

20240914

**Condensed matter physics:
from magnetism
to quantum spin liquid II**

Sophia University Ryui Kaneko (金子隆威)

Rough outline

Hamiltonian for electrons in atoms

$$\mathcal{H} = - \sum_j^{N_e} \frac{\hbar^2}{2m} \nabla_j^2 - \sum_\alpha^{N_i} \frac{\hbar^2}{2M_\alpha} \nabla_\alpha^2 - \sum_j^{N_e} \sum_\alpha^{N_i} \frac{Z_\alpha e^2}{|\vec{r}_j - \vec{R}_\alpha|} + \sum_{j \ll k}^{N_e} \frac{e^2}{|\vec{r}_j - \vec{r}_k|} + \sum_{\alpha \ll \beta}^{N_j} \frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha - \vec{R}_\beta|}$$

Hubbard model

$$\hat{H} = - \sum_{\langle i,j \rangle} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Heisenberg model

$$\hat{H} = \sum_{\langle i,j \rangle} J_{ij} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j$$

magnetism, quantum spin liquid, ...

Outline

- Brief review of itinerant electron systems
 - Electrons in crystals
 - Second quantization
 - Hubbard models
 - Solving models for simple cases
 - Noninteracting and atomic limits
 - Mean-field approximation
 - Exact diagonalization (2 sites)
 - Strong coupling limit: Heisenberg model (spin system)
- Magnetism and quantum spin liquid
 - Spin models
 - Frustrated magnetism and quantum spin liquid
 - Kitaev honeycomb spin liquid

Spin models

- Heisenberg model

$$H = \sum_{ij} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j = \sum_{ij} J_{ij} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z)$$

- XXZ model

$$H = \sum_{ij} [J_{ij}^{xy} (S_i^x S_j^x + S_i^y S_j^y) + J_{ij}^z S_i^z S_j^z]$$

- XY model ($J_{ij}^z=0$)

$$H = \sum_{ij} J_{ij}^{xy} (S_i^x S_j^x + S_i^y S_j^y)$$

- Classical Ising model ($J_{ij}^{xy}=0$)

$$H = \sum_{ij} J_{ij}^z S_i^z S_j^z$$

- Transverse-field Ising model

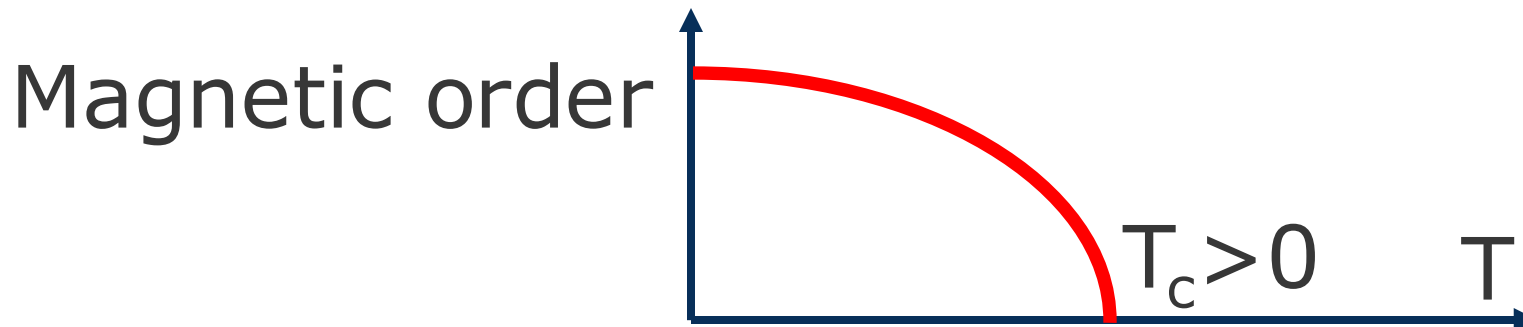
$$H = \sum_{ij} J_{ij} S_i^z S_j^z - \sum_i \Gamma_i S_i^x$$

Mermin-Wagner theorem

- Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $D \leq 2$.

N. D. Mermin and H. Wagner, PRL.17.1133 ('66)

Spatial dimension	$T_c > 0$?
1D	x
2D	x
3D	✓
4D	✓
...	...



Mermin-Wagner theorem

- Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions $D \leq 2$.
N. D. Mermin and H. Wagner, PRL.17.1133 ('66)

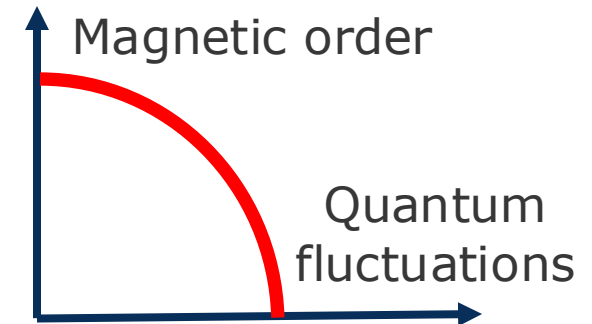
- Note 1: Of course, discrete symmetries can be spontaneously broken even in $D=2$ (e.g., $T_c > 0$ in 2D Ising models).
- Note 2: MW theorem does not state anything about the topological phase transition (e.g., Berezinskii-Kosterlitz-Thouless (BKT) transition occurs in systems with $U(1)$ symmetry in 2D).

“Mermin-Wagner theorem” at $T=0$

- Quantum fluctuations in low spatial dimensions sometimes behave like thermal fluctuations

- Consider

- Continuous spin systems on lattices
- Interaction J_{ij} is short-range
- J_{ij} is not ferromagnetic



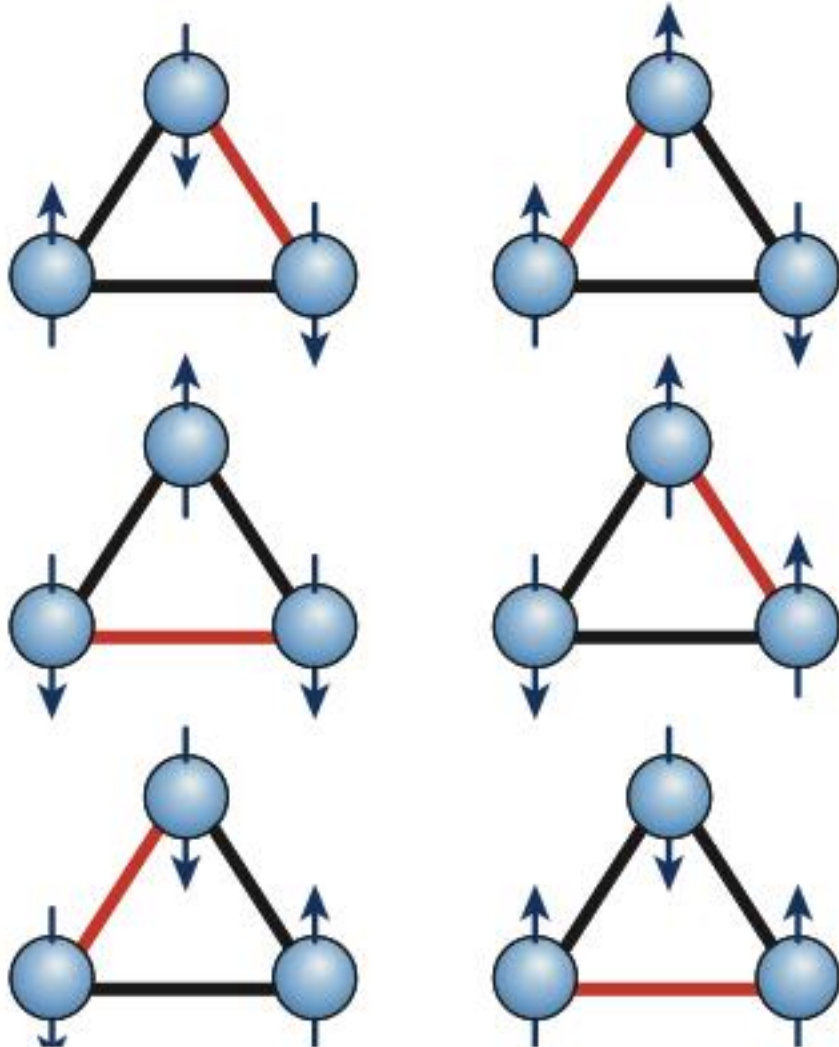
(c.f. for more rigorous argument, see H. Watanabe et al., arXiv:2310.16881)

Then,	Spatial dimension	Magnetic Long-range order at $T=0$?
	1D	x
	2D	✓
	3D	✓

Pitaevskii and Stringari, JLowTempPhys.85.377('91)

No long-range order even in 2D, 3D at $T=0$?

- Example 1: **Classical** triangular Ising model



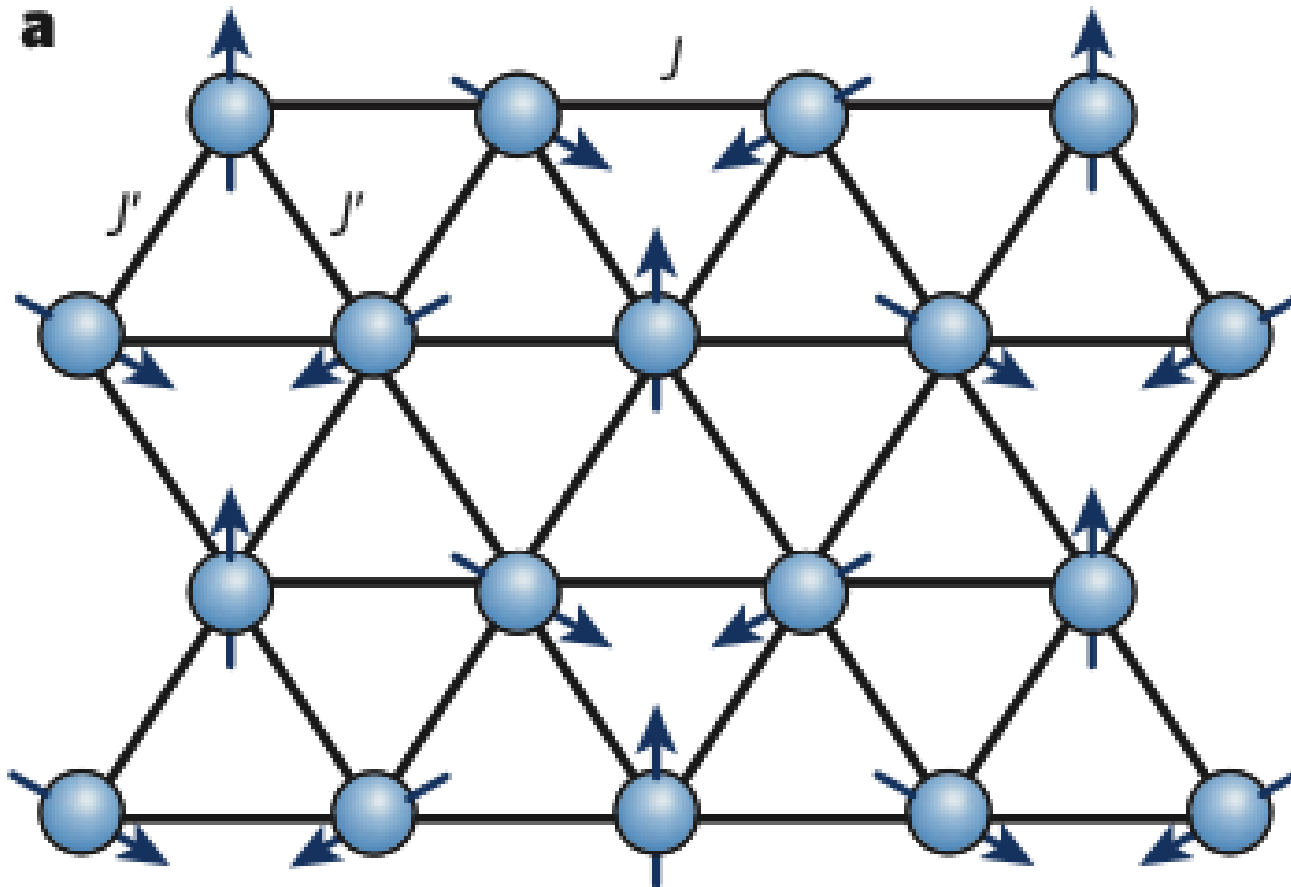
- Consider antiferromagnetic (AF) interaction $J > 0$
- Degenerate ground states for 3 sites
- For infinite sites, spin correlation shows **power-law decay** at $T=0$
- $\langle S_0 S_r \rangle \sim r^{-\eta}$ ($\eta = 1/2$)
- $\langle S_i \rangle = 0$ (**no long-range order**)

J. Stephenson, J. Math. Phys. 11, 413 (1970);
S. Alexander and P. Pincus, J. Phys. A: Math. Gen. 13, 263 (1980)

[Geometrical frustration](#)

No long-range order even in 2D, 3D at $T=0$?

- Example 2: **Classical** triangular Heisenberg model
(**ordered case**)



120° Neel order
at $T=0$

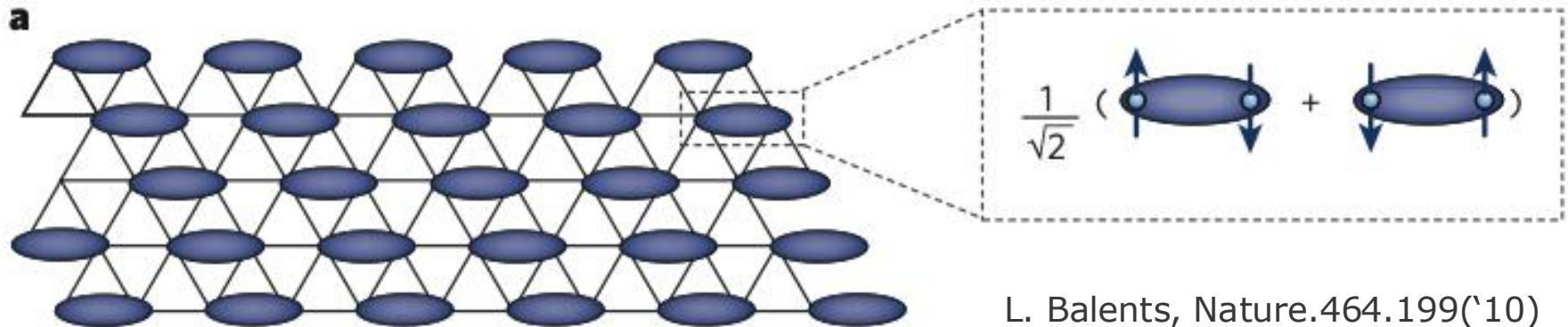
No long-range order even in 2D, 3D at $T=0$?

- In **quantum spin 1/2** triangular Heisenberg model
 - Ground state has **no magnetic order**?!

P. W. Anderson

“Resonating valence bonds: a new kind of insulator”

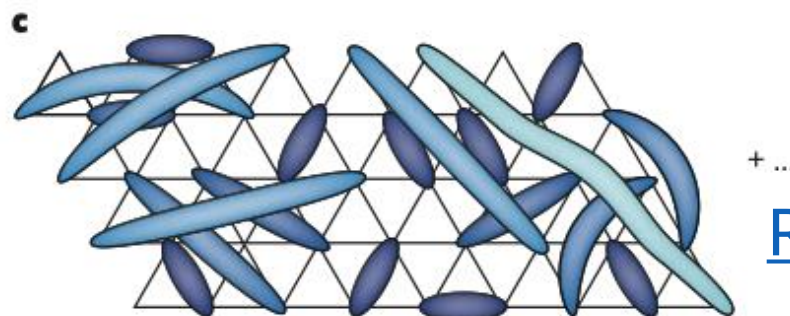
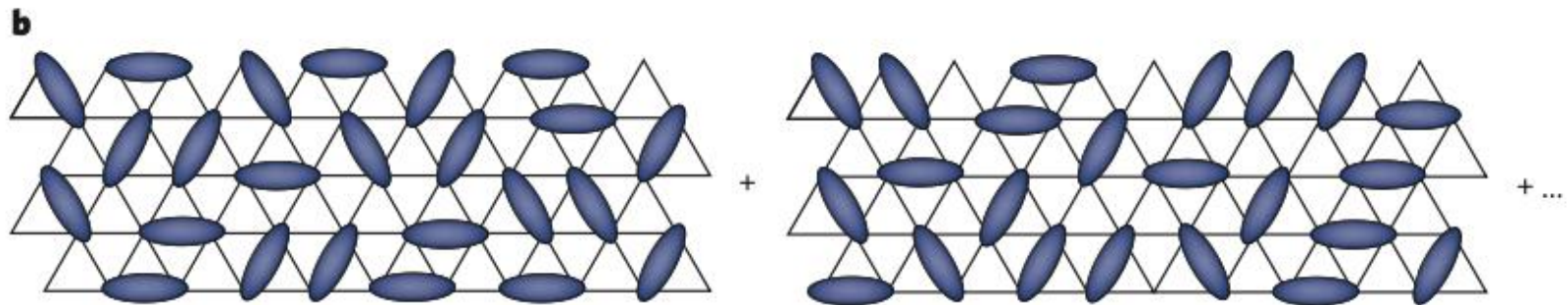
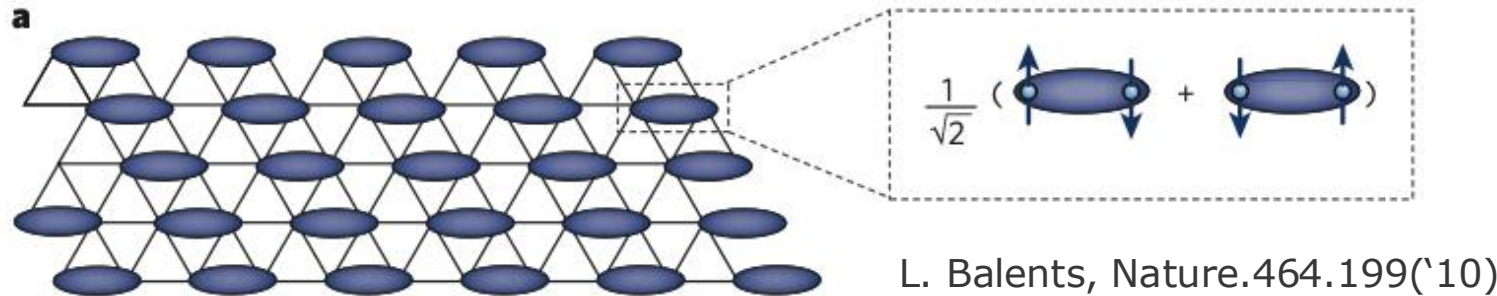
Mater. Res. Bull. 8, 153–160 (1973)



Example of a singlet dimerized state

No long-range order even in 2D, 3D at $T=0$?

- In **quantum spin 1/2** triangular Heisenberg model



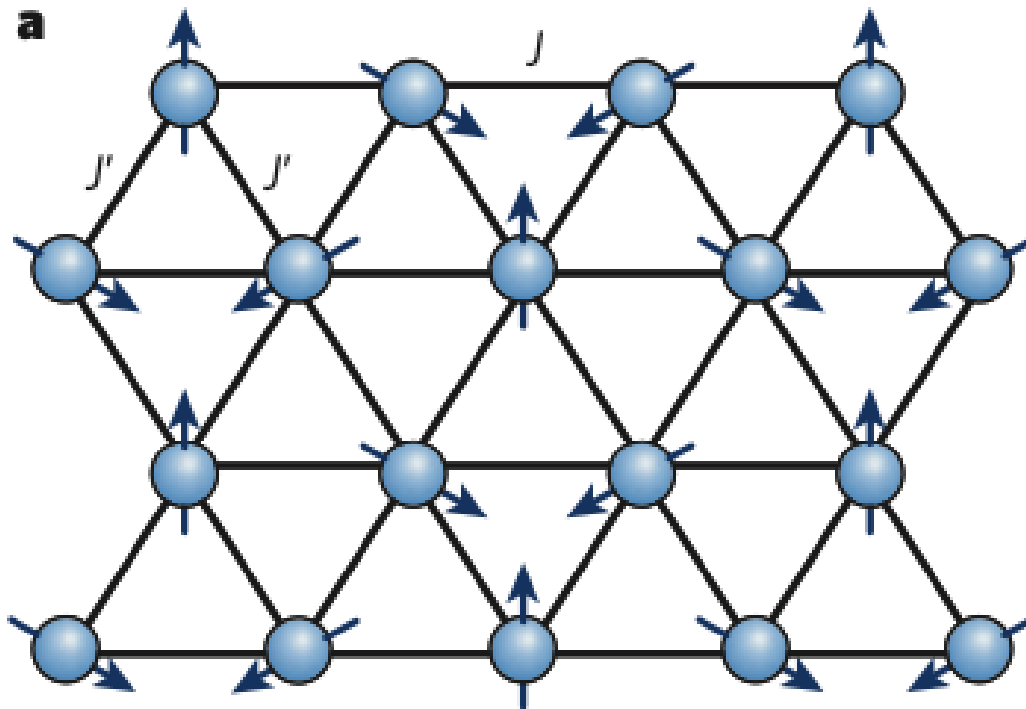
Dimer order is also absent?
Dimer dynamically moves?

+ ...

Resonating valence bond state
(RVB state)

No long-range order even in 2D, 3D at $T=0$?

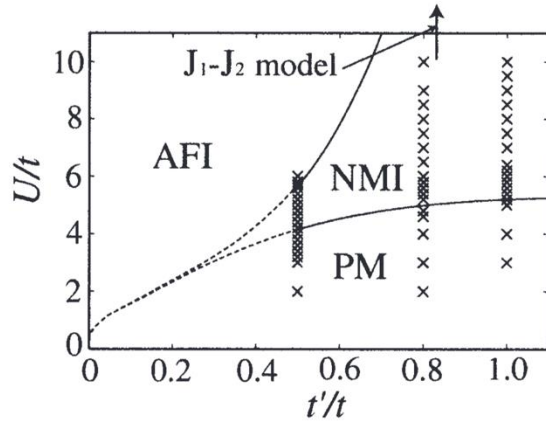
- In **quantum spin 1/2** triangular Heisenberg model
- Unfortunately, it is now widely believed that the true ground state has long-range magnetic order



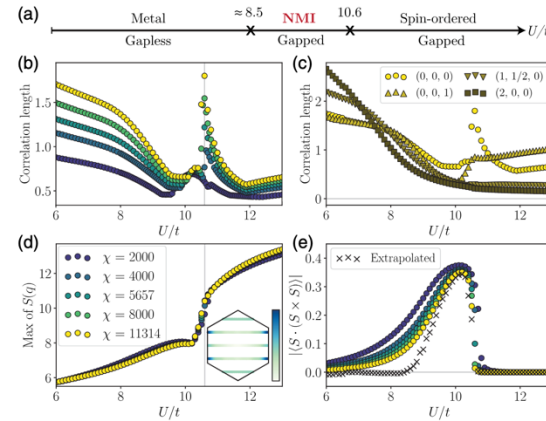
- Exact diagonalization
 - B. Bernu et al., PRB.50.10048('94)
- Variational Monte Carlo (VMC)
 - L. Capriotti et al., PRL.82.3899 ('99)
- Density matrix renormalization group (DMRG)
 - S. White and A. L. Chernyshev, PRL.99.127004('07)
- $\langle S_i \rangle / S_{\max} = 0.41(3)$ ($S_{\max} = 1/2$)

To realize quantum spin liquid...

- Effects of charge fluctuations

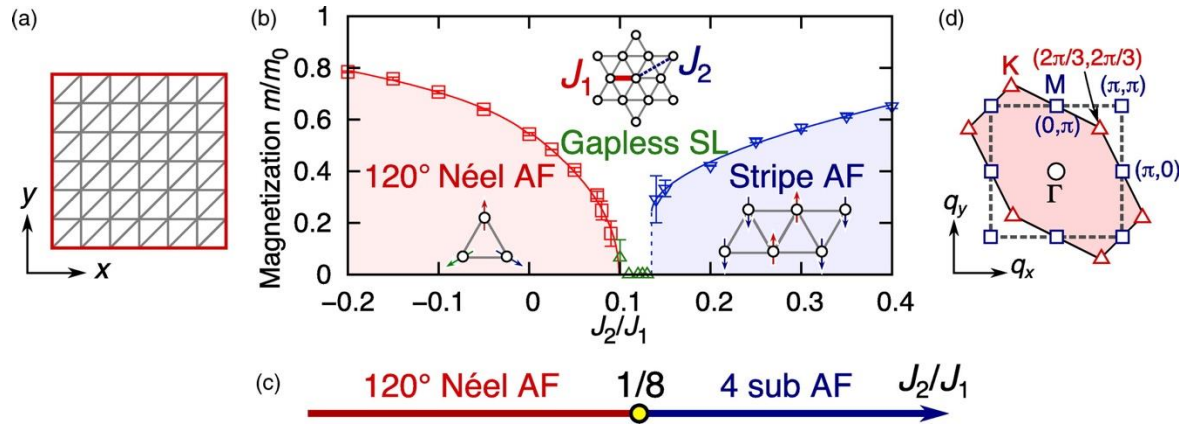


H. Morita et al.,
JPSJ.71.2109 ('02)



A. Szasz et al.,
PRX.10.021042 ('20)

- Effects of next-nearest-neighbor interaction

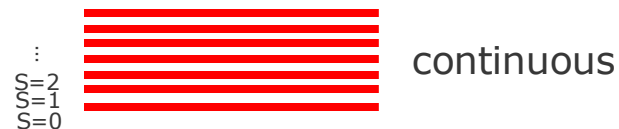
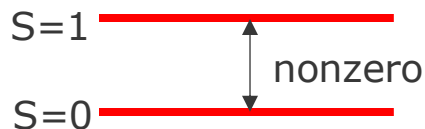


R. Kaneko et al.,
JPSJ.83.093707 ('14)

- And so on...

Quantum spin liquid (QSL)

- No long-range order of spin, dimer, ...
- Insulating (charge excitation: open)
 - Metal shows no order, but it is not quantum spin liquid
- Characterized by spin excitation (for $N_s \rightarrow \infty$)
 - Open: Gapped spin liquid
 - Often characterized by topological entanglement entropy
 - Closed: Gapless spin liquid
 - Sometimes characterized by spinon pairing symmetry (just as in the case of pairing symmetry in superconductors)



Example? Candidate materials?

- Triangular lattice

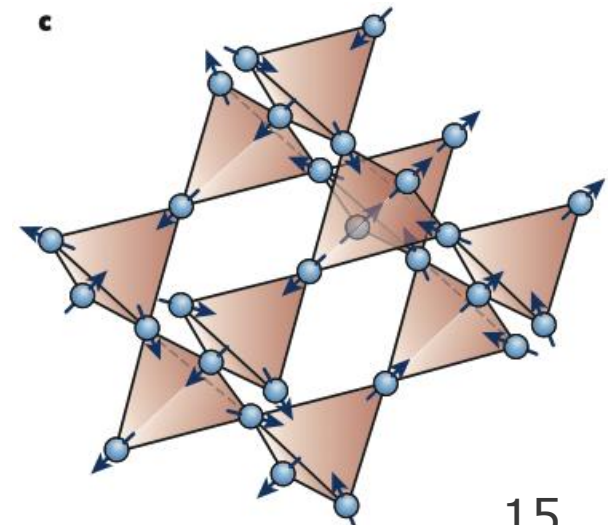
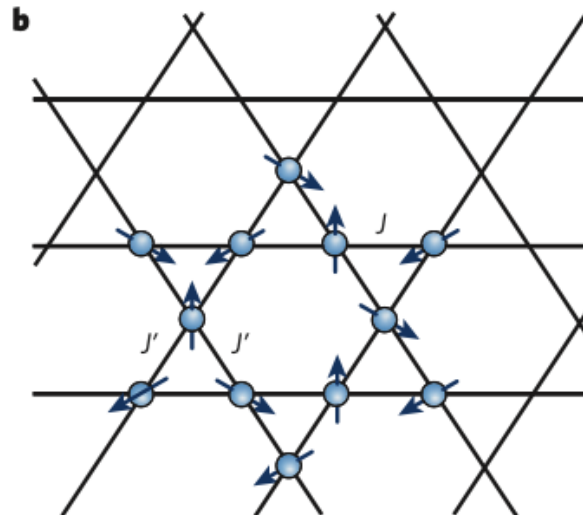
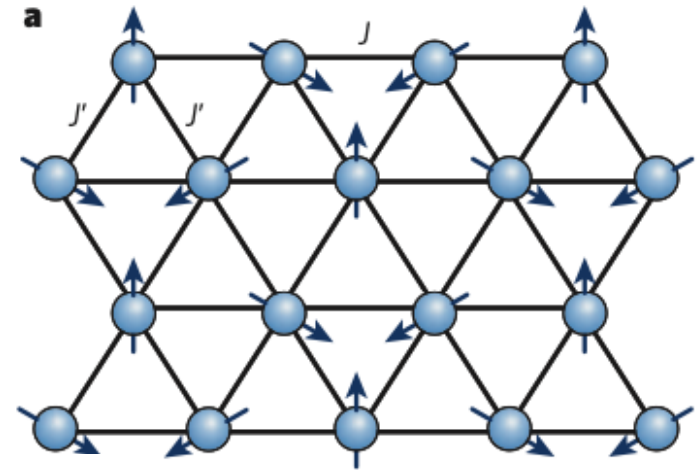
- Organic compounds
 - κ -(BEDTTTF) $_2$ Cu $_2$ (CN) $_3$
 - EtMe $_3$ Sb[Pd(dmit) $_2$] $_2$
- Antiferromagnets
 - YbMgGaO $_4$

- Kagome lattice

- Antiferromagnets
 - Herbertsmithite
 - Volborthite
 - Vesignieite
 - Kapellasite

- Pyrochlore lattice

- Antiferromagnets
 - Tb $_2$ Hf $_2$ O $_7$, Tb $_2$ Hf $_2$ O $_7$, Ce $_2$ Zr $_2$ O $_7$, ...



Why do we study QSL?

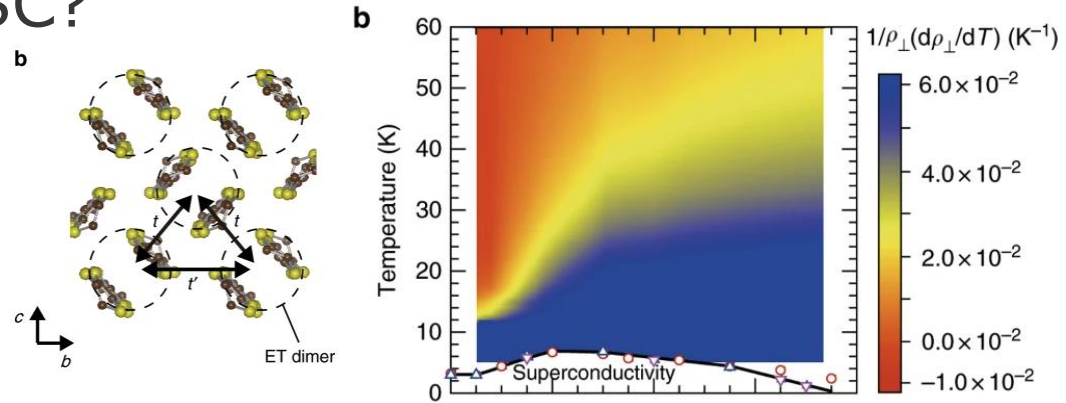
- Related to superconductivity (SC)
 - Doping QSL \rightarrow High T_c SC?

Article | [Open access](#) | Published: 02 October 2017

Anomalous metallic behaviour in the doped spin liquid candidate κ -(ET)₄Hg_{2.89}Br₈

[Hiroshi Oike](#) , [Yuji Suzuki](#), [Hiromi Taniguchi](#), [Yasuhide Seki](#), [Kazuya Miyagawa](#) & [Kazushi Kanoda](#) 


[Nature Communications](#) **8**, Article number: 756 (2017) | [Cite this article](#)



- Quantum computation
 - Using Majorana fermion in Kitaev spin liquid

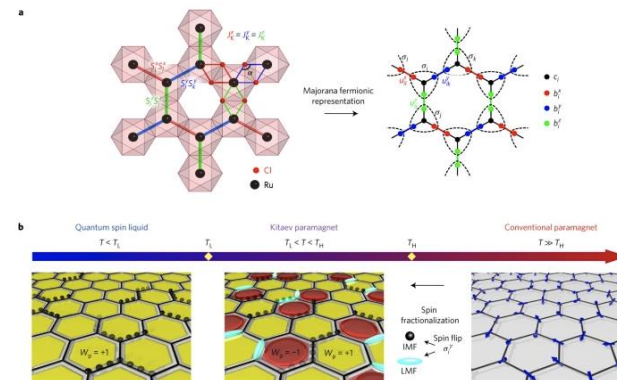
Letter | Published: 18 September 2017

Majorana fermions in the Kitaev quantum spin system α -RuCl₃

[Seung-Hwan Do](#), [Sang-Youn Park](#), [Junki Yoshitake](#), [Joji Nasu](#), [Yukitoshi Motome](#), [Yong Seung Kwon](#), [D. T. Adroja](#), [D. J. Voneshen](#), [Kyoo Kim](#), [T.-H. Jang](#), [J.-H. Park](#) , [Kwang-Yong Choi](#)  & [Sungdae Ji](#) 

[Nature Physics](#) **13**, 1079–1084 (2017) | [Cite this article](#)

Figure 1: Kitaev bonding geometry and cartoon of emergent Majorana fermions.



- (Just for fun)
 - Unconventional quasiparticles, statistics, ...

Difficulty in searching for QSL theoretically

- However, no analytical solution
 - Exception 1: “QSL” in 1D (Tomonaga-Luttinger liquid)
 - Exception 2: Kitaev QSL in 2D
- Mean-field approximation is not applicable
 - Any order parameter is 0
- No universal numerical methods
 - Exact diagonalization: Size too small
 - Quantum Monte Carlo method: Negative sign problem
- We often use **variational Monte Carlo** and **Tensor-network** methods

Kitaev QSL (rare example of solvable QSL)

What is unconventional about Kitaev QSL?

(in my opinion)

- It is often the case that
 - Gapped QSL → Short-range magnetic order
 $\langle S_0 \cdot S_r \rangle \sim \exp(-r/\xi)$
 - Gapless QSL → Quasi-long-range magnetic order
 $\langle S_0 \cdot S_r \rangle \sim r^{-\eta}$

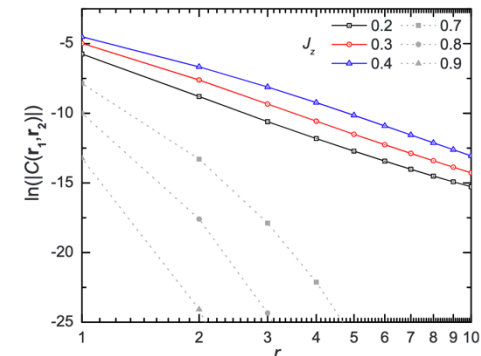
- In Kitaev QSL

- Gapless QSL → Short-range magnetic order
 $\langle S_0 \cdot S_r \rangle \sim \exp(-r/\xi)$

(Because spin rotational symmetry is explicitly broken and total spin is not a good quantum number in Kitaev model)

- In contrast, dimer-dimer correlation shows quasi-long-range order

S. Yang et al., PRA.78.012304 ('08)



Candidate material

PRL **102**, 017205 (2009)

PHYSICAL REVIEW LETTERS

week ending
9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

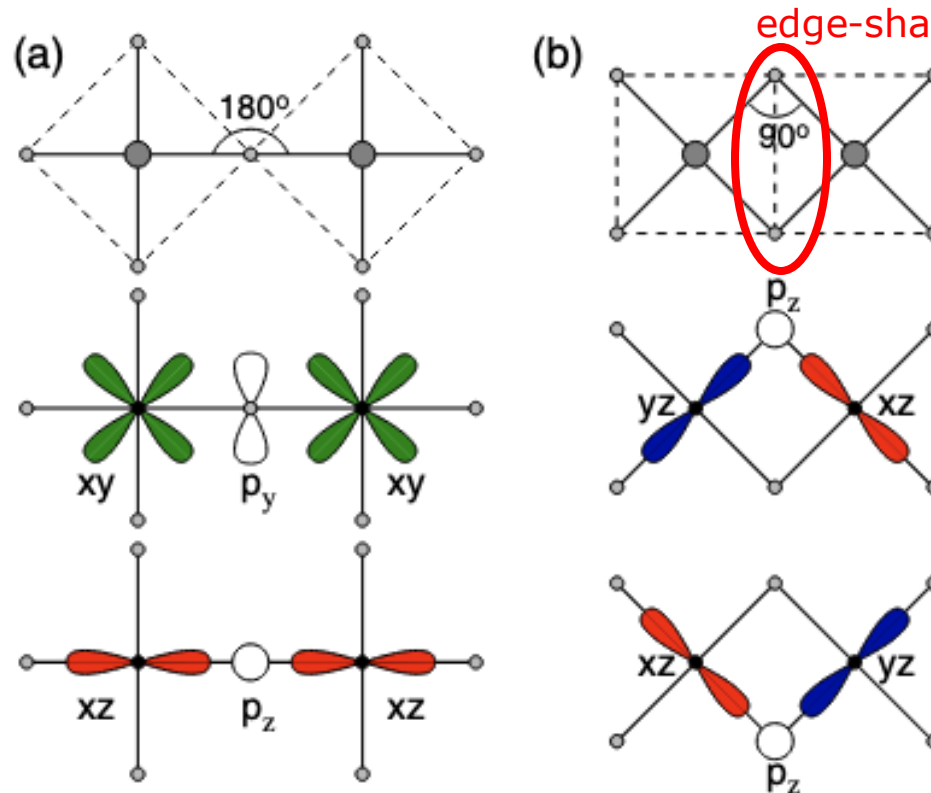
G. Jackeli^{1,*} and G. Khaliullin¹

¹Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
(Received 21 August 2008; published 6 January 2009)

We study the magnetic interactions in Mott-Hubbard systems with partially filled t_{2g} levels and with strong spin-orbit coupling. The latter entangles the spin and orbital spaces, and leads to a rich variety of the low energy Hamiltonians that extrapolate from the Heisenberg to a quantum compass model depending on the lattice geometry. This gives way to “engineer” in such Mott insulators an exactly solvable spin model by Kitaev relevant for quantum computation. We, finally, explain “weak” ferromagnetism, with an anomalously large ferromagnetic moment, in Sr_2IrO_4 .

DOI: [10.1103/PhysRevLett.102.017205](https://doi.org/10.1103/PhysRevLett.102.017205)

PACS numbers: 75.30.Et, 71.70.Ej, 75.10.Jm



- Consider Hubbard-type model with spin-orbit interaction
- Just as in the case of obtaining Heisenberg model, consider large U limit

Candidate: Sr_2IrO_4

$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij})(\vec{r}_{ij} \cdot \vec{S}_j)$$

$$\mathcal{H}_{ij}^{(\gamma)} = -JS_i^\gamma S_j^\gamma$$

Candidate material

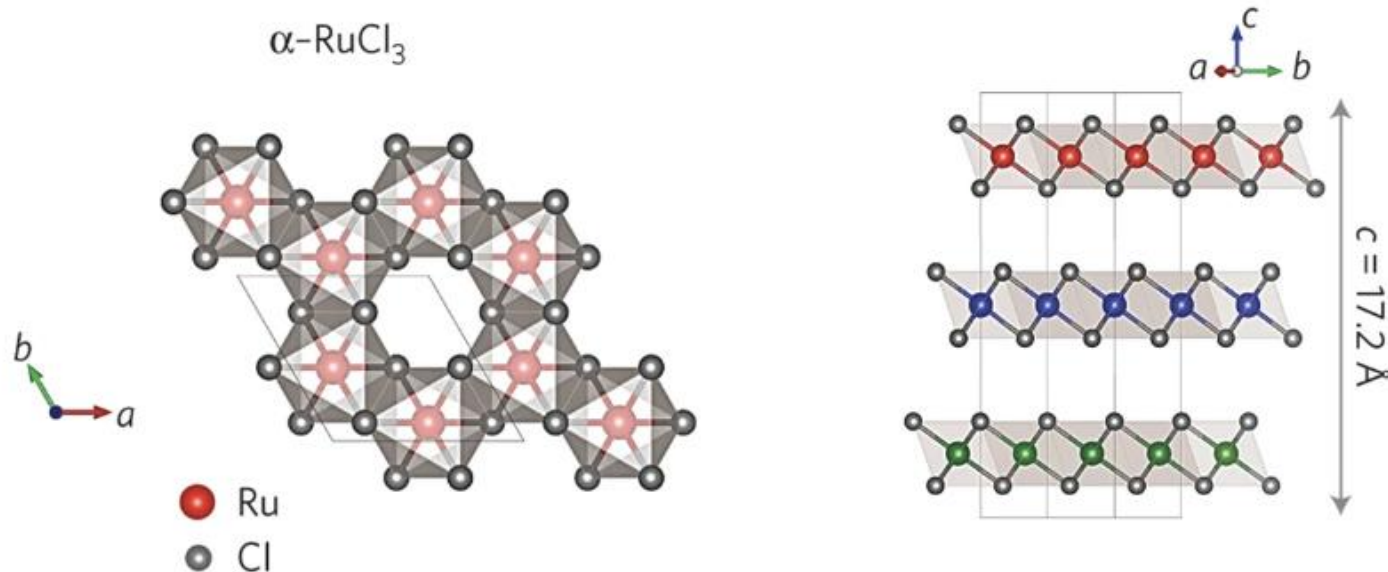
Article | Published: 04 April 2016

Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet

[A. Banerjee](#) , [C. A. Bridges](#), [J.-Q. Yan](#), [A. A. Aczel](#), [L. Li](#), [M. B. Stone](#), [G. E. Granroth](#), [M. D. Lumsden](#), [Y. Yiu](#), [J. Knolle](#), [S. Bhattacharjee](#), [D. L. Kovrizhin](#), [R. Moessner](#), [D. A. Tennant](#), [D. G. Mandrus](#) & [S. E. Nagler](#) 

[Nature Materials](#) **15**, 733–740 (2016) | [Cite this article](#)

a



- Ground state actually shows magnetic order
- At low temperatures, it exhibits QSL-like behavior

Candidate material

Letter | Published: 11 July 2018

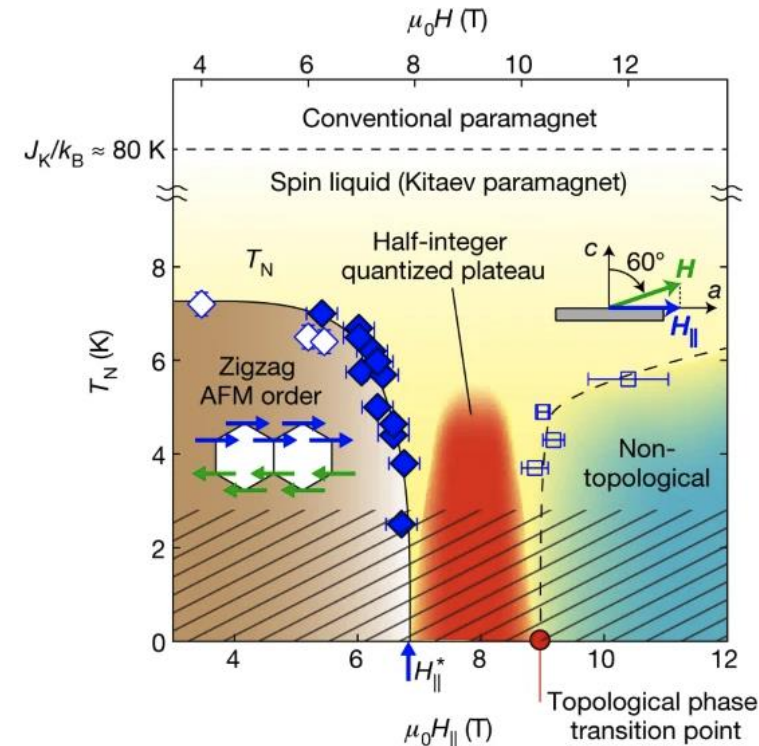
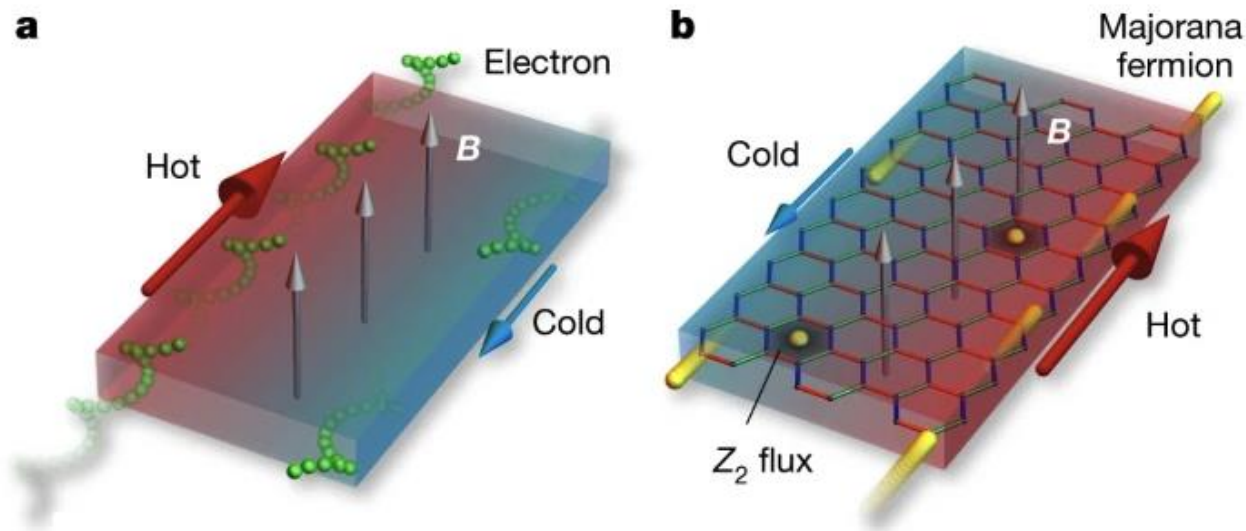
Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid

[Y. Kasahara](#), [T. Ohnishi](#), [Y. Mizukami](#), [O. Tanaka](#), [Sixiao Ma](#), [K. Sugii](#), [N. Kurita](#), [H. Tanaka](#), [J. Nasu](#), [Y.](#)

[Motome](#), [T. Shibauchi](#) & [Y. Matsuda](#) ✉

[Nature](#) **559**, 227–231 (2018) | [Cite this article](#)

Find QSL
under
magnetic
field



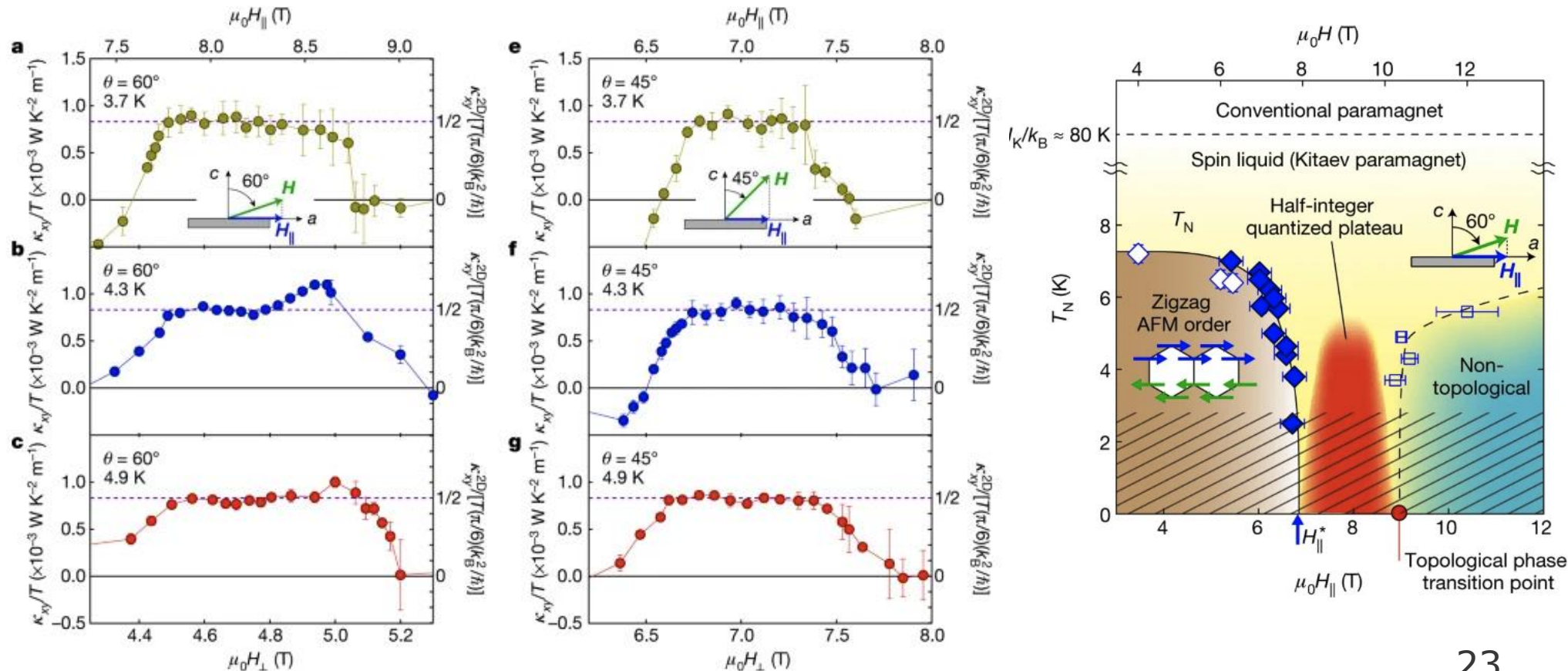
Candidate material

Letter | Published: 11 July 2018

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Find QSL
under
magnetic
field



Candidate “material”

- Ultracold atoms in optical lattices, Rydberg atom arrays

Open Access

Engineering and Probing Non-Abelian Chiral Spin Liquids Using Periodically Driven Ultracold Atoms

Bo-Ye Sun, Nathan Goldman, Monika Aidelsburger, and Marin Bukov
PRX Quantum **4**, 020329 – Published 19 May 2023

Open Access

Non-Abelian Floquet Spin Liquids in a Digital Rydberg Simulator

Marcin Kalinowski, Nishad Maskara, and Mikhail D. Lukin
Phys. Rev. X **13**, 031008 – Published 21 July 2023

Feasibility of Kitaev quantum spin liquids in ultracold polar molecules

Kiyu Fukui, Yasuyuki Kato, Joji Nasu, and Yukitoshi Motome
Phys. Rev. B **106**, 014419 – Published 25 July 2022

Recent topics (my research)

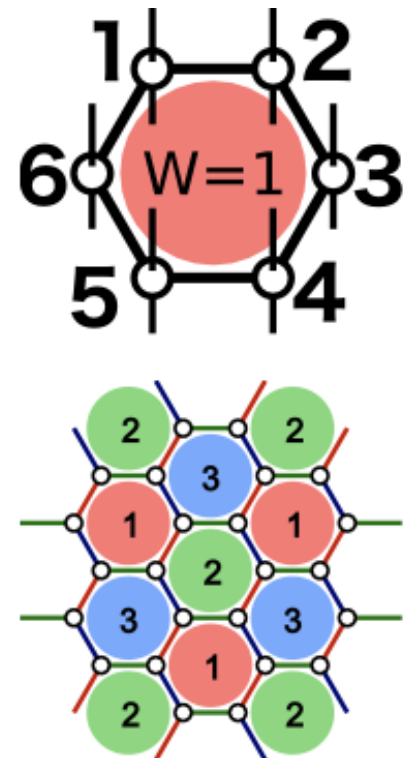
- How to efficiently represent **Kitaev gapless QSL** using **tensor network**?
- Gapless state
 - Often **logarithmic correction** in entanglement entropy
 - **1D tensor network** (matrix product state) is **not good** at representing gapless states
- 2D tensor network (projected entangled pair state (PEPS) / tensor product state)
 - **Do not prohibit** efficient description of **gapless** states (e.g. criticality of 2D classical Ising model by $D_{\text{bond}}=2$)
[see R. Orus, AnnPhys.349.117('14)]
- Honeycomb gapless spin liquid
 - Spinon Dirac dispersion → **no logarithmic** correction
[see Y. Zhang et al., PRL.107.067202('11)]

Recent topics (my research)

- PEPS
 - Efficiently describe “2D classical Ising”-like gapless state
- Kitaev gapless QSL
 - “2D classical Ising”-like in a sense that solvable by Jordan-Wigner transformation (quantum 1D Ising-like)
 - Gapless but no log correction in entanglement
- Is there any efficient PEPS representation of Kitaev gapless QSL?
 - Yes!
 - [H. Y. Lee et al., PRL.123.087203('19)]
- c.f. Representation in fermion basis: [P. Schmoll and R. Orus, PRB.95.045112('17)]
- We are interested in representation in spin basis

Recent topics (my research)

- Prepare eigenstates of flux: $|\text{trial}\rangle = \mathcal{P}_{W=1}|\psi\rangle$
 - $\mathcal{P}_{W=1}$: written by **3** tensor product operators
 - $|\psi\rangle$: can be anything
 - Magnetization is **0** by Elitzur's theorem
- Apply simple update and see how symmetry evolves
- First, focus on the isotropic FM Kitaev model
- Then, add perturbations

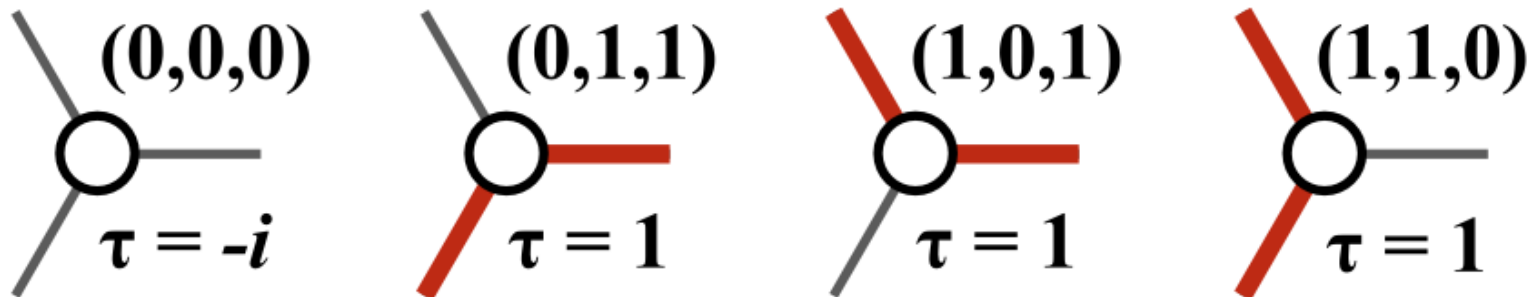


Recent topics (my research)

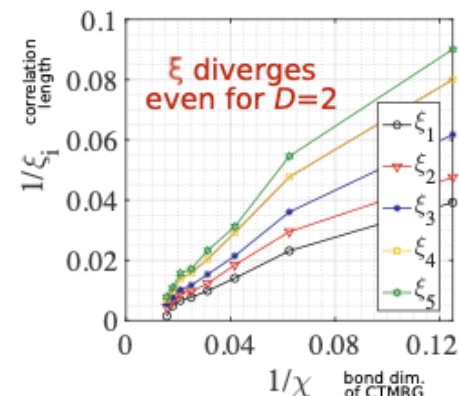
- Choose $|D = 4\rangle = \mathcal{P}_{W=1}|\vec{S} \propto (1, 1, 1)\rangle$
- Written in $D = 2$ by the Loop Gas operator:

$$|T_{xyz}\rangle = \hat{Q}_{\text{LG}}|\vec{S} \propto (1, 1, 1)\rangle \quad \hat{Q}_{\text{LG}} = \text{Tr} \prod_{\{\text{site}\}} Q_{xyzm_1m_2}^{(\text{site})} |m_1\rangle\langle m_2|$$

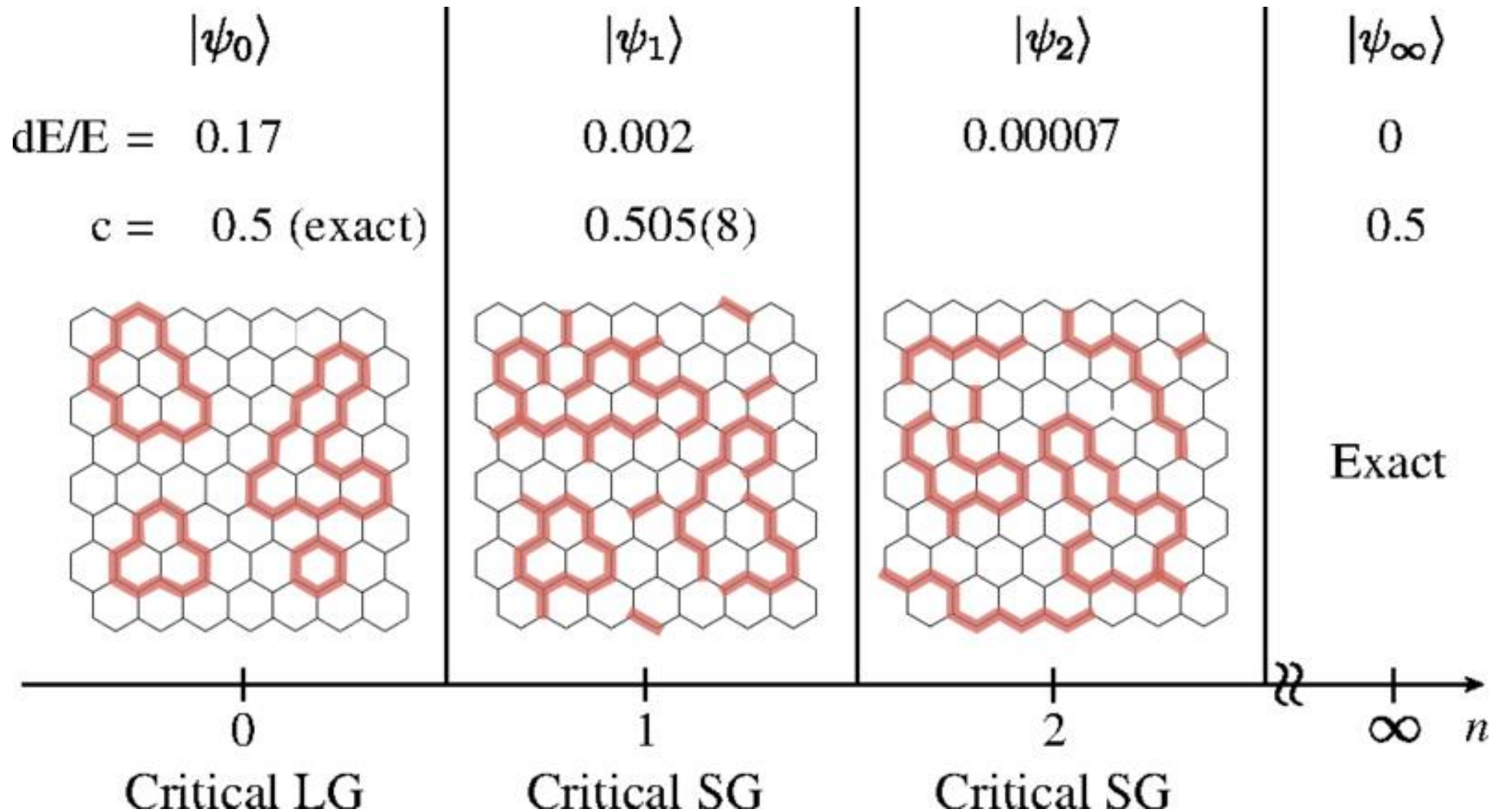
$$Q_{xyzm_1m_2} = \tau_{xyz} [(\sigma^x)^{1-x} (\sigma^y)^{1-y} (\sigma^z)^{1-z}]_{m_1m_2}$$



- Satisfy the following conditions even before optimization:
 - Nonmagnetic
 - Rotational symmetry: $E_x = E_y = E_z$
 - Energy better than classical: $E = -0.16349$
cf. $E_{\text{classical}} = -0.125$, $E_{\text{exact}} = -0.19682$
 - Criticality of KSL: $c = 1/2$ (2D Ising)



Recent topics (my research)



Recent topics (my research)

Article | [Open access](#) | Published: 02 April 2020

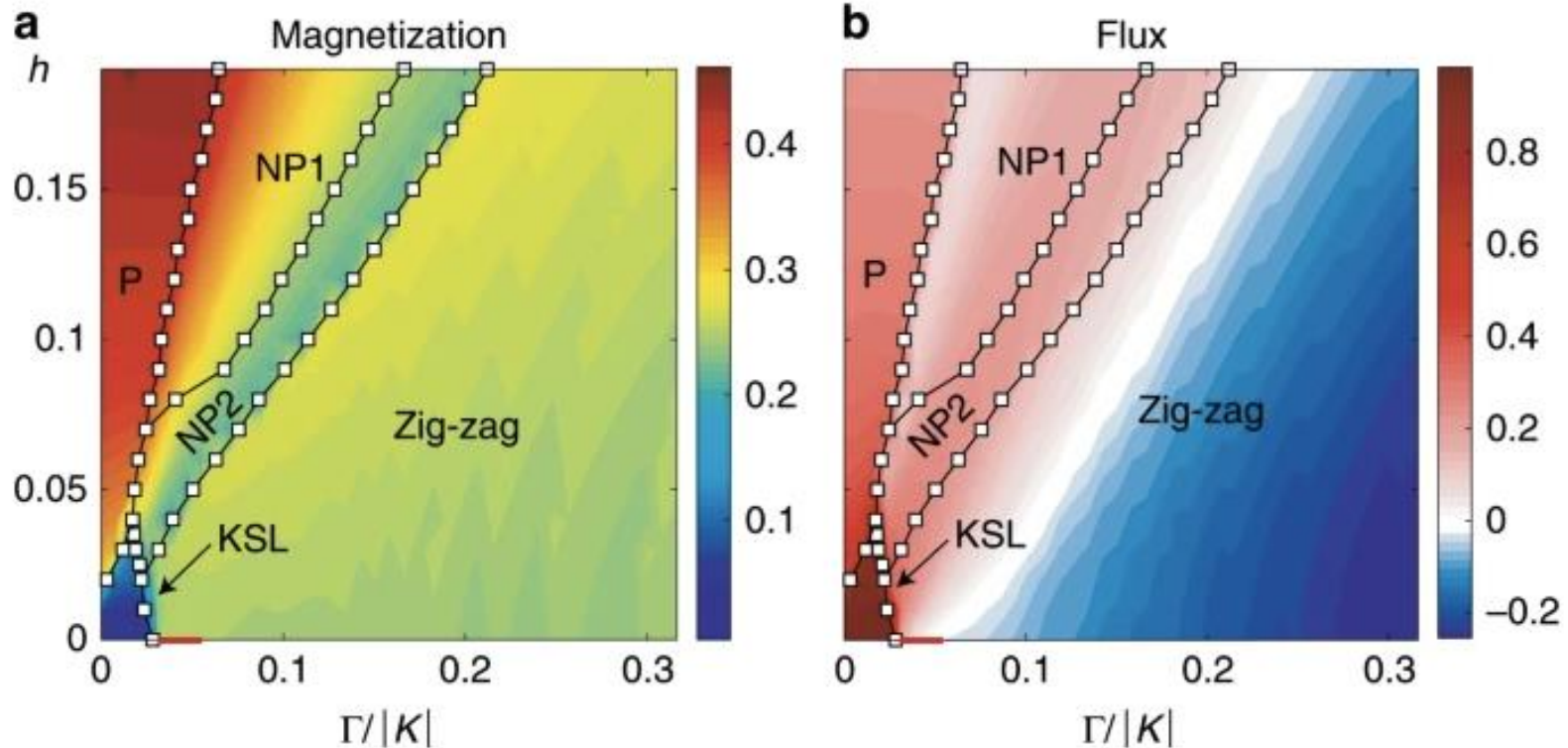
Magnetic field induced quantum phases in a tensor network study of Kitaev magnets

[Hyun-Yong Lee](#), [Ryui Kaneko](#), [Li Ern Chern](#), [Tsuyoshi Okubo](#), [Youhei Yamaji](#), [Naoki Kawashima](#) & [Yong Baek Kim](#) 

[Nature Communications](#) 11, Article number: 1639 (2020) | [Cite this article](#)

$$\hat{H}_{ij}^{\gamma} = -\frac{\hbar}{3} \cdot (\mathbf{S}_i + \mathbf{S}_j) + K S_i^{\gamma} S_j^{\gamma} + \Gamma (S_i^{\mu} S_j^{\nu} + S_i^{\nu} S_j^{\mu}) + \Gamma' (S_i^{\mu} S_j^{\gamma} + S_i^{\gamma} S_j^{\mu} + S_i^{\nu} S_j^{\gamma} + S_i^{\gamma} S_j^{\nu}),$$

Fig. 1: Ground-state phase diagram.



Today's summary

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