kitaev phase: Spectra and Excitations

- **Conserved Z_2 values**



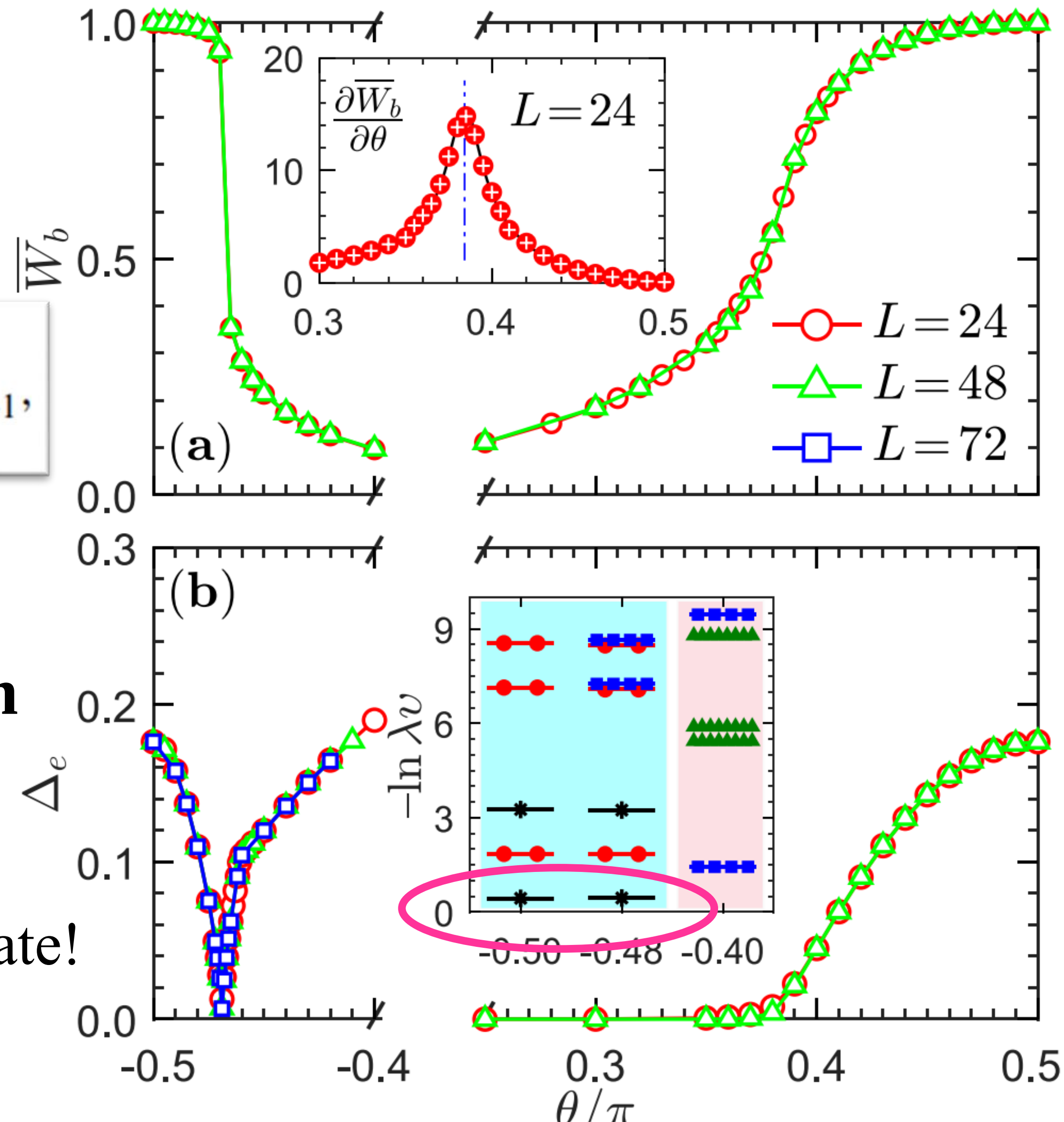
$$\hat{W}_{2l-1} = \Sigma^y_{2l-1}\Sigma^y_{2l}, \quad \hat{W}_{2l} = \Sigma^x_{2l}\Sigma^x_{2l+1},$$

$$\Sigma^\alpha_l = e^{i\pi S^\alpha_l}$$

- **Entanglement spectrum**

❑ gapped with unique G.S.

❑ Lowest E.S. is nondegenerate!



Sen, *et al.*, PRB **82**, 195435 (2007)

Double-peak specific heat in Kitaev phase

Thermodynamics

partition function $\boldsymbol{\Xi} = \mathbf{Tr}\left(e^{-\beta H}\right)$

- internal energy $U = -\dfrac{\partial \ln \Xi}{\partial \beta}$
- free energy $F = -\beta^{-1} \ln \Xi$

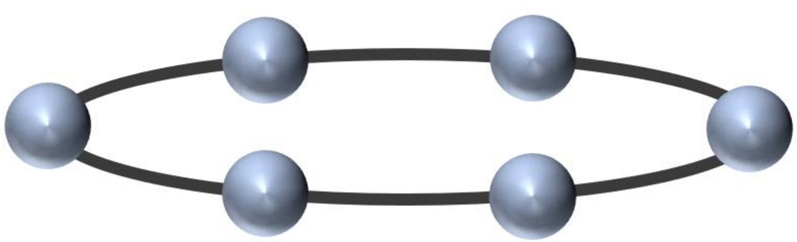
$$C_v = \frac{1}{N}\left(\frac{\partial U}{\partial T}\right)_V = -\frac{\beta^2}{N}\frac{\partial U}{\partial \beta}$$

(Specific heat)

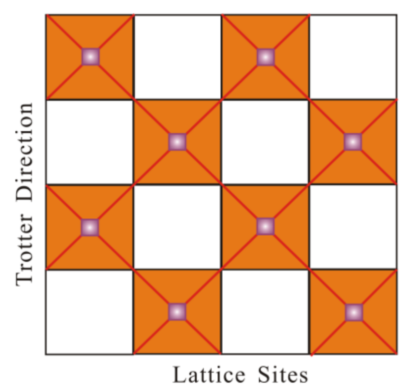
$$\mathcal{S} = \frac{\beta}{N}(U - F) = \mathcal{S}_0 + \int_0^T \frac{C_v(T')}{T'} dT'$$

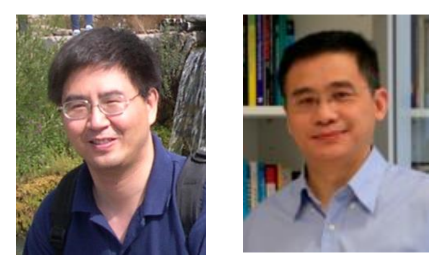
(thermal entropy)

Exact diagonalization



Transfer-matrix RG

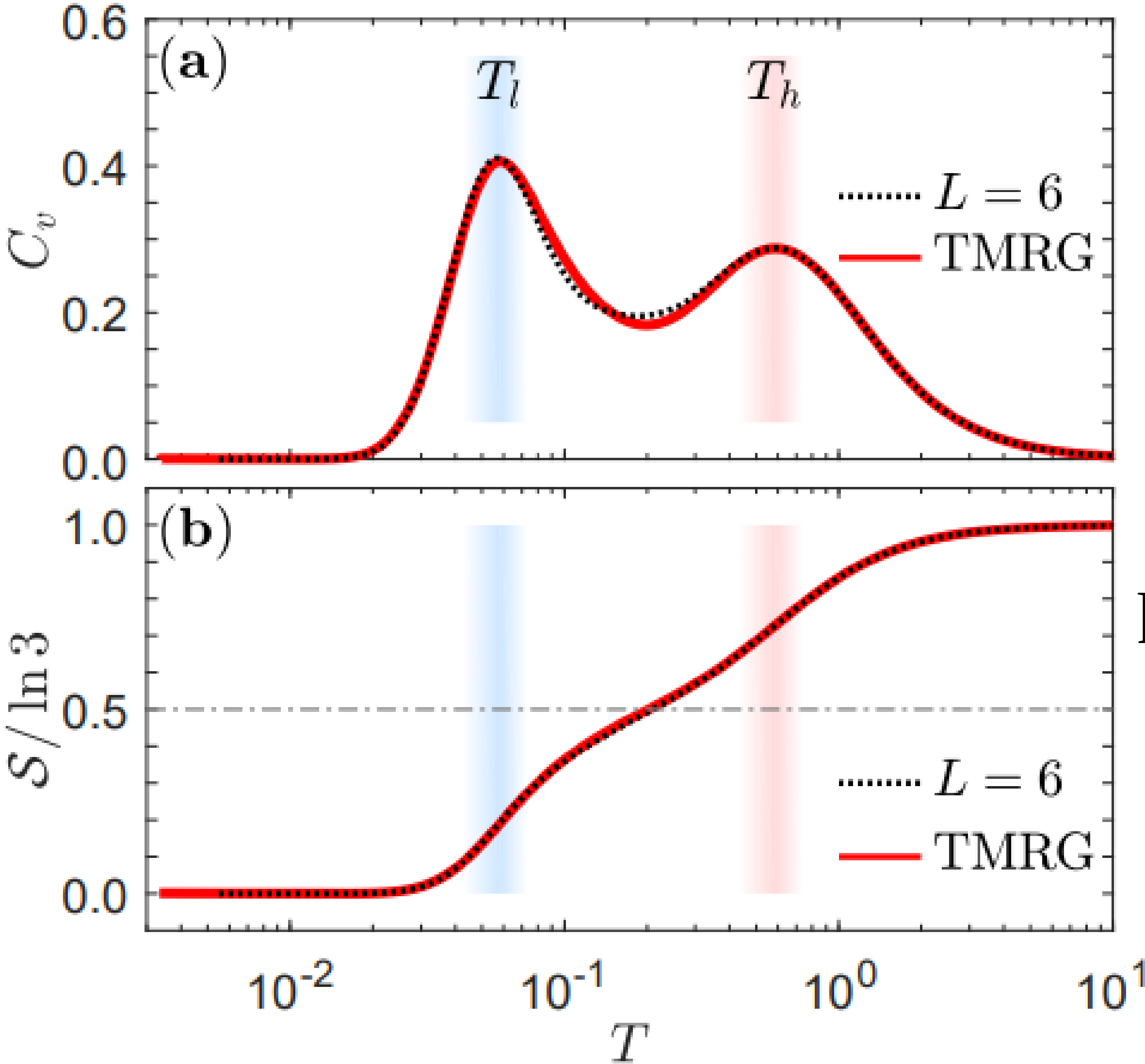




Wang, Xiang, *et al.*, (90's)

Double-peak specific heat in Kitaev phase

- **Specific heat & thermal entropy in spin-1 Kitaev chain**

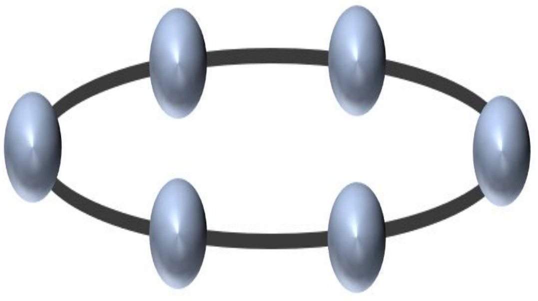


double peak in C_v

$T_h \simeq 0.5860$

$T_l \simeq 0.0582$

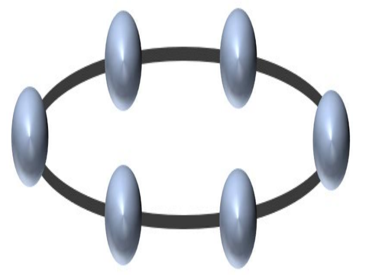
half-plateau is absent



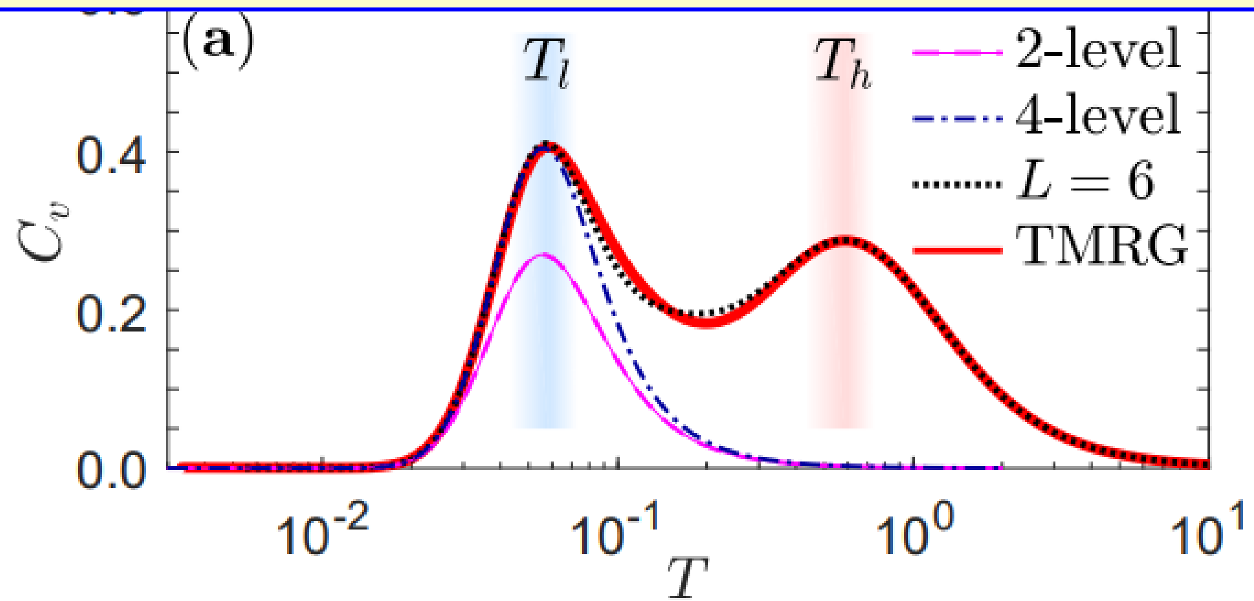
Double-peak specific heat in Kitaev phase

Understanding of low-T peak in specific heat

υ	E_υ	degeneracy	Δ_υ	$\tilde{\Delta}_\upsilon/\Delta_\kappa$
0	−3.63027662	1	0.00000000	0
1	−3.45009088	6	0.18018574	1
2	−3.38928222	6	0.24099440	∼4/3
3	−3.33005874	2	0.30021788	∼5/3



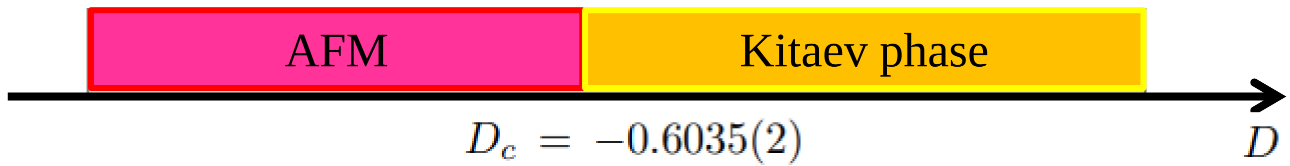
The low-T peak relates to the large degeneracy of the low-lying excited states.

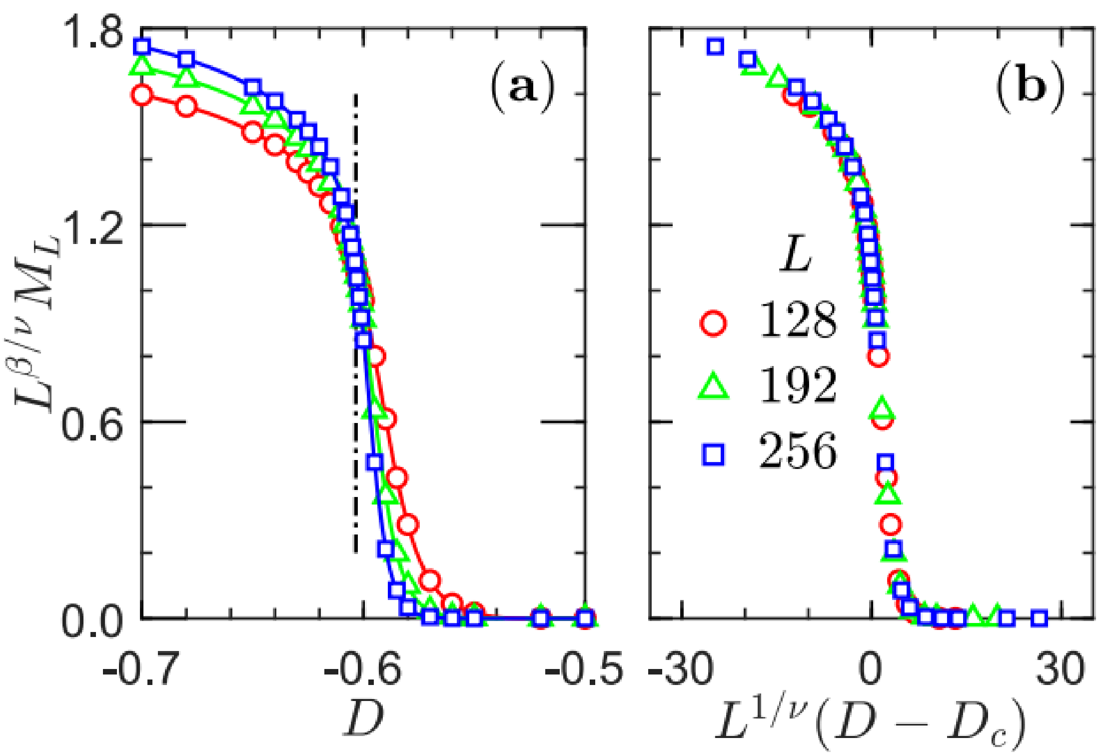


Spin-nematicity in Kitaev phase

Spin-1 Kitaev chain with single-ion anisotropy

$$\mathcal{H} = K \sum_{i=1}^{L/2} \left(S_{2i-1}^x S_{2i}^x + S_{2i}^y S_{2i+1}^y \right) + D \sum_{i=1}^{L} \left(\frac{S_i^x + S_i^y + S_i^z}{\sqrt{3}} \right)^2$$





Finite-size scaling

$$M_L(D) \simeq L^{-\beta/\nu} f_M\left(|D - D_c| L^{1/\nu}\right)$$

$$M_L = \sqrt{\left(\langle S_{L/2}^x \rangle\right)^2 + \left(\langle S_{L/2}^y \rangle\right)^2 + \left(\langle S_{L/2}^z \rangle\right)^2}.$$

critical exponents

$$\beta = 0.127(3) \text{ and } \nu = 0.99(2)$$

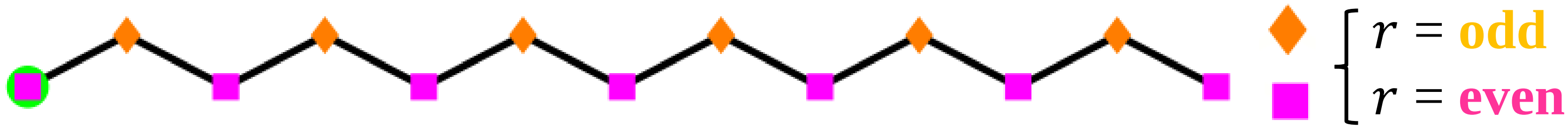
Ising universality class

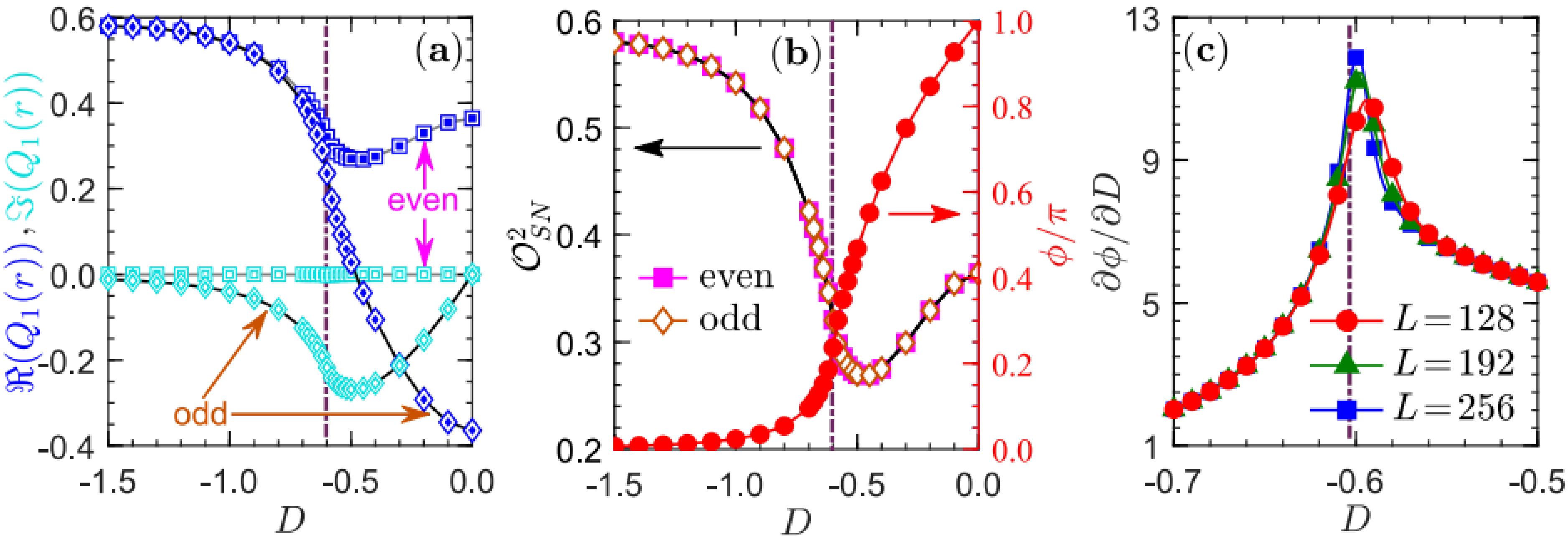
Spin-nematicity in Kitaev phase

Spin-nematic correlation

Q. Luo, *et al.*, PRB 107, 245131 (2023)

$$Q_{\delta=1}(i,j) = \langle S_i^+ S_{i+\delta}^+ S_j^- S_{j+\delta}^- \rangle \simeq \mathcal{O}_{SN}^2 e^{-\imath\phi}, r \equiv |j-i| \to \infty$$

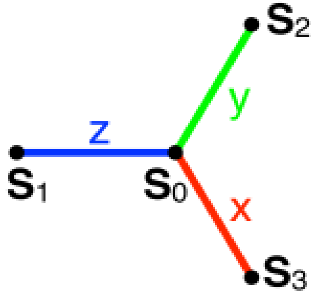




The Kitaev phase might be a spin-nematic phase.

Classical 2D Kitaev-Γ model: $K > 0$

Setup and Definition



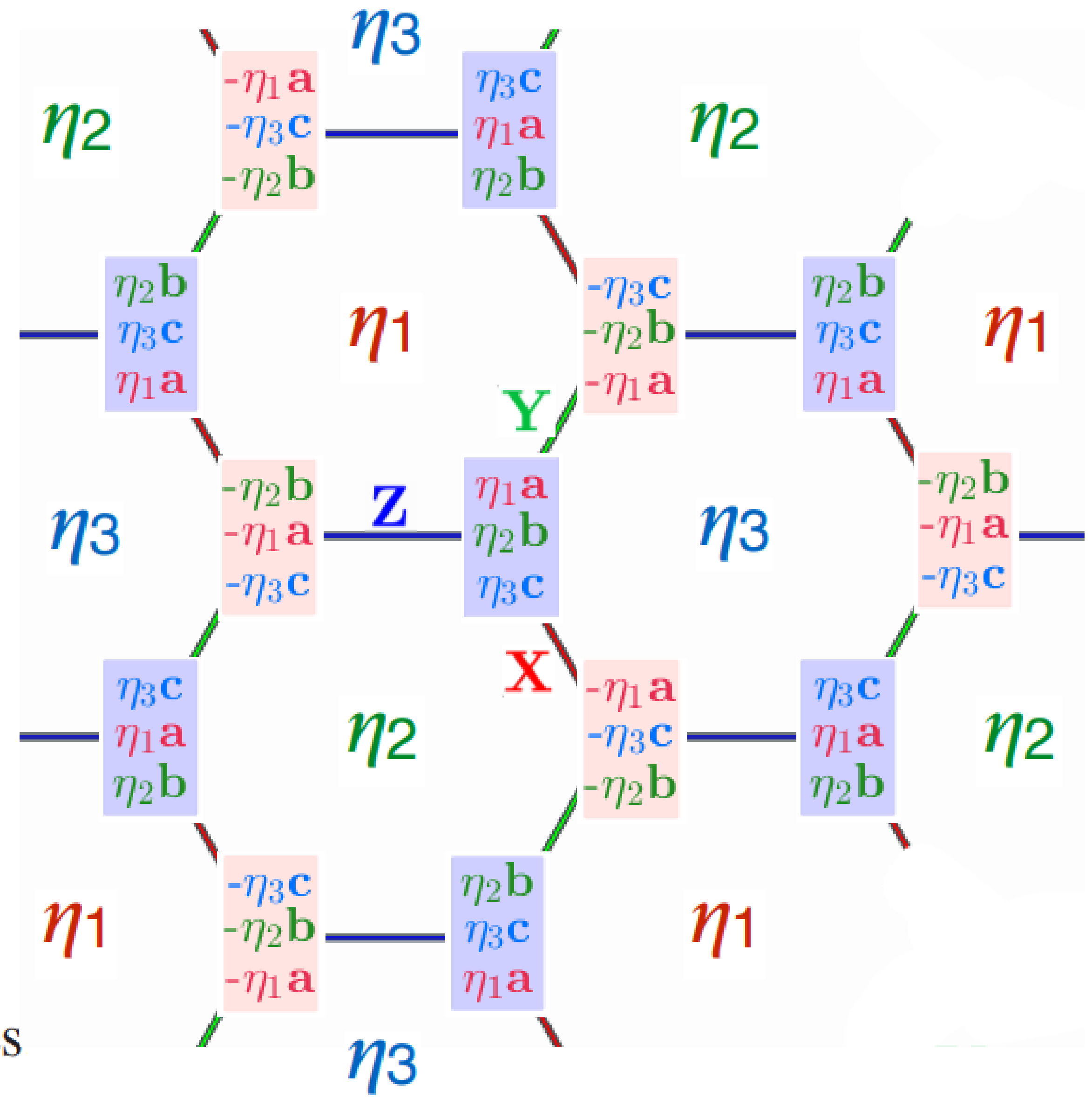
$$\mathbf{S}_0 = (\eta_1 a, \eta_2 b, \eta_3 c),$$

$$a = |S_0^x|,\ \eta_1 = \mathrm{sgn}(S_0^x)$$
$$b = |S_0^y|,\ \eta_2 = \mathrm{sgn}(S_0^y)$$
$$c = |S_0^z|,\ \eta_3 = \mathrm{sgn}(S_0^z)$$

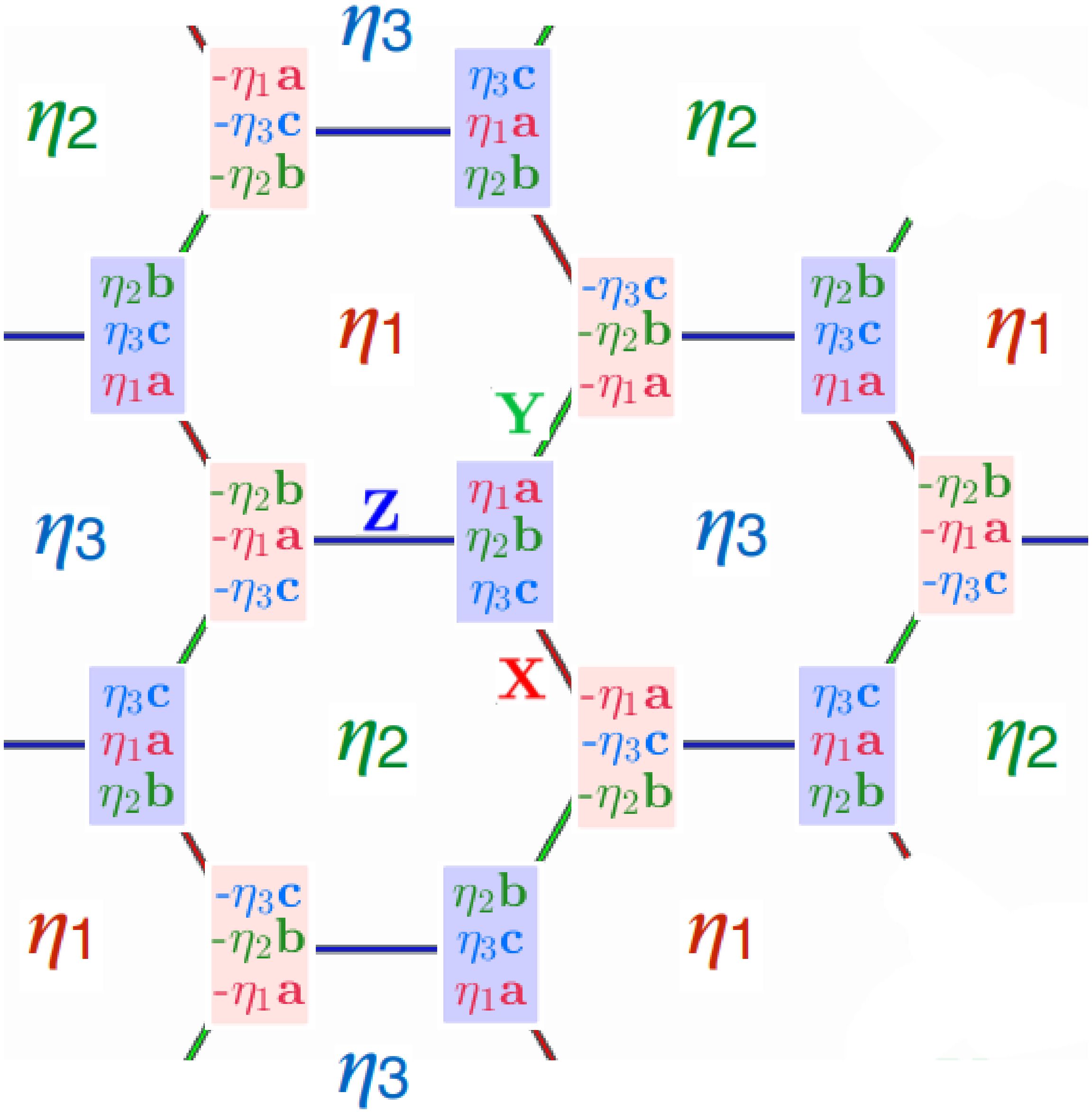
Restrictions

$$a^2 + b^2 + c^2 = S^2$$

$\eta_i = \pm 1$ are Ising variables



Classical Kitaev-Γ model: $K > 0$



for ∀ fixed (a, b, c)

- ❑ # sublattice: 3
- ❑ # G.S.: $2^3 = 8$
- ➢ **magnetically ordered state**

for $(a, b, c) = S/\sqrt{3}$

- ❑ AFM: $\eta_1 = \eta_2 = \eta_3$
  - ■ two sublattice
  - ■ 2-fold degeneracy
- ❑ 120 order: otherwise
  - ■ six sublattice
  - ■ 6-fold degeneracy

Chiral spin state (手性自旋态)

Real-space perturbation theory

$$\mathbf{S}_i = S_i^z \mathbf{e}_i^z + S_i^+ \mathbf{e}_i^- + S_i^- \mathbf{e}_i^+$$

$$\mathbf{e}_i^\pm = \frac{1}{2}(\mathbf{e}_i^x \pm i\mathbf{e}_i^y)$$

$$\mathcal{H} = \frac{1}{2}\sum_{ij} \mathbf{S}_i \cdot \mathbf{A}_{ij} \cdot \mathbf{S}_j = \mathcal{H}_0 + \mathcal{V}$$

$$\mathcal{H}_0 = E_{cl} + \sum\nolimits_j B_j n_j$$

$$E_{cl} = \frac{S^2}{2}\sum_{ij} A_{ij}^{zz}$$

$$\mathbf{B}_j = -S\sum_i \mathbf{e}_i^z \cdot \mathbf{A}_{ij} = -B_j \mathbf{e}_j^z$$

$$\left[n_i = S - S_i^z,\, A_{ij}^{\alpha\beta} = \mathbf{e}_i^\alpha \cdot \mathbf{A}_{ij} \cdot \mathbf{e}_j^\beta\right]$$

$$\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2 + \mathcal{V}_3$$

$$\mathcal{V}_1 = \frac{1}{2}\sum_{ij}\left(A_{ij}^{++} S_i^- S_j^- + h.c.\right),$$

$$\mathcal{V}_2 = \frac{1}{2}\sum_{ij}\left(A_{ij}^{+-} S_i^- S_j^+ + h.c.\right),$$

$$\mathcal{V}_3 = -\frac{1}{2}\sum_{ij}\left(A_{ij}^{z+} n_i S_j^- + A_{ij}^{+z} S_i^- n_j + h.c.\right)$$

energy correlation

$$e_{cl} = -(\Gamma + K/2)S^2 - \frac{(\Gamma - K)^2 S}{32|\Gamma + 2K|}\left[\left(\frac{a}{S}\right)^4 + \left(\frac{b}{S}\right)^4 + \left(\frac{c}{S}\right)^4\right]$$

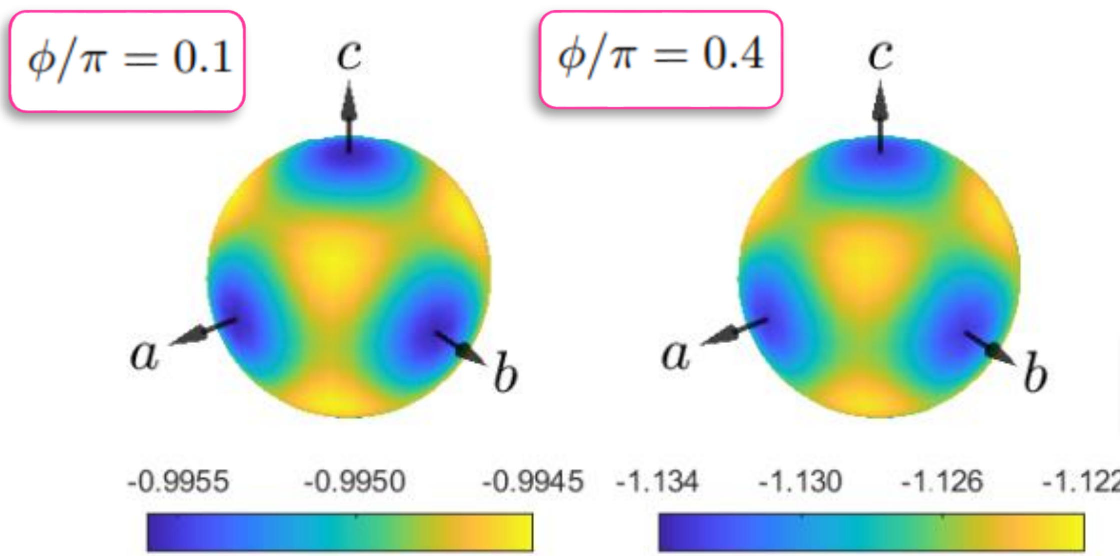
Chiral spin state (手性自旋态)

- **Linear spin-wave theory**

$$\tilde{S}_i^+ \simeq \sqrt{2S}a_i, \quad \tilde{S}_i^- \simeq \sqrt{2S}a_i^\dagger, \quad \tilde{S}_i^n = S - a_i^\dagger a_i$$

$$\mathcal{H}_{SW} = -NS(S+1)e_g + \frac{S}{2}\sum_{\boldsymbol{q}} \hat{\mathbf{x}}_{\boldsymbol{q}}^\dagger \hat{\mathbf{H}}_{\boldsymbol{q}} \hat{\mathbf{x}}_{\boldsymbol{q}}, \quad \hat{\mathbf{H}}_{\boldsymbol{q}} = \begin{pmatrix} \hat{\Lambda}_{\boldsymbol{q}} & \hat{\Delta}_{\boldsymbol{q}} \\ \hat{\Delta}_{\boldsymbol{q}}^\dagger & \hat{\Lambda}_{-\boldsymbol{q}}^T \end{pmatrix}$$

$$e_{sw} = \left(1 + \frac{1}{S}\right) e_{cl} + \frac{S}{2}\sum_{\upsilon\mathbf{q}} \omega_{\upsilon\mathbf{q}}.$$



The energy is minimized when one of the three spin components is unitary.

Cubic axes are selected!

QL, et al., arXiv:2403.08382.

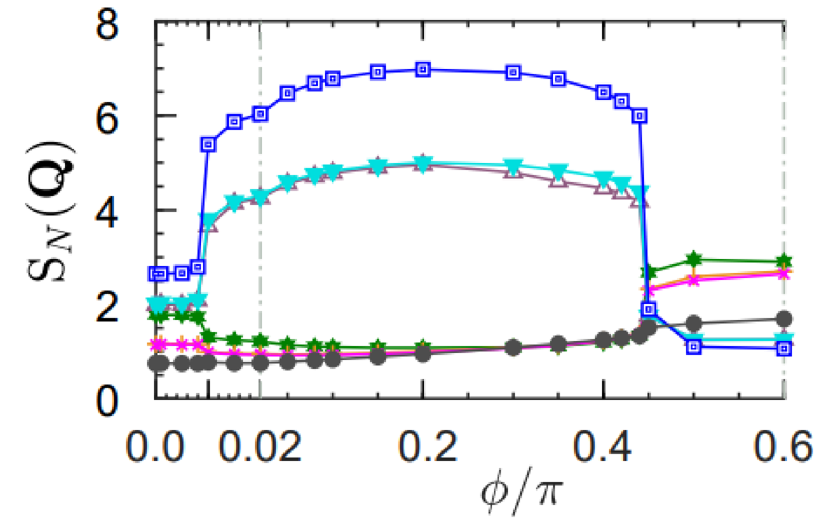
Chiral spin state (手性自旋态)

Static structure factor: $S(\mathrm{K})/S(\Gamma') = 2/3$

$$\mathbb{S}_N(\mathbf{q}) = \frac{1}{N}\sum_{ij}\sum_{\gamma}\langle S_i^{\gamma} S_j^{\gamma}\rangle e^{\imath\mathbf{q}\cdot(\boldsymbol{R}_i-\boldsymbol{R}_j)}$$

$$\mathbb{S}_N(\boldsymbol{\Gamma}') \propto \frac{S^2}{4} + \frac{\eta_a\eta_b ab + \eta_b\eta_c bc + \eta_c\eta_a ca}{2} = \frac{S^2}{4}$$

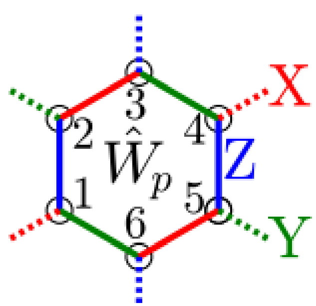
$$\mathbb{S}_N(\mathbf{K}) \propto \frac{S^2}{6} - \frac{\eta_a\eta_b ab + \eta_b\eta_c bc + \eta_c\eta_a ca}{6} = \frac{S^2}{6}$$

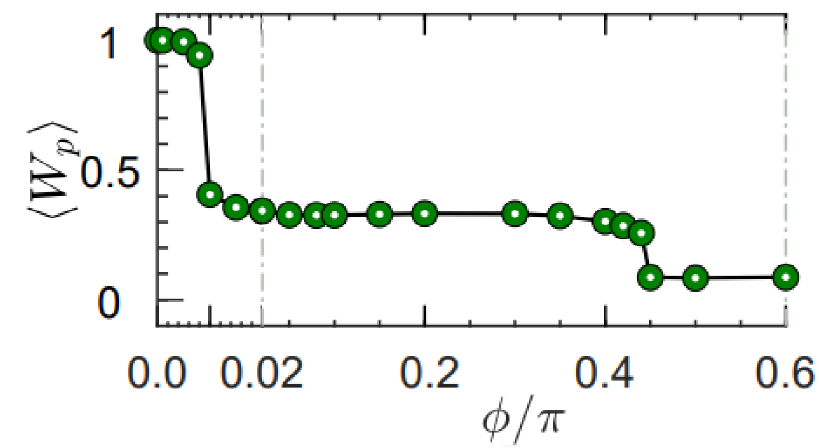


Hex. plaquette operator: Evidence of trimerization

$$\hat{W}_p = e^{\imath\pi(S_1^x + S_2^y + S_3^z + S_4^x + S_5^y + S_6^z)}$$

$$\begin{cases} W_{p,a} = 1 \\ W_{p,b} = 0 \\ W_{p,c} = 0 \end{cases}$$



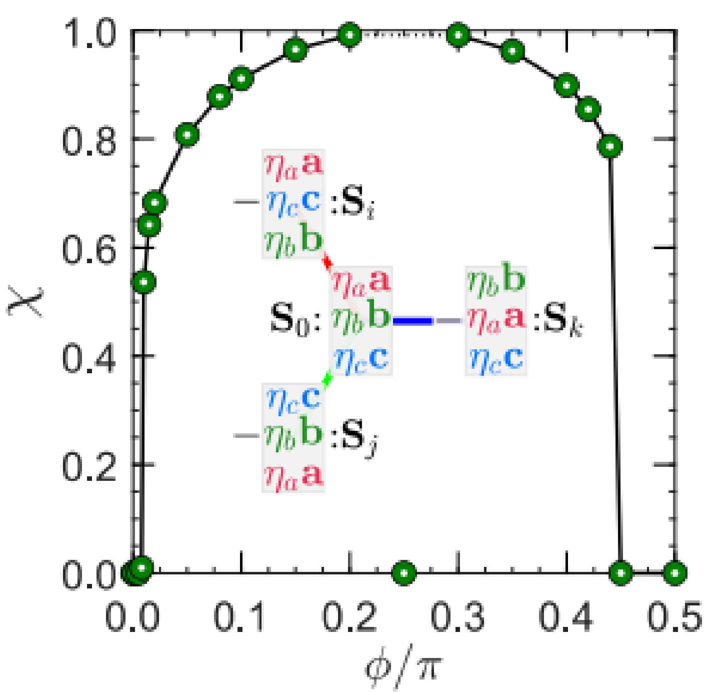


Chiral spin state (手性自旋态)

Scalar spin chirality

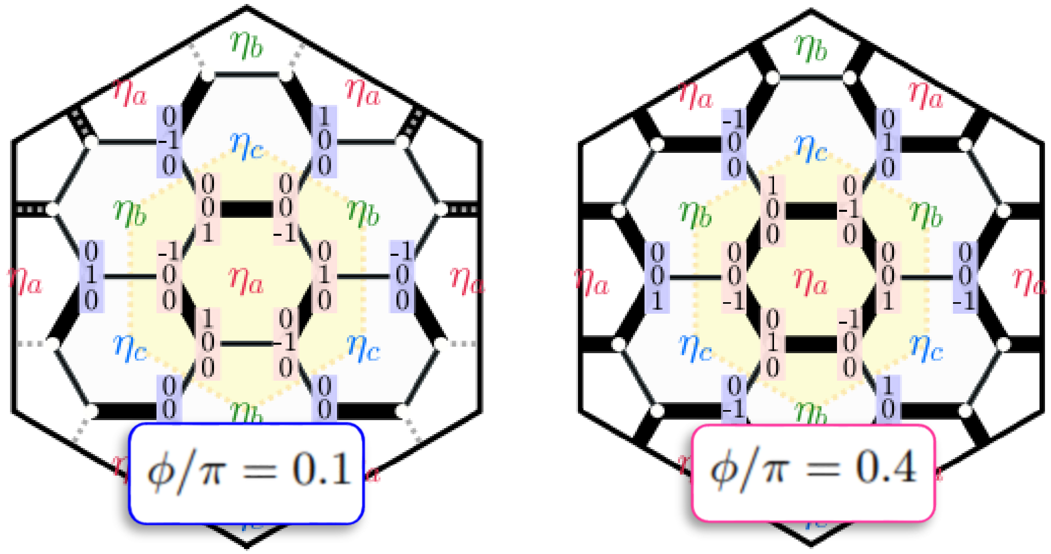
$$\chi_{ijk}^{\triangle} = \left\langle \hat{\mathbf{S}}_i \cdot (\hat{\mathbf{S}}_j \times \hat{\mathbf{S}}_k) \right\rangle$$

$$\chi_{ijk}^{\triangle} = (\eta_a a)^3 + (\eta_b b)^3 + (\eta_c c)^3 - 3\eta_a\eta_b\eta_c abc = \eta S^3$$



Columnar vs Plaquette pattern

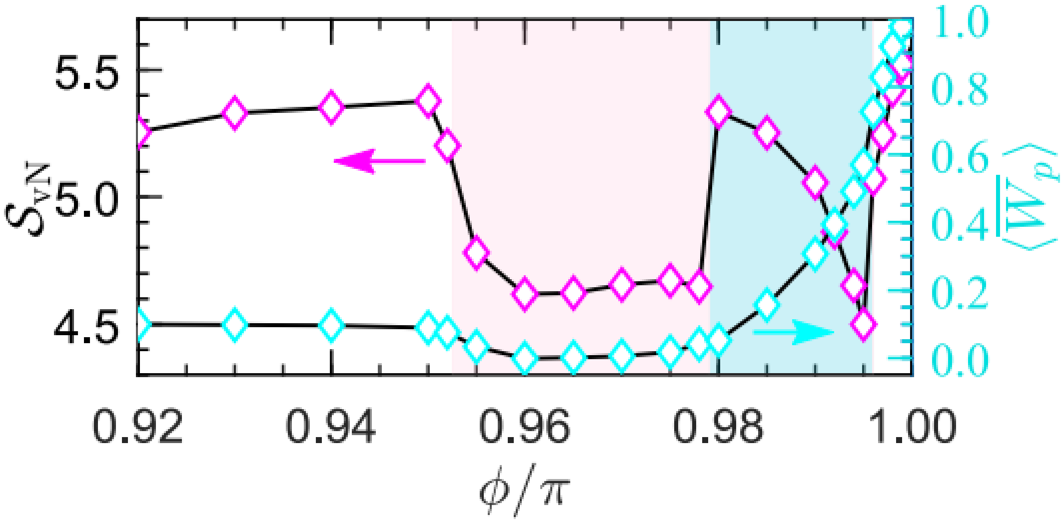
When $\boldsymbol{K} > \boldsymbol{\Gamma}$ $(\phi/\pi < 0.25)$,
K-bonds should be stronger,
leading to **columnar-like** dimer pattern



When $\boldsymbol{K} < \boldsymbol{\Gamma}$ $(\phi/\pi > 0.25)$,
Γ-bonds should be stronger,
leading to **plaquette-like** dimer pattern

Nematic ferromagnets (向列铁磁体)

Quantum phase transition (24-site hexagonal cluster)

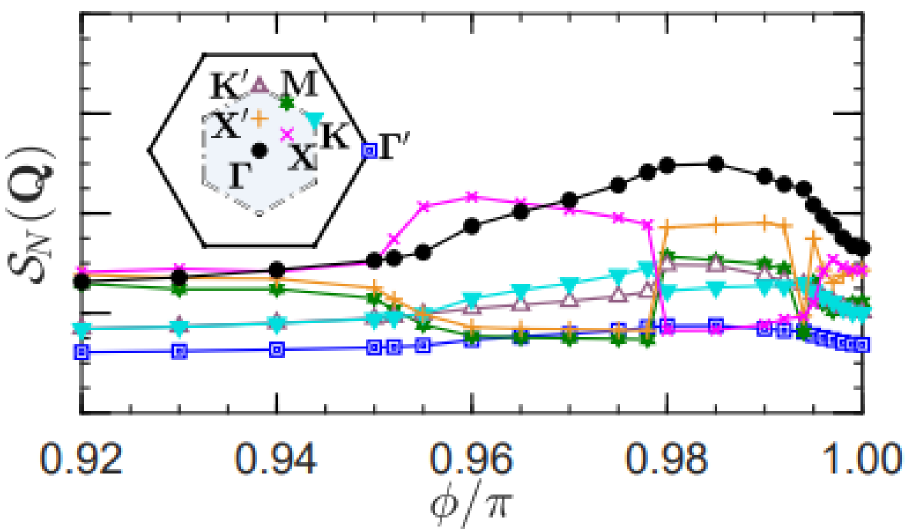


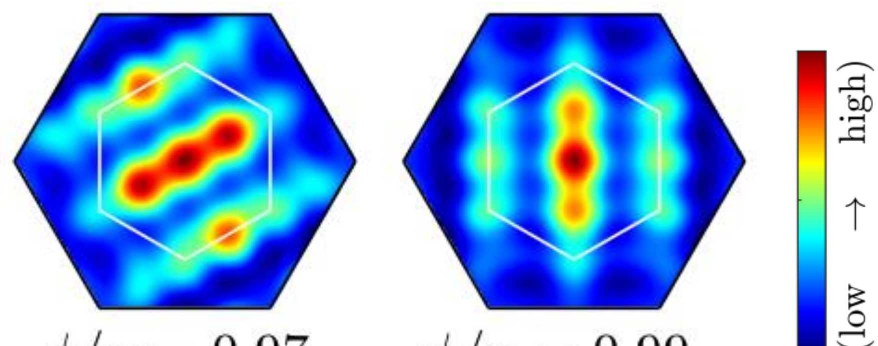
- von Neumann entropy

$$\mathcal{S}_{\rm vN}(l) = -\mathrm{tr}\,(\rho_l \ln \rho_l)$$

- hex. plaquette operator

$$\hat{W}_p = e^{\imath\pi(S_1^x+S_2^y+S_3^z+S_4^x+S_5^y+S_6^z)}$$



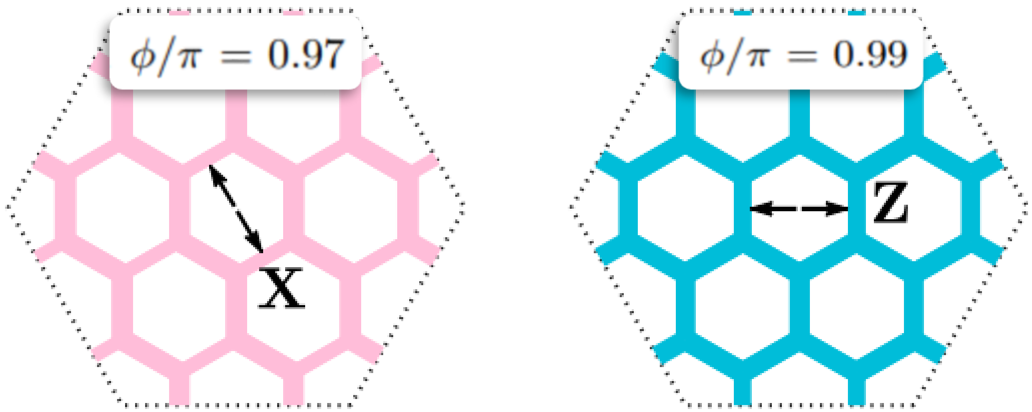


$\phi/\pi = 0.97$ $\phi/\pi = 0.99$

leading peak at **Γ** point!

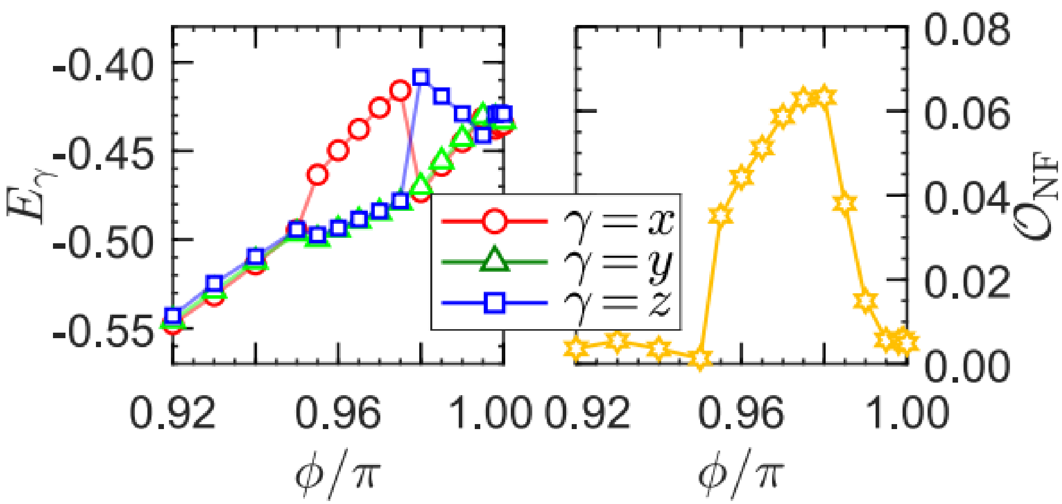
Nematic ferromagnets (向列铁磁体)

Nematic order is the breaking of **rotational** symmetry in the presence of translational invariance.



One of the bond energy is different from the remaining.

C_3 Rot. Sym. Breaking!



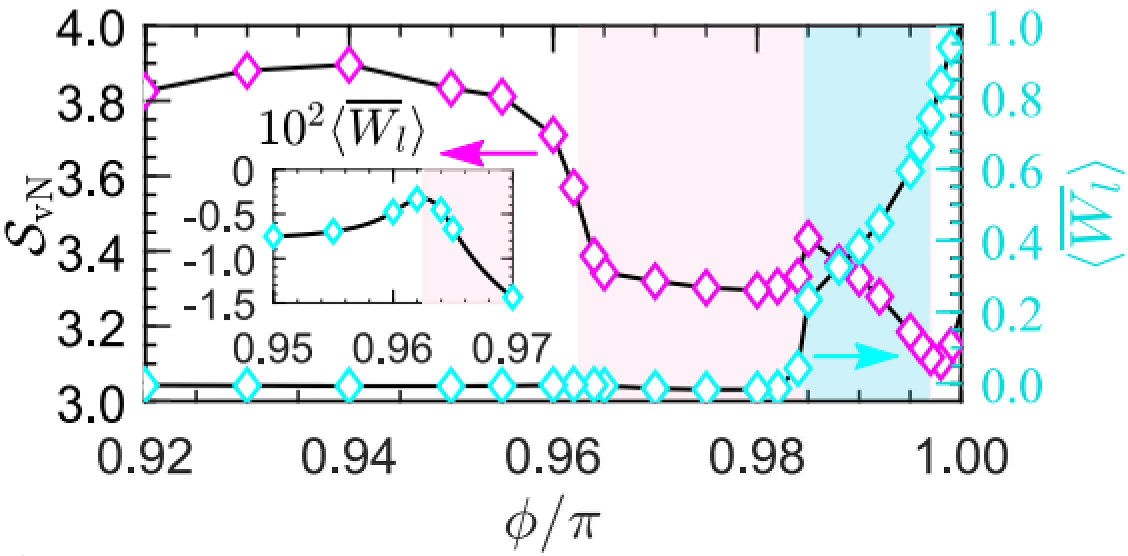
❑ Nematic order parameter

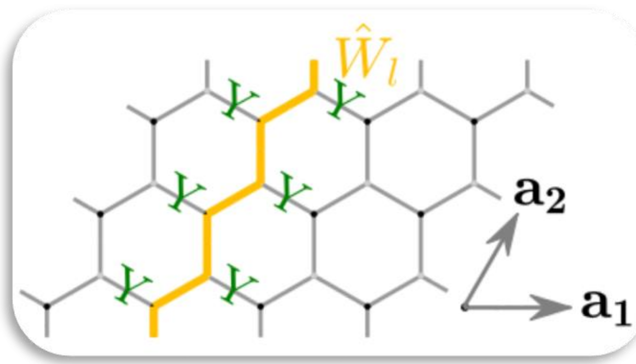
$$\mathcal{O}_{\rm NF} = |\min(E^\gamma) - \max(E^\gamma)|$$

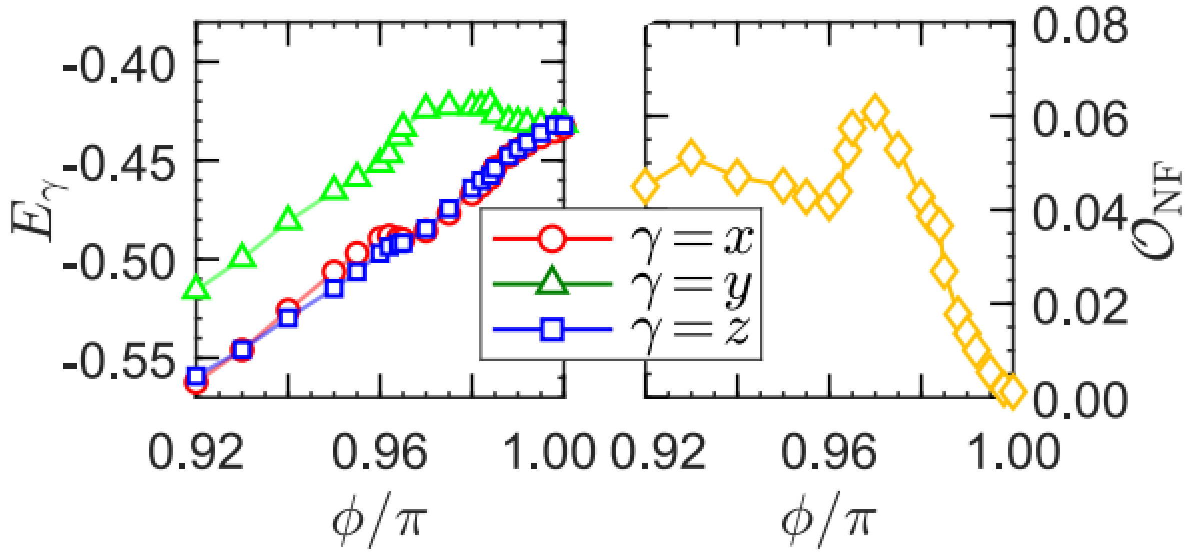
QL, et al., arXiv:2403.08382.

Nematic ferromagnets (向列铁磁体)

- **Quantum phase transition (24-site rhombic cluster)**

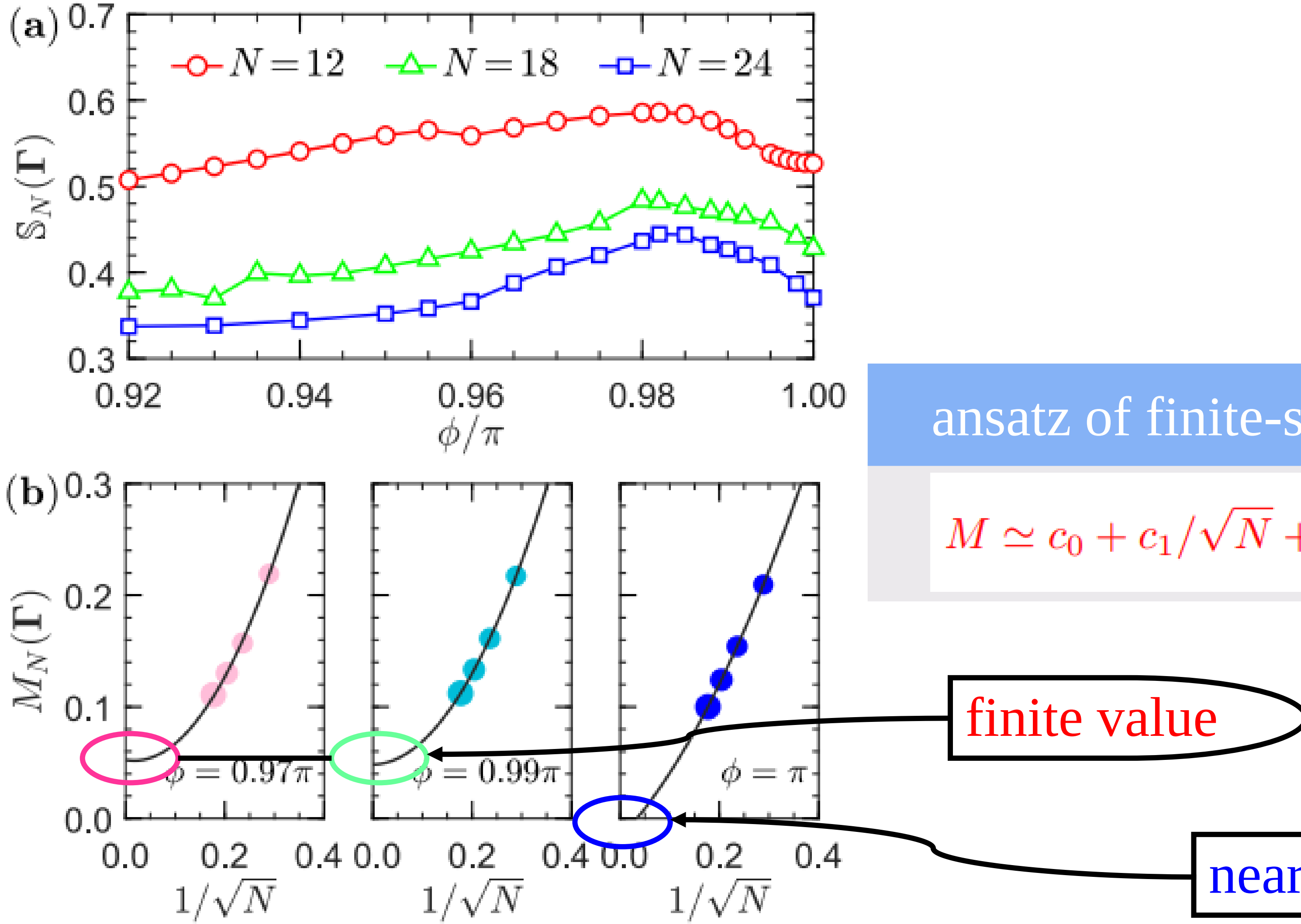






Nematic ferromagnets (向列铁磁体)

Magnetic order parameter



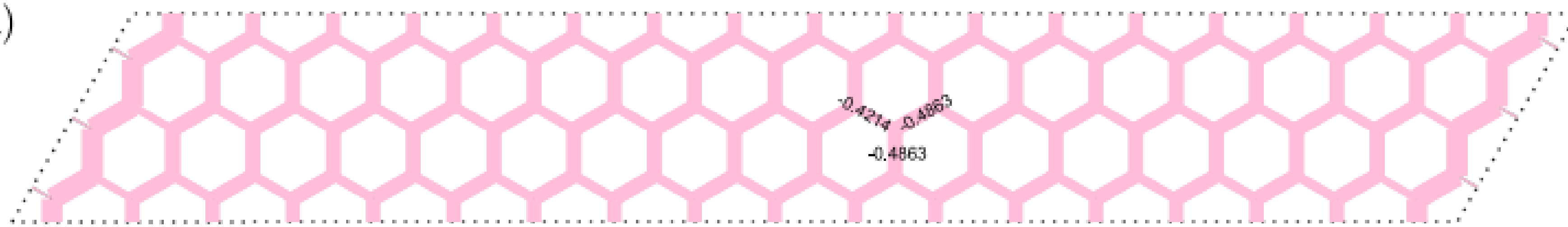
ansatz of finite-size scaling

$$M \simeq c_0 + c_1/\sqrt{N} + c_2/N + \cdots$$

Nematic ferromagnets (向列铁磁体)

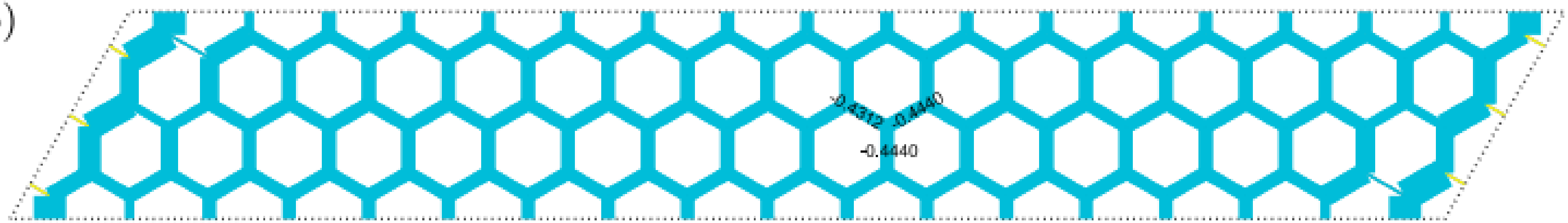
Nematicity on long 2 × 18 × 3 cylinder

(a)



$E^{\gamma} = (-0.4863, -0.4214, -0.4863) \longrightarrow \mathcal{O}_{\mathrm{NF}} = 0.0649$

(b)

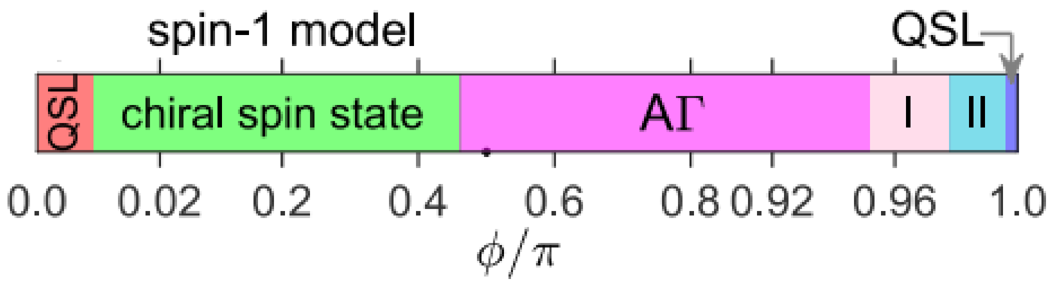


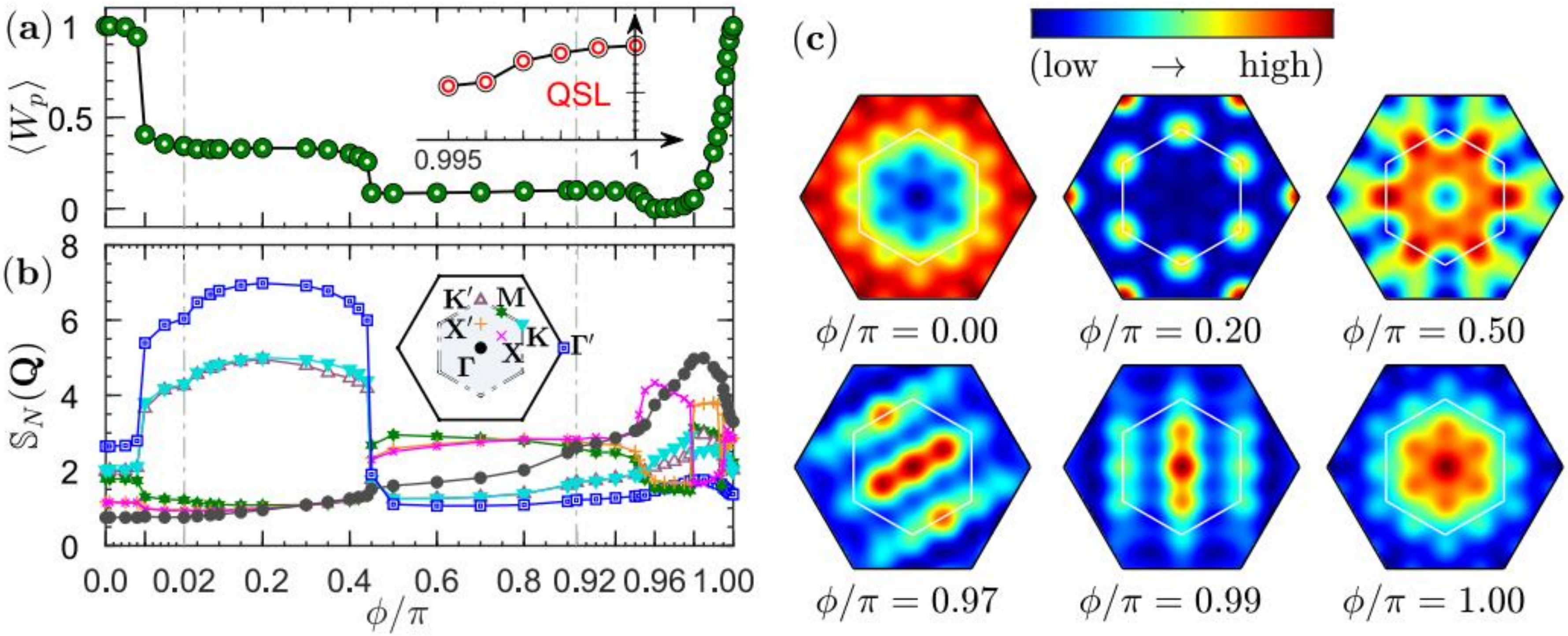
$E^{\gamma} = (-0.4440, -0.4312, -0.4440) \longrightarrow \mathcal{O}_{\mathrm{NF}} = 0.0128$

Robustness of the nematic order parameter

Phase	Parameter	$N = 24$	$2 \times 4 \times 3$	$2 \times 18 \times 3$
NF-I	$\phi/\pi = 0.97$	0.0592	0.0615	0.0649
NF-II	$\phi/\pi = 0.99$	0.0158	0.0139	0.0128

The quantum phase diagram





Remark: The AΓ phase is a likely disordered phase, but more computational efforts are required.

Outline

- 朗道相变理论和新突破
  - Ising模型中的相变
  - Kosterlitz-Thouless相变和去禁闭量子临界点
  - Luttinger液体和Haldane相
- 量子自旋液体和自旋轨道耦合型材料
  - 量子自旋液体简介
  - 三角晶格上的量子材料
  - 蜂窝晶格上的量子材料
- Kitaev-Γ模型中的物理
  - 自旋S=1/2和1的Kitaev-Γ自旋链
  - 自旋S=1的Kitaev-Γ模型

感谢各位老师同学批评指正！