20240914 Condensed matter physics: from magnetism to quantum spin liquid II

Sophia University Ryui Kaneko (金子隆威)

https://github.com/ryuikaneko/lecturenote_2024_condmat

Rough outline

Hamiltonian for electrons in atoms

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

Heisenberg model
$$\hat{H} = \sum_{ij} J_{ij} \hat{S}_{i} \cdot \hat{S}_{j}$$

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 $(J_{ij}^z=0)$

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

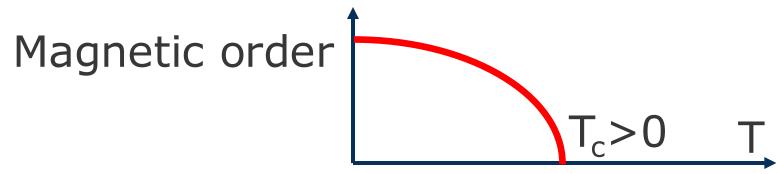
• Classical Ising model $(J_{ij}^{xy}=0)$ $H = \sum_{i:J_{ij}^z S_i^z S_j^z} J_{ij}^z S_i^z S_j^z$

• 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<=2.
 N. D. Mermin and H. Wagner, PRL.17.1133 ('66)

Spatial dimension	Tc>0?
1D	X
2D	X
3D	✓
4D	✓



Mermin-Wagner theorem

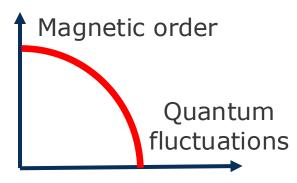
- Continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions in dimensions D <= 2.

 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., Tc>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_{ii} is short-range
 - J_{ii} is not ferromagnetic

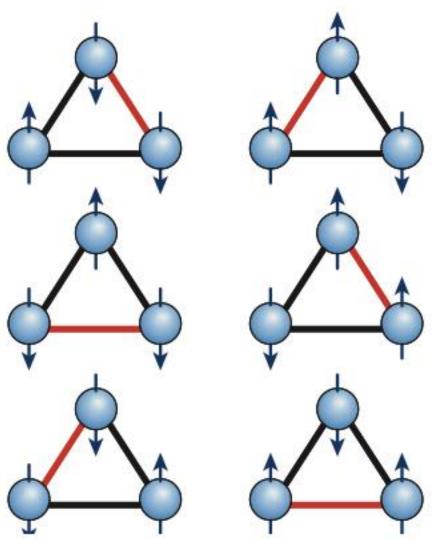


(c.f. for more rigorous argument, see H. Watanabe et al., arXiv:2310.16881)

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

L. Pitaevskii and S. Stringari, JLowTempPhys.85.377('91)

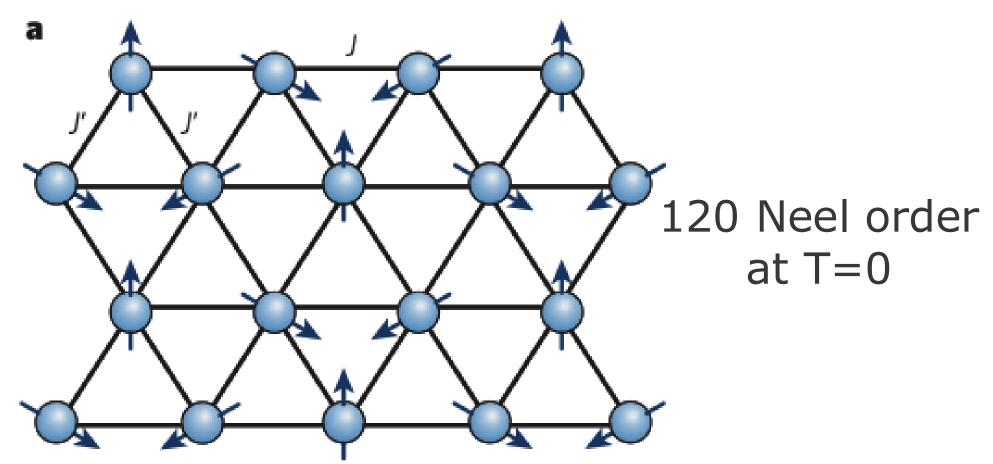
Example 1: Classical triangular Ising model



- Consider antiferromagnetic (AF) interaction J>0
- For 3 sites, degenerate ground states
- For infinite sites, spin correlation shows power-law decay at T=0 $< S_0 S_r > \sim r^{-\eta} (\eta = 1/2)$
- But no long-range order $\Sigma_i \exp(iQr_i) < S_i > = 0$ $(Q=(2\pi/3, 2\pi/3))$
 - J. Stephenson, J.Math.Phys.11.413 ('70); S. Alexander and P. Pincus, J.Phys.A:Math.Gen.13.263 ('80)

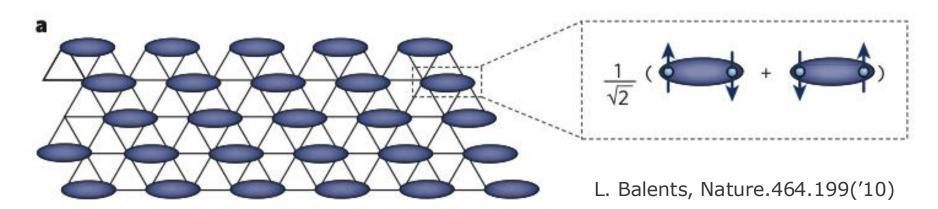
Geometrical frustration

• Example 2: Classical triangular Heisenberg model (ordered case)



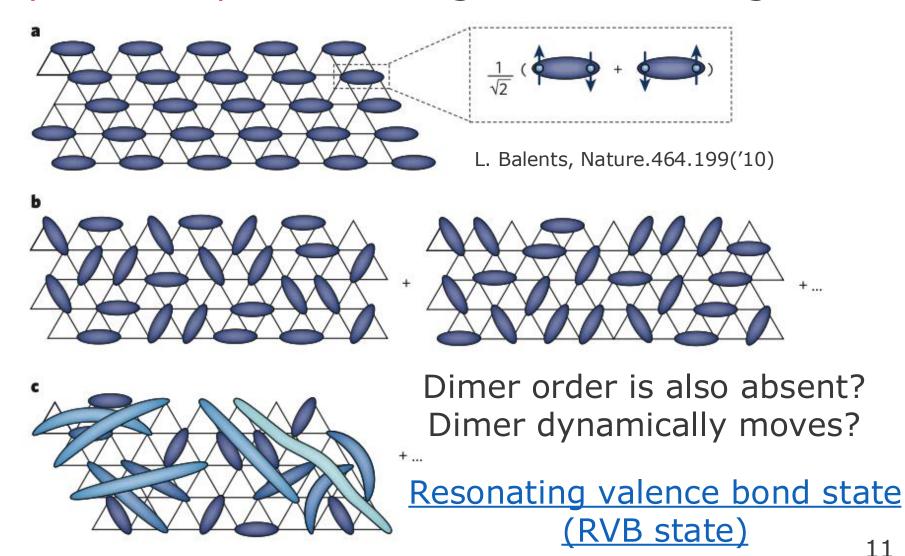
- In quantum spin 1/2 triangular Heisenberg model
 - Ground state has no magnetic order?!
 P. W. Anderson

"Resonating valence bonds: a new kind of insulator" Mater. Res. Bull. 8, 153–160 (1973)



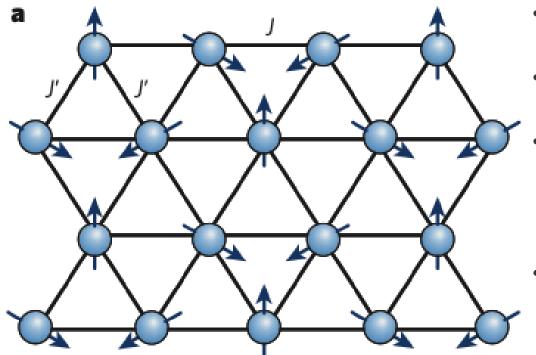
Example of a singlet dimerized state

• In quantum spin 1/2 triangular Heisenberg model



• In quantum spin 1/2 triangular Heisenberg model

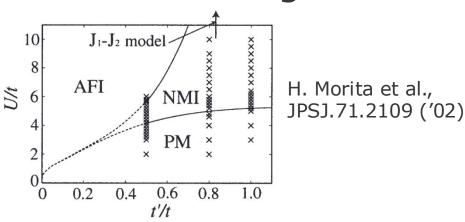
 Unfortunately, it is now widely believed that the true ground state has long-range magnetic order

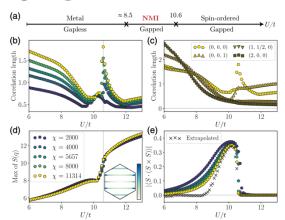


- Exact diagonalization
 - B. Bernu et al., PRB.50.10048('94)
- Variational Monte Carlo (VMC)
 - L. Capriotti et al., PRL.82.3899 ('99)
- Density matrix renormalization group (DMRG)
 - S. White and A. L. Chernyshev, PRL.99.127004('07)
- $\Sigma_{i} \exp(iQr_{i}) < S_{i} > /S_{max} = 0.41(3)$ (Q=(2\pi/3,2\pi/3),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

To realize quantum spin liquid...

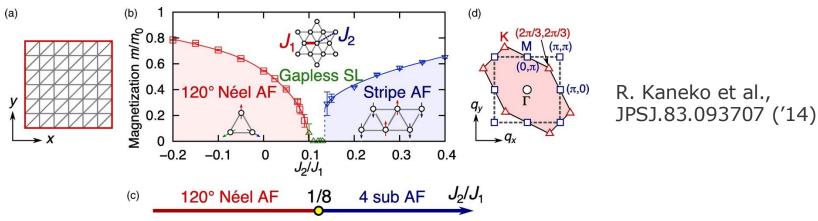
Effects of charge fluctuations





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

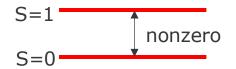
Effects of next-nearest-neighbor interaction



And so on...

Quantum spin liquid (QSL)

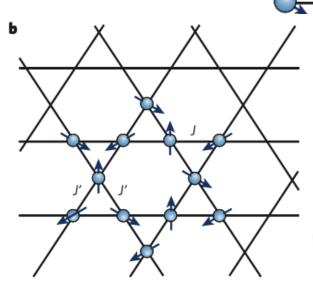
- No long-range order of spin, dimer, ...
- Insulating (charge excitation: open)
 - Metal shows no order, but it is not quantum spin liquid
- Characterized by spin excitation (for $N_s \rightarrow \infty$)
 - Open: Gapped spin liquid
 - Often characterized by topological entanglement entropy
 - Closed: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

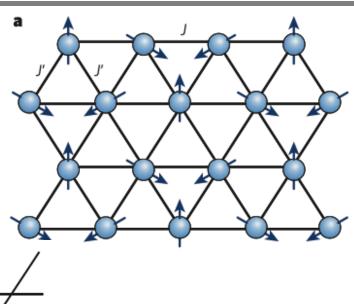


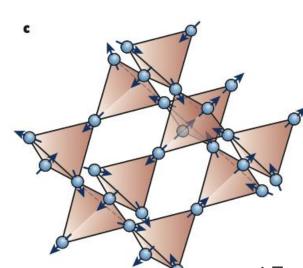


Example? Candidate materials?

- Triangular lattice
 - Organic compounds
 - κ-(BEDTTTF)₂Cu₂(CN)₃
 - EtMe₃Sb[Pd(dmit)₂]₂
 - Antiferromagnets
 - YbMgGaO₄
- Kagome lattice
 - Antiferromagnets
 - Herbertsmithite
 - Volborthite
 - Vesignieite
 - Kapellasite
- Pyrochlore lattice
 - Antiferromagnets
 - Tb₂Hf₂O₇, Tb₂Hf₂O₇, Ce₂Zr₂O₇, ...







Why do we study QSL?

Related to superconductivity (SC)

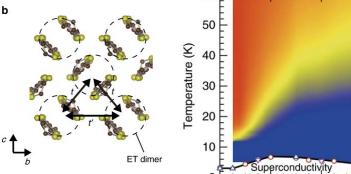
Doping QSL → High T_c SC?

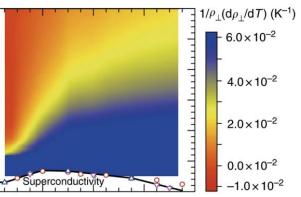
Article Open access Published: 02 October 2017

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 Tensornetwork methods

Model

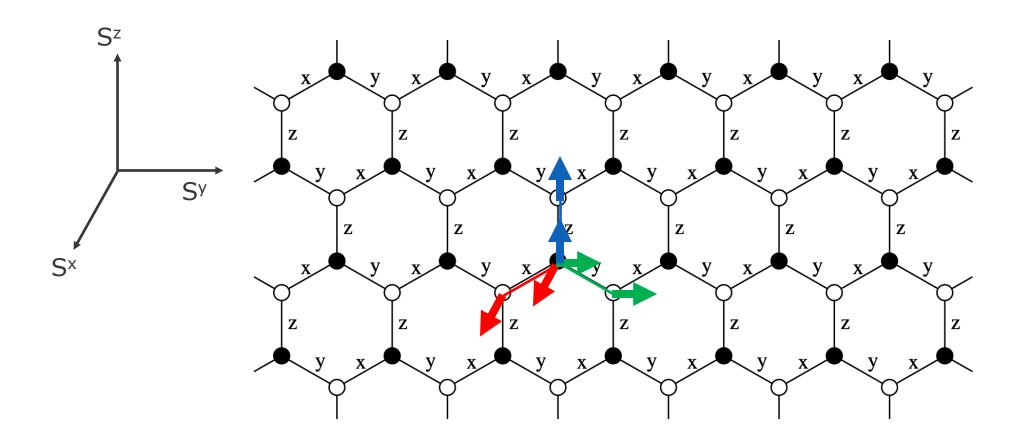
A. kitaev, AnnPhys.321.2 ('06)



Bond-dependent Ising interaction

$$H = -J_{x} \sum_{x-\text{links}} \sigma_{j}^{x} \sigma_{k}^{x} - J_{y} \sum_{y-\text{links}} \sigma_{j}^{y} \sigma_{k}^{y} - J_{z} \sum_{z-\text{links}} \sigma_{j}^{z} \sigma_{k}^{z}$$

Intuitive understanding (bond frustration)



- Common way of solving the problem
 - Using conserved quantities, extending the Hilbert space (original way)

[A. Kitaev, AnnPhys.321.2('06)]

Apply Jordan-Wigner transformation

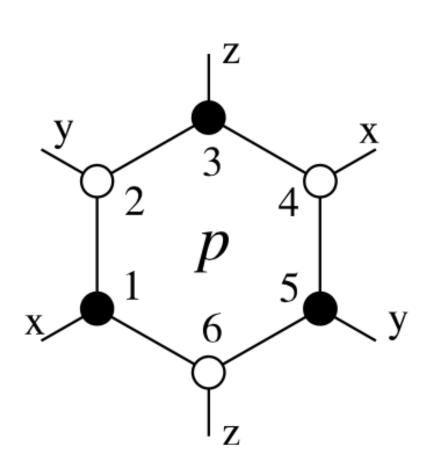
[X.-Y. Feng et al., PRL.98.087204('07); H.-D. Chen and J. Hu, PRB.76.193101('07); H.-D. Chen and Z. Nussinov, JPhysA:MathTheor.41.075001('08); S. Mandal et al., JPhysA:MathTheor.45.335304('12)]

Similar to the original way,
 but without extending the Hilbert space

[J. Fu et al., PRB.97.115142 ('18)]

Focus on the original way

Conserved quantities



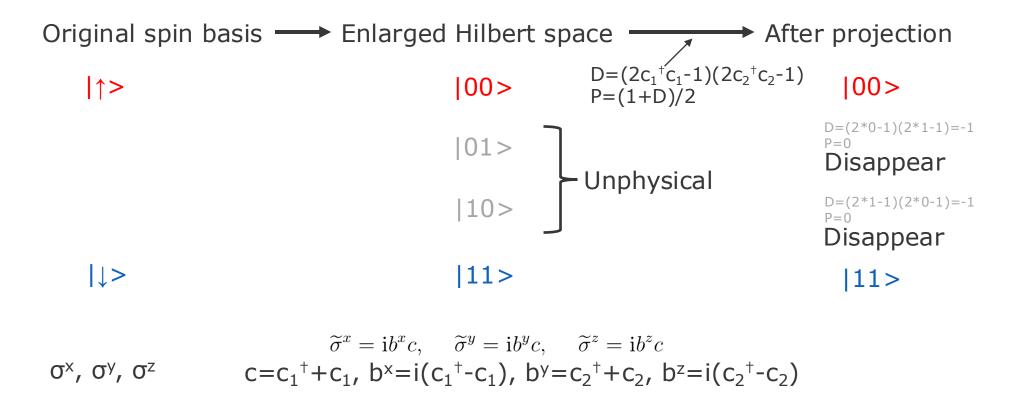
$$W_p = \sigma_1^x \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

After some tedious calculations, we obtain

- $[H,W_p]=0$ for all p
- $[W_p, W_{p'}] = 0$ for all p, p'
- $W_p^2=1 \rightarrow W_p=+1 \text{ or } -1$

Describe eigenstates of H using eigenstates of W_p

• Enlarge Hilbert space using Majorana fermions (c=c[†])



Solve the problem in the enlarged Hilbert space and finally apply the projection to obtain the physical state

Enlarge Hilbert space using Majorana fermions

$$H = -J_x \sum_{x-\text{links}} \sigma_j^x \sigma_k^x - J_y \sum_{y-\text{links}} \sigma_j^y \sigma_k^y - J_z \sum_{z-\text{links}} \sigma_j^z \sigma_k^z$$

$$\sigma_j^x \mapsto -\operatorname{i} b_j^y b_j^z, \quad \sigma_j^y \mapsto -\operatorname{i} b_j^z b_j^x, \quad \sigma_j^z \mapsto -\operatorname{i} b_j^x b_j^y$$

$$(\operatorname{i} b_j^\alpha c_j)(\operatorname{i} b_k^\alpha c_k) = -\operatorname{i} (\operatorname{i} b_j^\alpha b_k^\alpha) c_j c_k$$

$$\widetilde{H} = rac{\mathrm{i}}{4} \sum_{j,k} \hat{A}_{jk} c_j c_k,$$

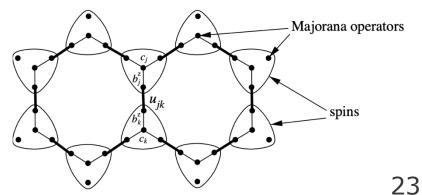
Quadratic-"like" Hamiltonian

Looks not free because of uik

$$\hat{A}_{jk} = \left\{ egin{array}{l} 2{J}_{lpha_{jk}}\hat{u}_{jk} \ 0 \end{array}
ight.$$

 $\hat{u}_{jk}=\mathrm{i}b_{j}^{\alpha_{jk}}b_{k}^{\alpha_{jk}}.$

 $\widetilde{H} = \frac{i}{4} \sum_{j,k} \hat{A}_{jk} c_j c_k, \quad \hat{A}_{jk} = \begin{cases} 2J_{\alpha_{jk}} \hat{u}_{jk} & \text{if } j \text{ and } k \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases}$



It IS actually a quadratic Hamiltonian

After some tedious calculations, we obtain

- $u_{jk} = -u_{kj}$
- $[H,u_{jk}]=0$ for all j, k
- $[u_{jk}, u_{j'k'}] = 0$ for all j, k, j', k'
- $u_{jk}^2 = 1 \rightarrow u_{jk} = +1 \text{ or } -1$

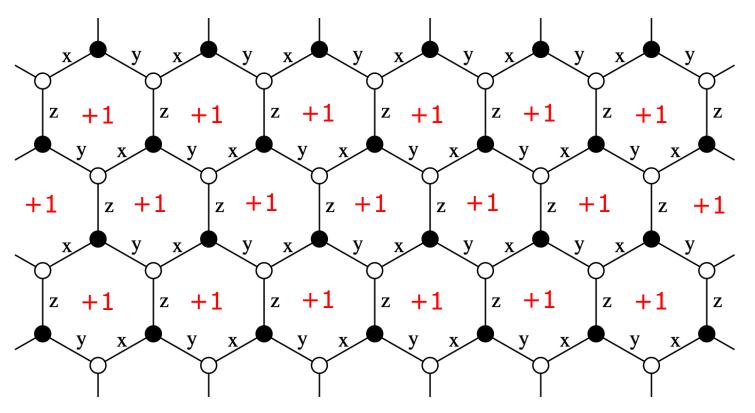
$$w_p = \prod_{(j,k) \in \text{boundary}(p)} u_{jk}$$
 $(j \in \text{even sublattice}, k \in \text{odd sublattice})$
The role of u_{ik} and W_p

The role of u_{jk} and W_p is the same

$$\widetilde{H} = rac{\mathrm{i}}{4} \sum_{j,k} \hat{A}_{jk} c_j c_k$$

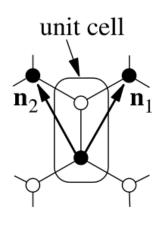
Quadratic Hamiltonian because u_{jk} is just a number

- Configuration of u_{ik}?
 - According to Lieb's theorem, [E. H. Lieb, PRL.73.2158 ('94)] u_{jk} =+1 (W_p =+1) for all j, k (p) in the ground state
 - Often called "flux free" or "Vortex free"



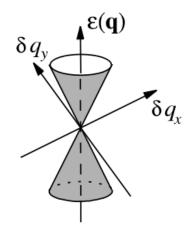
Spectrum of the quadratic Hamiltonian

$$H_{\text{vortex-free}} = \frac{\mathrm{i}}{4} \sum_{j,k} A_{jk} c_j c_k, \quad A_{jk} = 2 J_{\alpha_{jk}} u_{jk}^{\mathrm{std}}$$



$$i\widetilde{A}(\mathbf{q}) = \begin{pmatrix} 0 & if(\mathbf{q}) \\ -if(\mathbf{q})^* & 0 \end{pmatrix}, \quad \varepsilon(\mathbf{q}) = \pm |f(\mathbf{q})|,$$

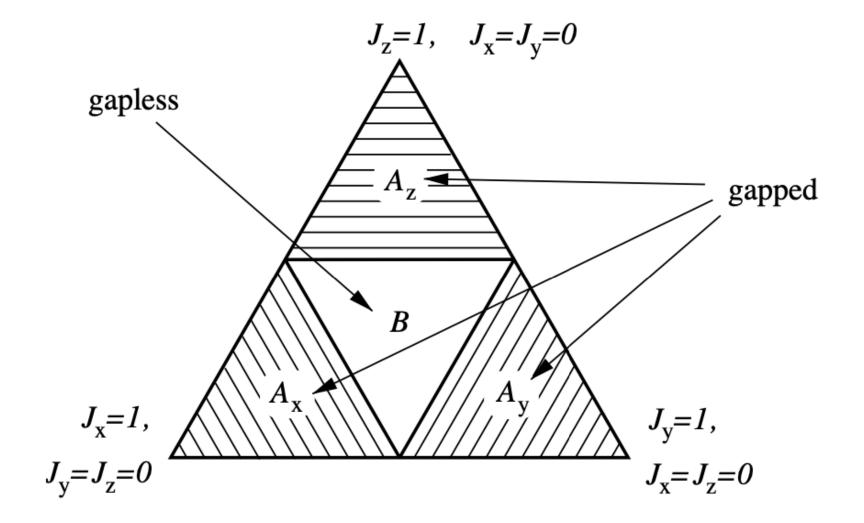
$$f(\mathbf{q}) = 2(J_x e^{i(\mathbf{q}, \mathbf{n}_1)} + J_y e^{i(\mathbf{q}, \mathbf{n}_2)} + J_z), \quad \mathbf{n}_1 = (\frac{1}{2}, \frac{\sqrt{3}}{2}), \, \mathbf{n}_2 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$$



When $J_x \sim J_y \sim J_z$, Dirac cone dispersion appears

- Reduce enlarged Hilbert space:
 Project out unphysical states
- Projection operator commutes with Hamiltonian!!
 - P=(1+D)/2
 - [H,P]=0
- As for the energy spectrum, we do not need to care about the projection
- As for the eigenstate, $|\Psi_w\rangle = \prod_j \left(\frac{1+D_j}{2}\right) |\widetilde{\Psi}_u\rangle$

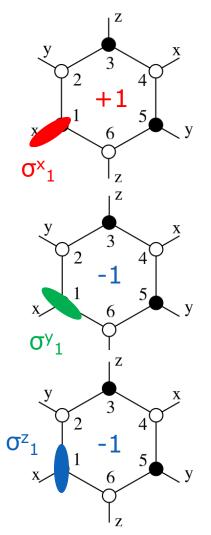
Ground state phase diagram



- Short-range spin correlation
- Applying σ^a flips the flux
 - $W_p \sigma^x_1 = + \sigma^x_1 W_p$ (commute)

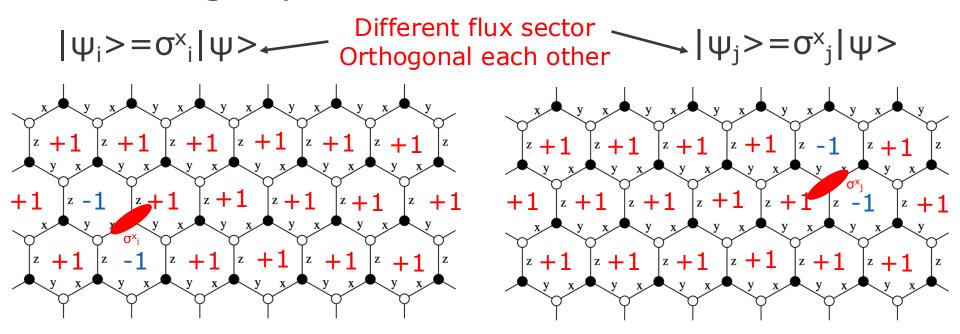
• $W_p \sigma^{y_1} = -\sigma^{y_1} W_p$ (anticommute)

• $W_p \sigma^z_1 = -\sigma^z_1 W_p$ (anticommute)



• $W_p \sigma_1^{\gamma} | eigenstate(+1) > = -\sigma_1^{\gamma} W_p | eigenstate(+1) > = -\sigma_1^{\gamma} | eigenstate(+1) >$

Short-range spin correlation



$$\langle \psi_i | \psi_j \rangle = 0 \rightarrow \langle \psi | \sigma^x_i \sigma^x_j | \psi \rangle = 0$$

Spin correlation is 0 except i and j on the same bond for all eigenstates |ψ>

Short-range QSL for any eigenstates

[G. Baskaran et al., PRL.98.247201 ('07)]

Relation to superconductivity

[F. J. Burnell and C. Nayak, PRB.84.125125(`11); S. Mandal et al., JPhysA: MathTheor.45.335304('12)]

- Solution by Jordan-Wigner transformation on a torus
- p-wave superconductor (but with projection)

$$H = \sum_{k} (\epsilon_{k} \psi_{k}^{\dagger} \psi_{k} - \epsilon_{k} \psi_{-k} \psi_{-k}^{\dagger} + i \delta_{k} \psi_{k}^{\dagger} \psi_{-k}^{\dagger} - i \delta_{k} \psi_{-k} \psi_{k})$$

$$+ \epsilon_{0,0} \psi_{0,0}^{\dagger} \psi_{0,0} + \epsilon_{\pi,0} \psi_{\pi,0}^{\dagger} \psi_{\pi,0} + \epsilon_{0,\pi} \psi_{0,\pi}^{\dagger} \psi_{0,\pi} + \sum_{k} \epsilon_{k} - MNJ_{z}$$

$$E_{k} = 2(J_{x} \cos k_{x} + J_{y} \cos k_{y} + J_{z})$$

$$\delta_{k} = 2(J_{x} \sin k_{x} + J_{y} \sin k_{y})$$

$$E_{k} = \sqrt{\epsilon_{k}^{2} + \delta_{k}^{2}} \cos 2\theta_{k} = \epsilon_{k}/E_{k}$$

$$H = \sum_{k} E_{k} (\alpha_{k}^{\dagger} \alpha_{k} - \beta_{k}^{\dagger} \beta_{k}) + \epsilon_{0,0} \psi_{0,0}^{\dagger} \psi_{0,0} + \epsilon_{\pi,0} \psi_{\pi,0}^{\dagger} \psi_{\pi,0} + \epsilon_{0,\pi} \psi_{0,\pi}^{\dagger} \psi_{0,\pi}$$

$$-\frac{1}{2} (\epsilon_{0,0} + \epsilon_{0,\pi} + \epsilon_{\pi,0}) + \left(\sum_{k} \frac{1}{2} \epsilon_{k} - N_{z} J_{z}\right).$$

$$\begin{pmatrix} \alpha_{k} \\ \beta_{k} \end{pmatrix} = \begin{pmatrix} \cos \theta_{k} & -i \sin \theta_{k} \\ -i \sin \theta_{k} & \cos \theta_{k} \end{pmatrix} \begin{pmatrix} \psi_{k} \\ \psi_{-k}^{\dagger} \end{pmatrix}$$

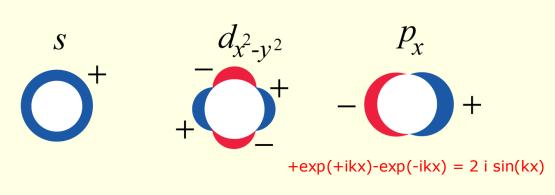
• This is also the case for SU(2) slave fermion formalism (although SU(2) slave fermion formalism is an approximation)

$$\hat{S}_{i}^{\alpha} = \frac{1}{2} f_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^{\alpha} f_{i\beta}$$
 $n_{i\uparrow} + n_{i\downarrow} = 1, \quad f_{i\uparrow}^{\dagger} f_{i\downarrow}^{\dagger} = 0, \quad f_{i\uparrow} f_{i\downarrow} = 0$

Relation to superconductivity

[F. J. Burnell and C. Nayak, PRB.84.125125('11); S. Mandal et al., JPhysA: MathTheor.45.335304('12)]

- Solution by Jordan-Wigner transformation on a torus
- p-wave superconductor (but with projection)



 $Taken\ from\ https://zvine-ap.eng.hokudai.ac.jp/{\sim}asano/research.html$

$$\epsilon_k = 2(J_x \cos k_x + J_y \cos k_y + J_z)$$
$$\delta_k = 2(J_x \sin k_x + J_y \sin k_y)$$

$$^{z}E_{k}=\sqrt{\epsilon_{k}^{2}+\delta_{k}^{2}}\cos2\theta_{k}=\epsilon_{k}/E_{k}$$

$$+ \exp(+ikx) - \exp(-ikx) = 2 i \sin(kx) \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} = \begin{pmatrix} \cos \theta_k & -i \sin \theta_k \\ -i \sin \theta_k & \cos \theta_k \end{pmatrix} \begin{pmatrix} \psi_k \\ \psi_{-k}^{\dagger} \end{pmatrix}$$

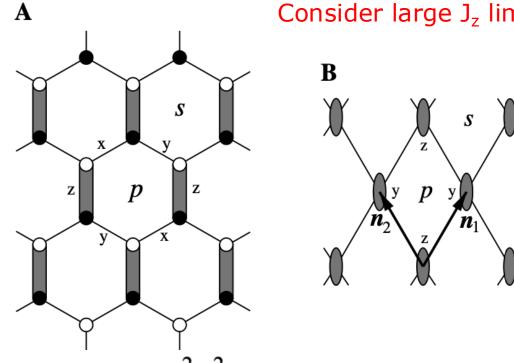
• This is also the case for SU(2) slave fermion formalism (although SU(2) slave fermion formalism is an approximation)

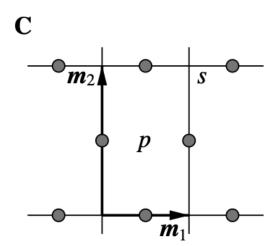
$$\hat{S}_{i}^{\alpha} = \frac{1}{2} f_{i\alpha}^{\dagger} \sigma_{\alpha\beta}^{\alpha} f_{i\beta}$$
 $n_{i\uparrow} + n_{i\downarrow} = 1, \quad f_{i\uparrow}^{\dagger} f_{i\downarrow}^{\dagger} = 0, \quad f_{i\uparrow} f_{i\downarrow} = 0$

Relation to Toric code model

$$H_0 = -J_z \sum \sigma_j^z \sigma_k^z, \quad V = -J_x \sum \sigma_j^x \sigma_k^x - J_y \sum \sigma_j^y \sigma_k^y$$

Consider large J₇ limit





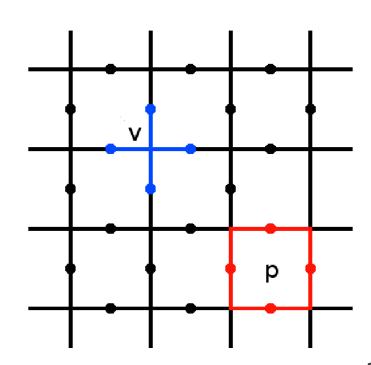
$$H_{\mathrm{eff}} = -rac{J_x^2 J_y^2}{16 |J_z|^3} \sum_p Q_p, \quad Q_p = \sigma_{\mathrm{left}(p)}^y \sigma_{\mathrm{right}(p)}^y \sigma_{\mathrm{up}(p)}^z \sigma_{\mathrm{down}(p)}^z$$

Relation to Toric code model

$$H_{ ext{eff}} = -J_{ ext{eff}} \left(\sum_{ ext{vertices}} Q_s + \sum_{ ext{plaquettes}} Q_p \right)$$
 $J_{ ext{eff}} = J_x^2 J_y^2 / (16 |J_z|^3)$

Unitary transformation
 $U = \prod_{ ext{zontal links}} X_j \prod_{ ext{vertical links}} Y_k$
 $H'_{ ext{eff}} = UH_{ ext{eff}} U^\dagger$
 $= -J_{ ext{eff}} \left(\sum_{ ext{vertices}} A_s + \sum_{ ext{plaquettes}} B_p \right)$

$$J_{\rm eff} = J_x^2 J_y^2 / (16|J_z|^3)$$



Relation to Toric code model



The **toric code** is a topological quantum error correcting code, and an example of a stabilizer code, defined on a two-dimensional spin lattice.^[1] It is the simplest and most well studied of the quantum double models.^[2] It is also the simplest example of topological order— Z_2 topological order (first studied in the context of Z_2 spin liquid in 1991).^{[3][4]} The toric code can also be considered to be a Z_2 lattice gauge theory in a particular limit.^[5] It was introduced by Alexei Kitaev.

The toric code gets its name from its periodic boundary conditions, giving it the shape of a torus. These conditions give the model translational invariance, which is useful for analytic study. However, some experimental realizations require open boundary conditions, allowing the system to be embedded on a 2D surface. The resulting code is typically known as the planar code. This has identical behaviour to the toric code in most, but not all, cases.

Original motivation seems to be quantum computation

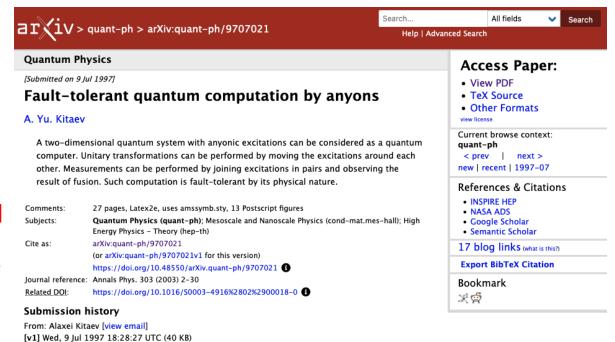
Strongly influences the field of condensed matter physics

1997: Toric code model

 \downarrow

2005: Kitaev honeycomb model

(Toric code model and RVB states are mentioned in introduction)



What is unconventional about Kitaev QSL?

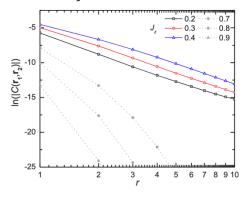
(in my opinion)

- It is often the case that
 - Gapped QSL \rightarrow Short-range magnetic order <S₀.S_r> \sim exp(-r/ ξ)
 - Gapless QSL \rightarrow Quasi-long-range magnetic order $< S_0.S_r > \sim r^{-\eta}$
- In Kitaev QSL
 - Gapless QSL \rightarrow Short-range magnetic order <S₀.S_r> \sim exp(-r/ ξ)

(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)]



What is unconventional about Kitaev QSL?

(in my opinion)

- It is often the case that
 - Only low-energy states exhibit QSL behavior
 - At high temperatures, we cannot see QSL behavior
- In Kitaev QSL
 - All the eigenstates are QSL
 - QSL behavior (short-range spin correlations) even at high temperatures
 - [G. Baskaran et al., PRL.98.247201 ('07)]
 - QSL behavior in real-time dynamics as well [A. Lavasani et al., PRB.108.115135 ('23)]
 - It can also be extended to general spin S [G. Baskaran et al., PRB.78.115116 ('08)]

PRL 102, 017205 (2009)

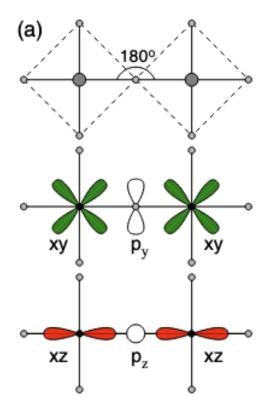
PHYSICAL REVIEW LETTERS

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)

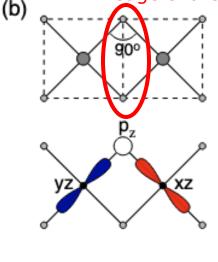


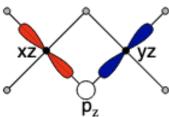
$$\mathcal{H}_{ij} = J_1 \vec{S}_i \cdot \vec{S}_j + J_2 (\vec{S}_i \cdot \vec{r}_{ij}) (\vec{r}_{ij} \cdot \vec{S}_j)$$

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







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

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

Candidates: Sr₂IrO₄, Na₂IrO₃, a-RuCl₃, ...

Article | Published: 04 April 2016

Proximate Kitaev quantum spin liquid behaviour in a honeycomb magnet

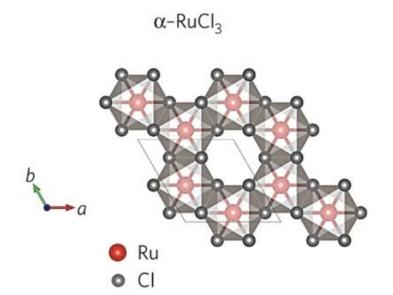
A. Banerjee [™], C. A. Bridges, J.-Q. Yan, A. A. Aczel, L. Li, M. B. Stone, G. E. Granroth, M. D. Lumsden, Y. Yiu, J. Knolle, S. Bhattacharjee, D. L. Kovrizhin, R. Moessner, D. A. Tennant, D. G. Mandrus & S. E.

<u>Nagler</u>

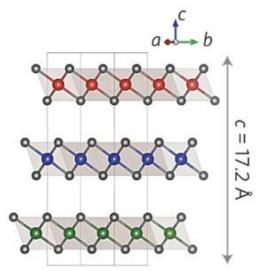
✓

Nature Materials 15, 733–740 (2016) Cite this article

a



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



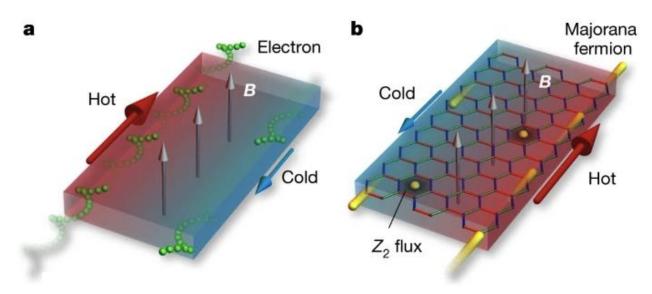
Letter | Published: 11 July 2018

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

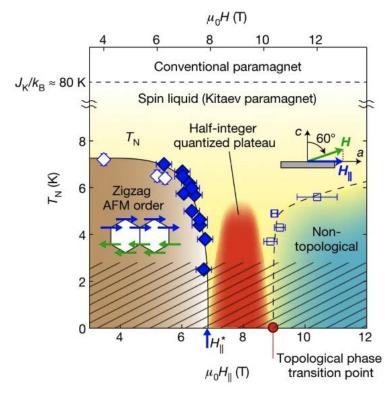
Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, Sixiao Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y.

Motome, T. Shibauchi & Y. Matsuda [™]

Nature 559, 227–231 (2018) Cite this article



Find QSL under magnetic field



Letter | Published: 11 July 2018

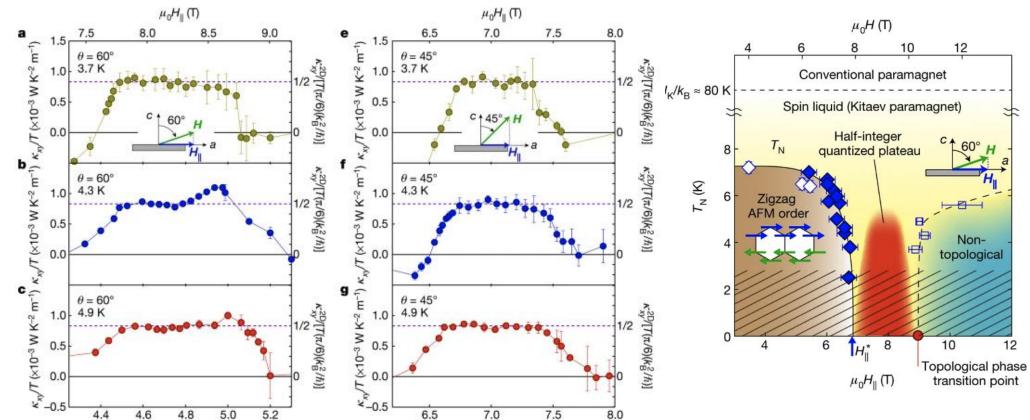
 $\mu_0 H_{\perp}$ (T)

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.

Find QSL under magnetic field

41



 $\mu_0 H_{\perp}$ (T)

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

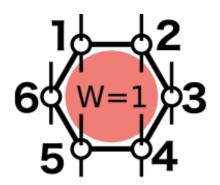
Feasibility of Kitaev quantum spin liquids in ultracold polar molecules

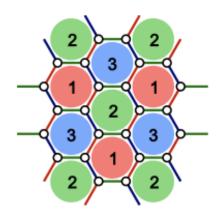
Kiyu Fukui, Yasuyuki Kato, Joji Nasu, and Yukitoshi Motome Phys. Rev. B **106**, 014419 – Published 25 July 2022

- 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 $D_{bond}=2$) [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)]

- 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

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

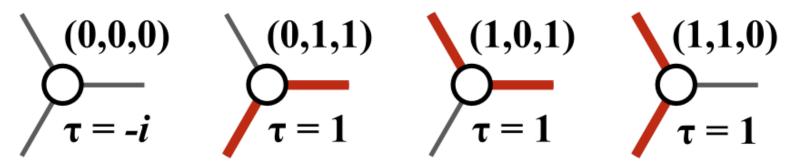




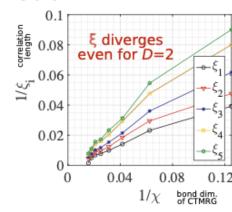
- Choose $|D=4
 angle=\mathcal{P}_{W=1}|ec{S}\propto (1,1,1)
 angle$
- Written in D = 2 by the Loop Gas operator:

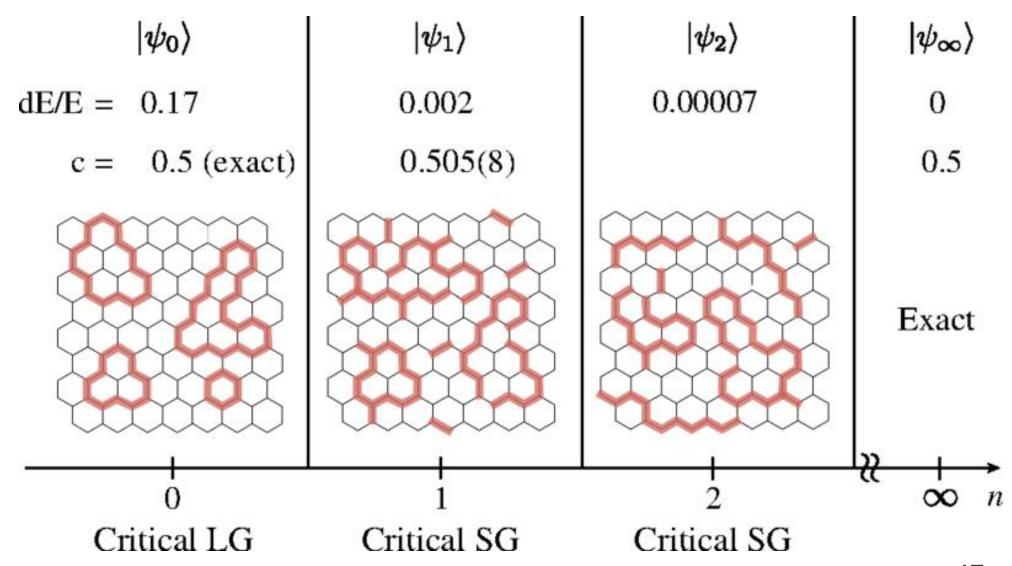
$$|T_{xyz}
angle = \hat{Q}_{\mathrm{LG}}|ec{S} \propto (1,1,1)
angle \hspace{0.5cm} \hat{Q}_{\mathrm{LG}} = \mathrm{Tr} \prod_{\{\mathrm{site}\}} Q_{xyzm_1m_2}^{(\mathrm{site})} |m_1
angle \langle m_2|$$

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



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





Article Open access | Published: 02 April 2020

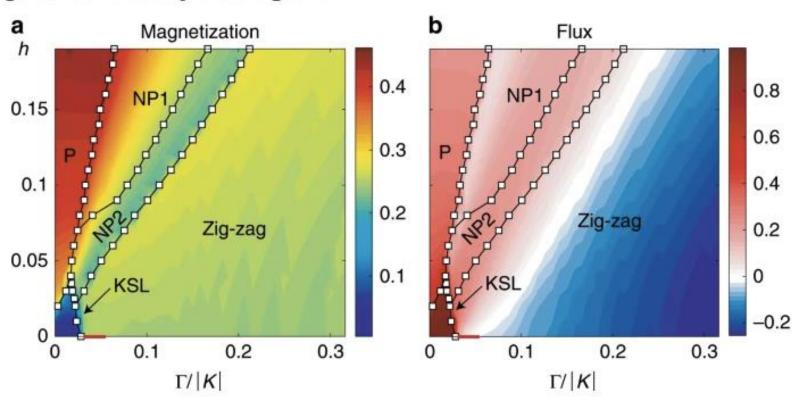
Magnetic field induced quantum phases in a tensor network study of Kitaev magnets

$$egin{aligned} \hat{H}_{ij}^{\gamma} &= -rac{\mathbf{h}}{3}\cdot(\mathbf{S}_i+\mathbf{S}_j) + KS_i^{\gamma}S_j^{\gamma} + \Gamma(S_i^{\mu}S_j^{
u} + S_i^{
u}S_j^{\mu}) \ &+ \Gamma'(S_i^{\mu}S_j^{\gamma} + S_i^{\gamma}S_i^{\mu} + S_i^{
u}S_j^{\gamma} + S_i^{
u}S_j^{\gamma}), \end{aligned}$$

<u>Hyun-Yong Lee, Ryui Kaneko, Li Ern Chern, Tsuyoshi Okubo, Youhei Yamaji, Naoki Kawashima</u> & <u>Yong</u>
Baek Kim[™]

Nature Communications 11, Article number: 1639 (2020) Cite this article

Fig. 1: Ground-state phase diagram.



Today's summary

- 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

https://github.com/ryuikaneko/lecturenote_2024_condmat