Kitaev Quantum Spin Liquids

Materials 286G

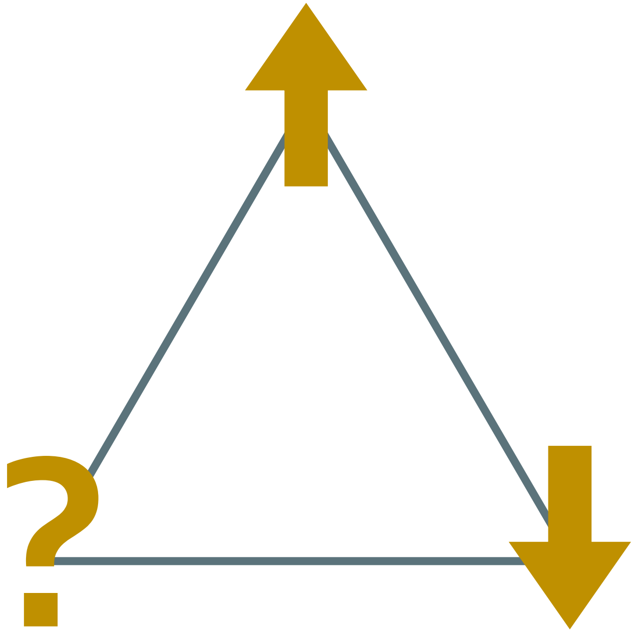
Aurland Hay

19 May 2022

Magnetic frustration

Geometric frustration: geometric constraints suppress of long-range order

Example:
Ising-type antiferromagnetically interacting spins on triangular network



Ramirez, Hayashi, Cava, Siddharthan, Shastry, *Nature* **399** (1999) 333-335
Pauling, *J. Am. Chem. Soc.* **57** (1935) 2680-2684.

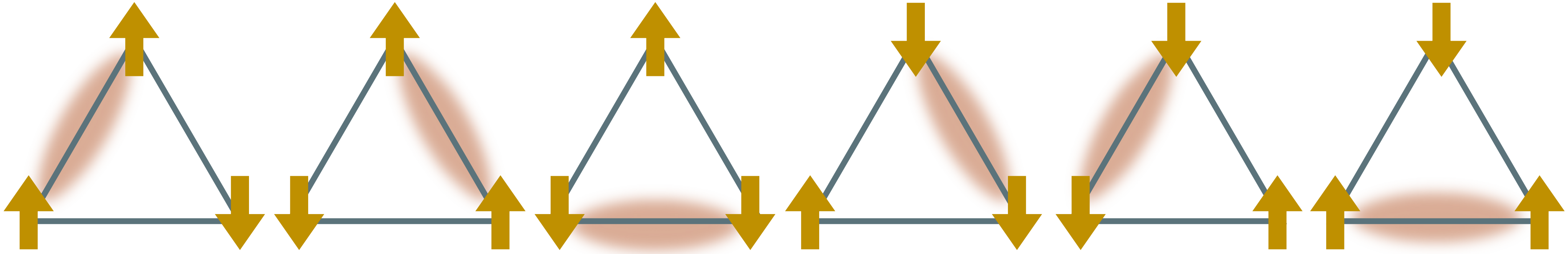
Geometric frustration creates ground state degeneracy

Geometric frustration: geometric constraints suppress of long-range order

Example:

Ising-type antiferromagnetically interacting spins on triangular lattice

- macroscopic ground state degeneracy
- “residual entropy”



Ramirez, Hayashi, Cava, Siddharthan, Shastry, *Nature* **399** (1999) 333-335
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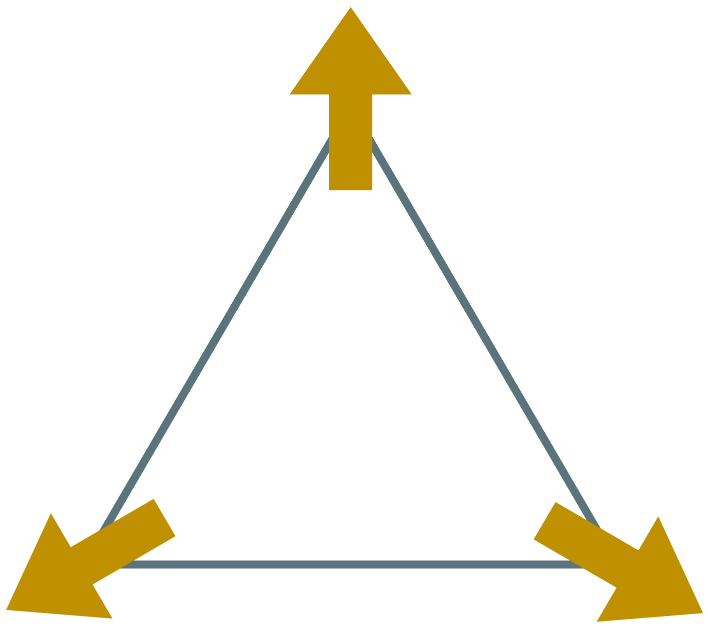
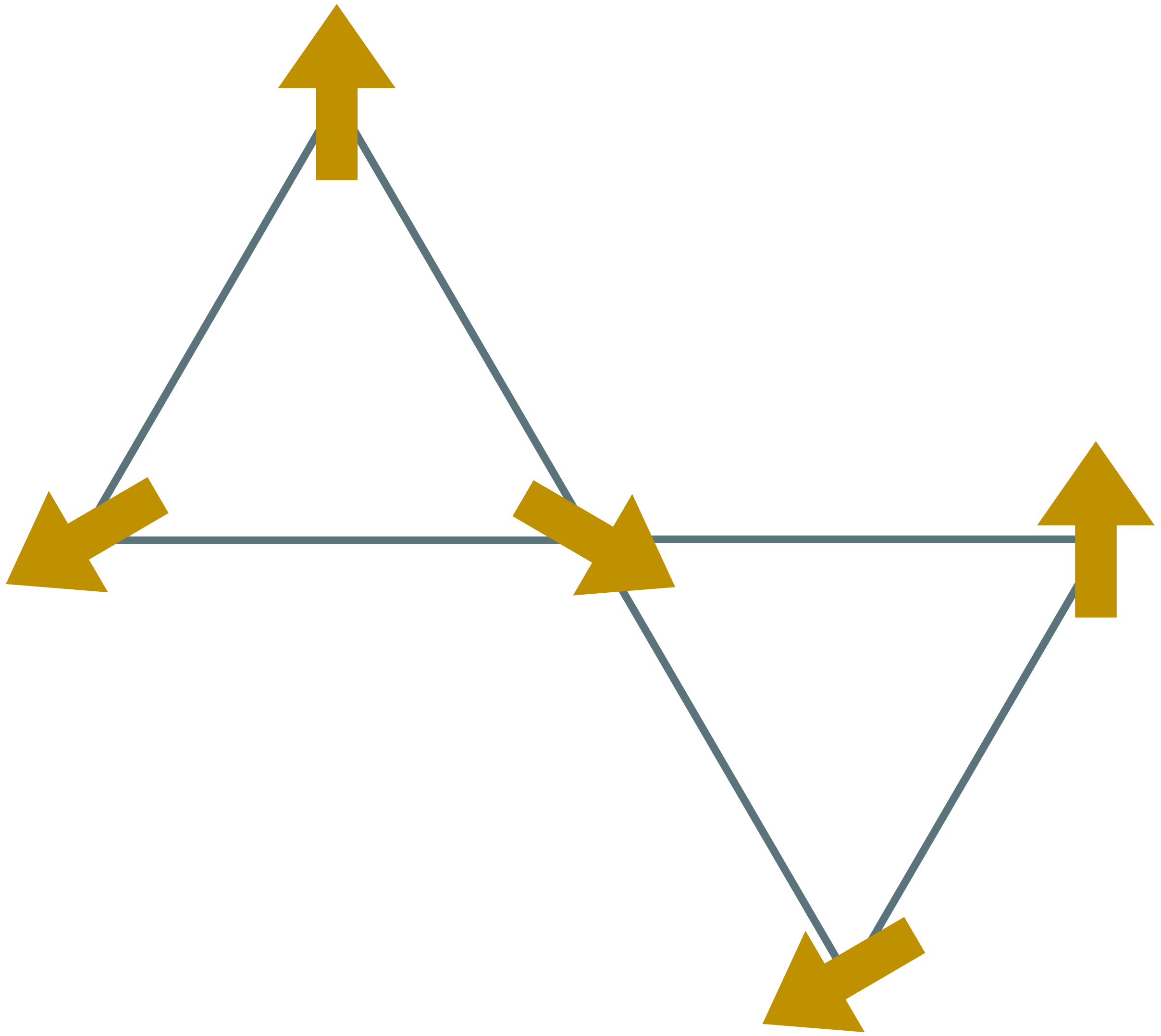
One ground state option: noncollinear spins



Anderson, *Mater. Res. Bull.* ***8*** (1973) 153-160.

One ground state option: noncollinear spins



Anderson, *Mater. Res. Bull.* ***8*** (1973) 153-160.

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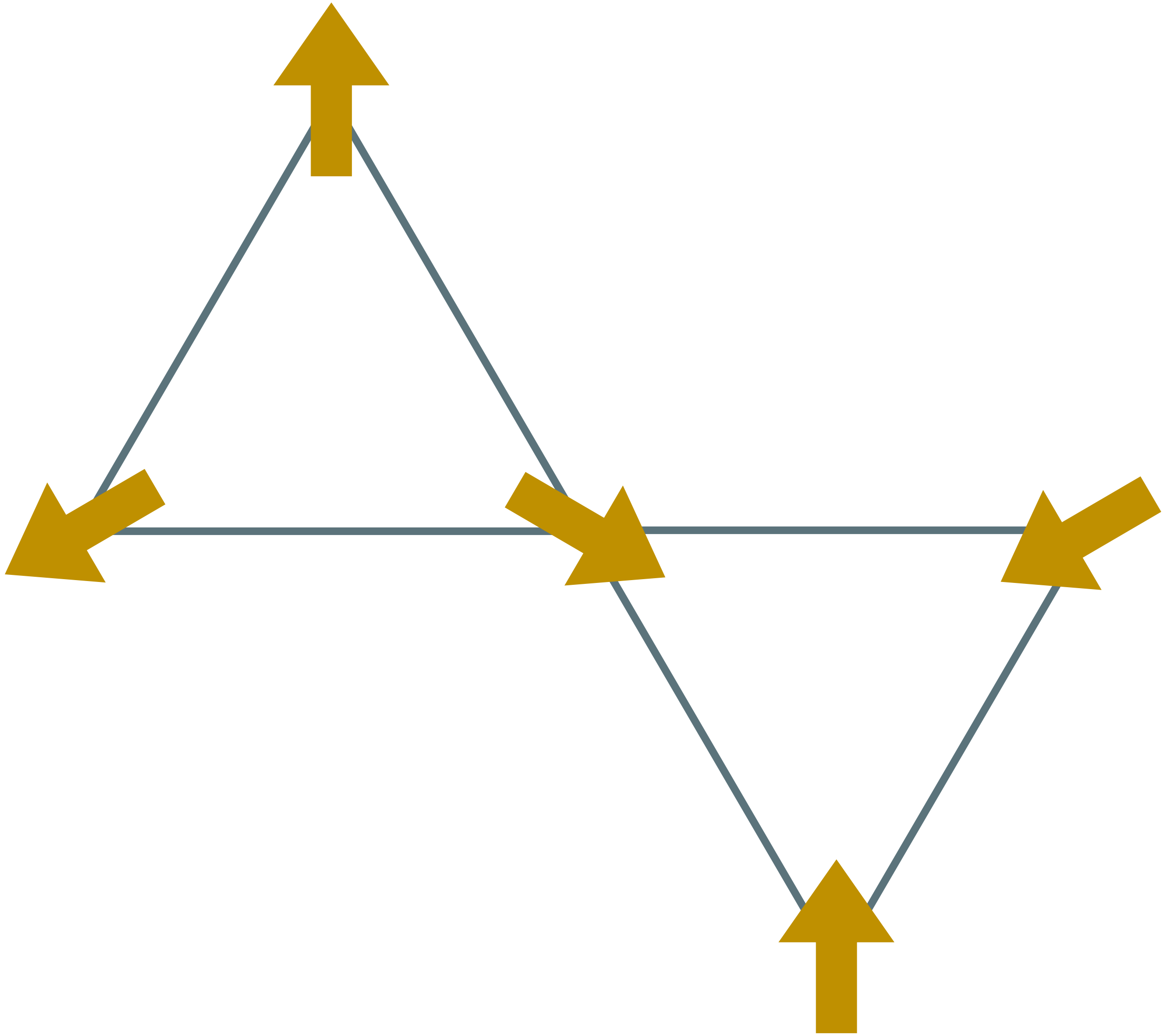
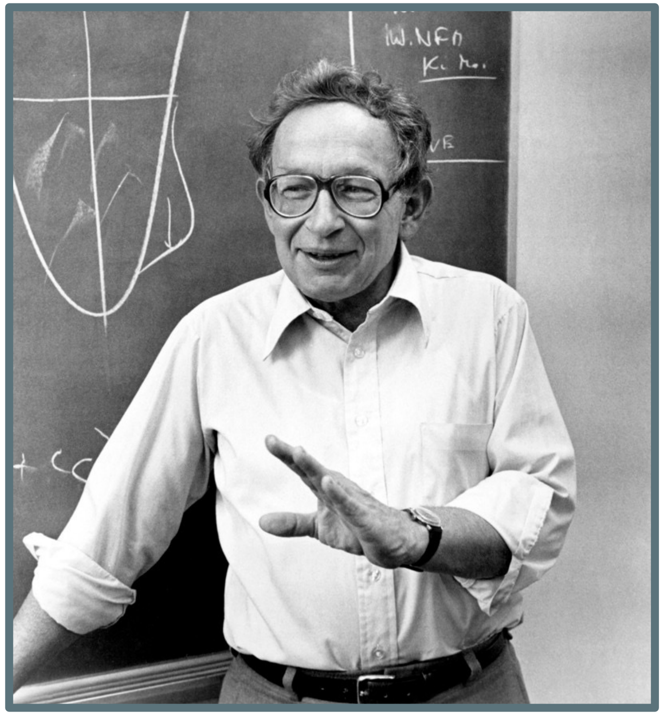
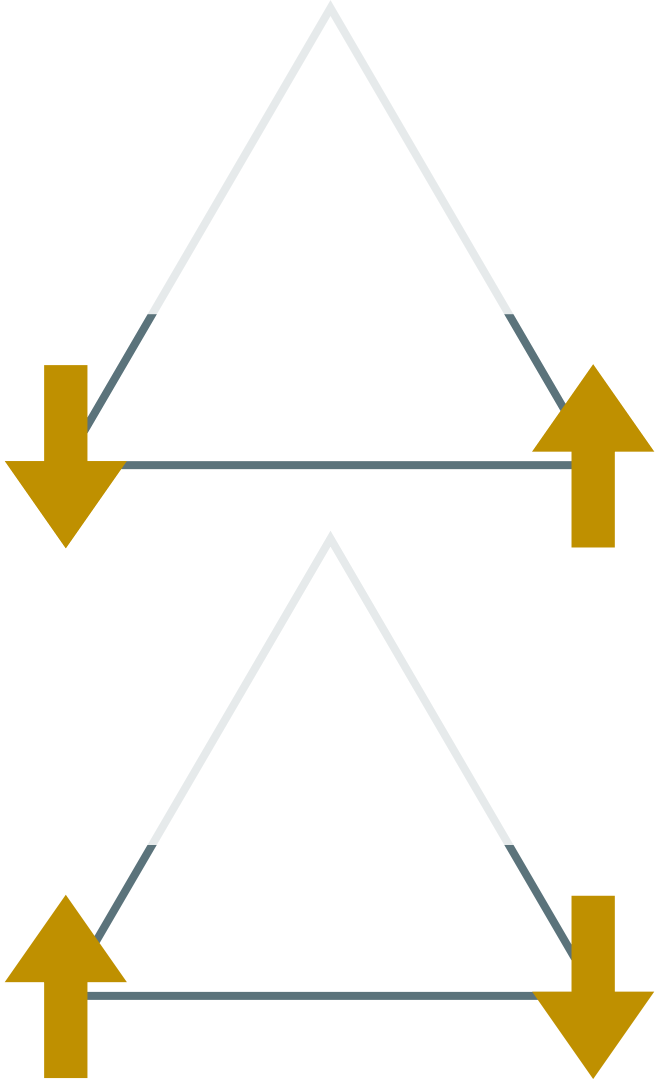


Anderson, *Mater. Res. Bull.* ***8*** (1973) 153-160.

Anderson: resonating valence bond (RVB) model





singlet state

$$\frac{1}{\sqrt{2}}(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle)$$

Image from www.nature.com/articles/d41586-020-01318-4
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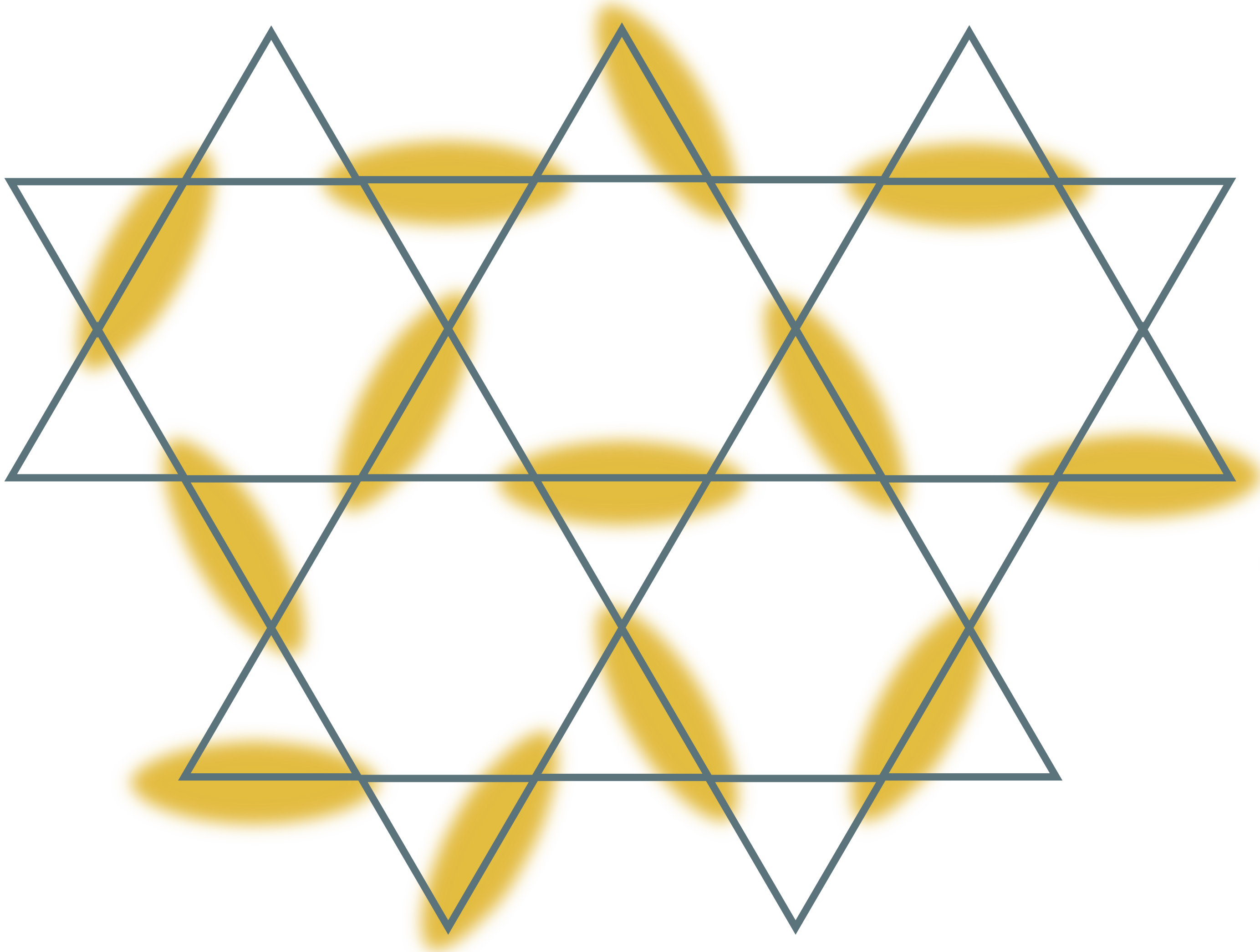

singlet state

$$= \frac{1}{\sqrt{2}}\left(|{\downarrow\uparrow}\rangle - |{\uparrow\downarrow}\rangle\right)$$

Image from www.nature.com/articles/d41586-020-01318-4

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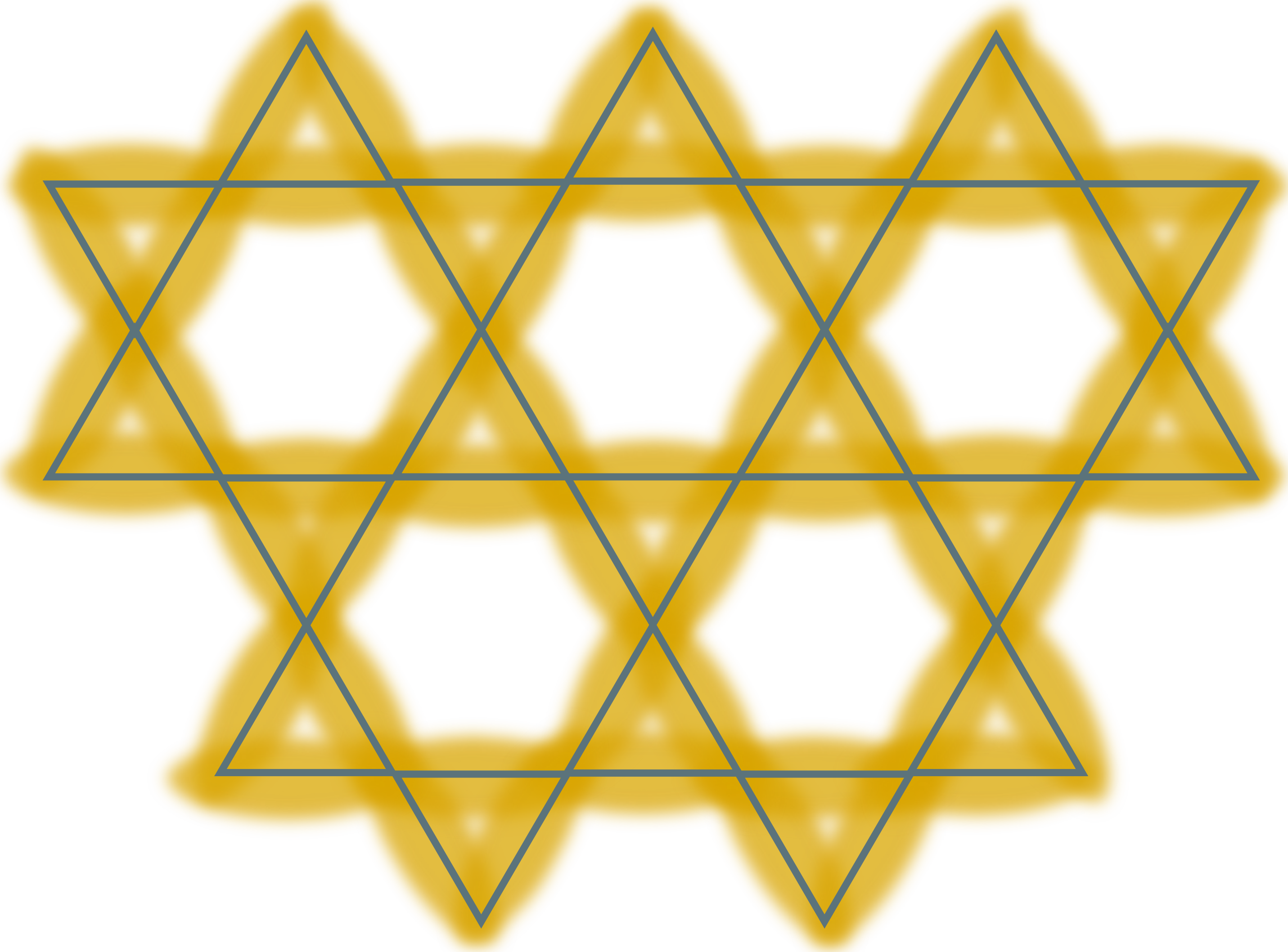


- entangled singlet state
- entangled superposition of singlets across network

Image from www.nature.com/articles/d41586-020-01318-4
Anderson, *Mater. Res. Bull.* ***8*** (1973) 153-160.

Defining a QSL

Quantum spin liquid

1) no long-range ordering of spins even at 0 K
2) no symmetry breaking
3) long-range entanglement of spins
4) fractional excitations
    - emergent mode with only part of the degrees of freedom of elementary particles in system
    - electron = bound state of spinon + chargon + orbiton

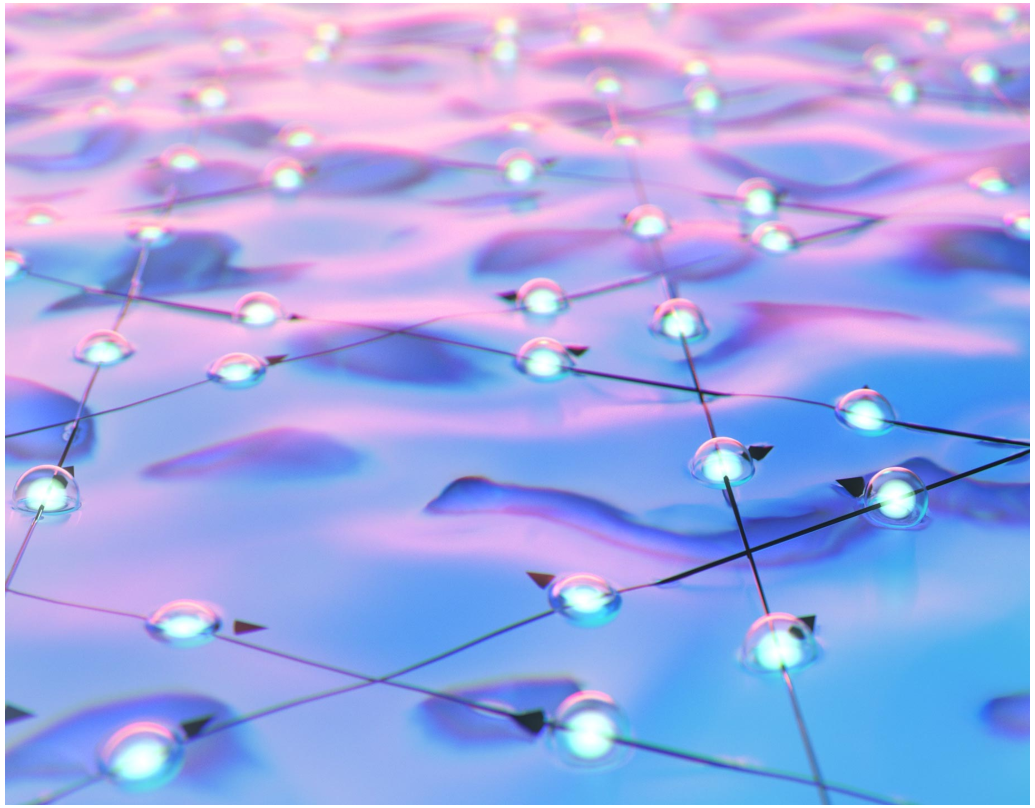
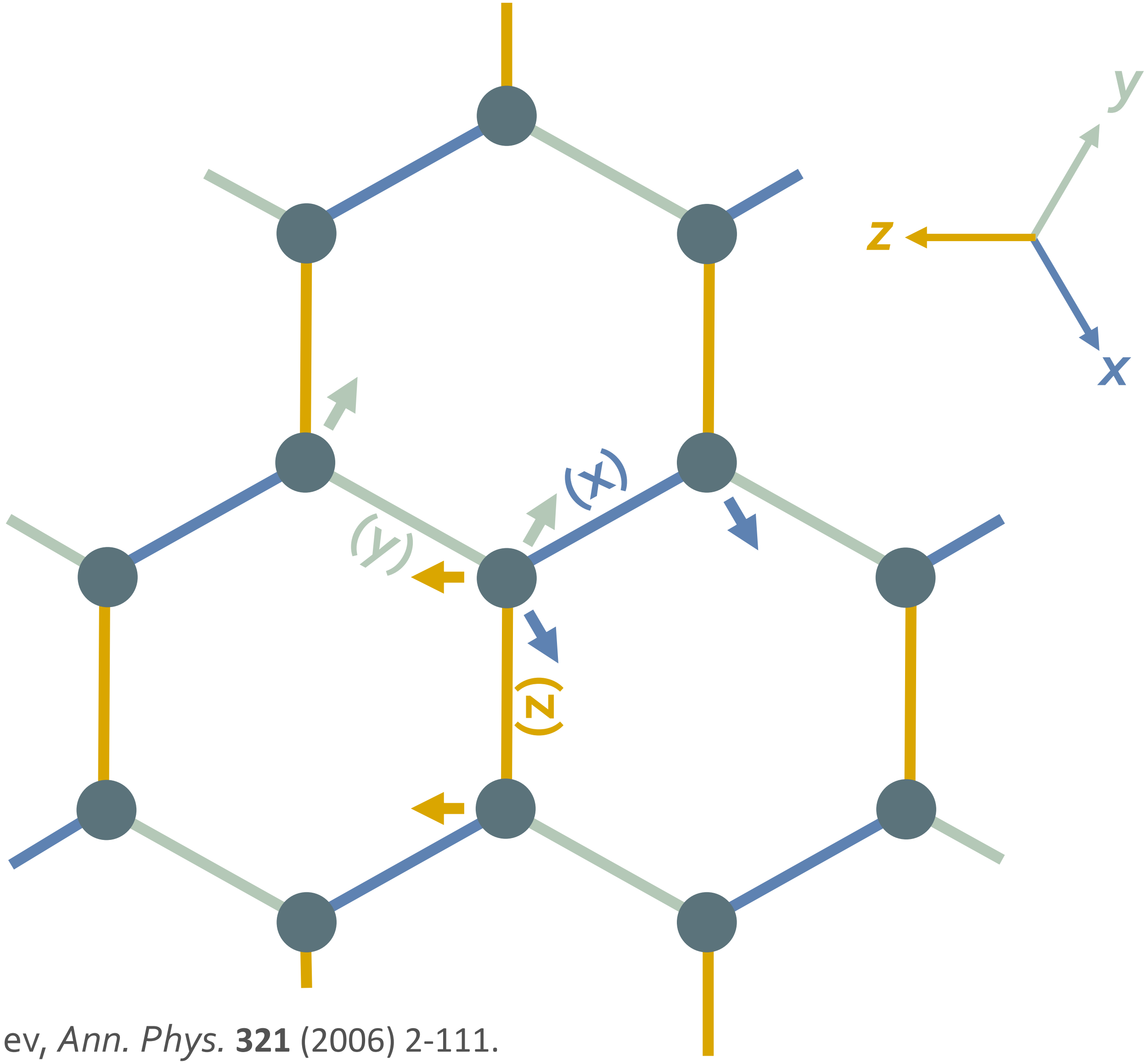


Image from www.quantamagazine.org/quantum-simulators-create-a-totally-new-phase-of-matter-20211202/
Jinsheng Wen, Shun-Li Yu, Shiyan Li, Weiqiang Yu, Jian-Xin Li, *npj Quantum Mater.* **4** (2019) 12.
Ye, Marchetti, *Phys. Scr.* **94** (2019) 115808.

Kitaev model

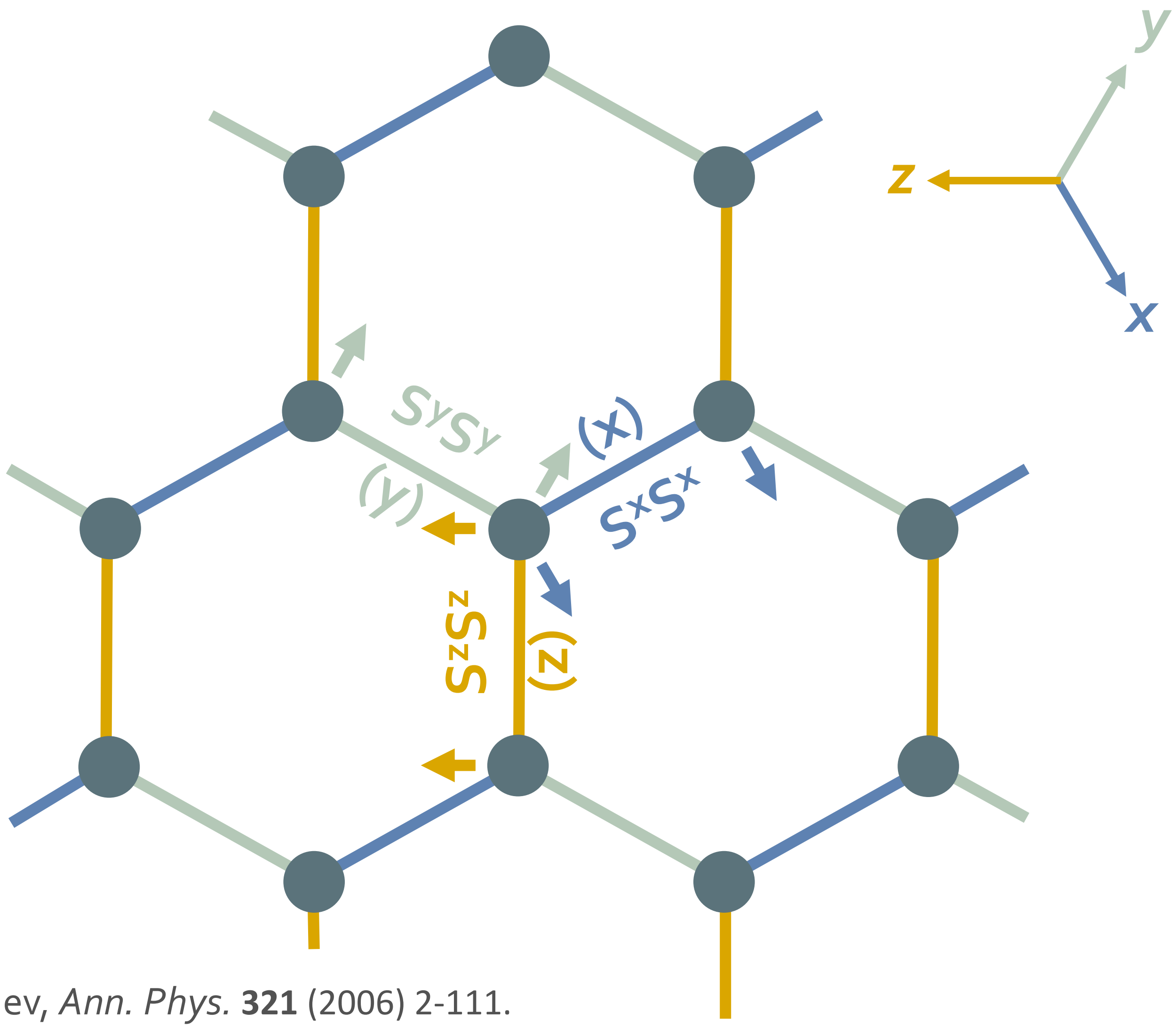


- S = ½ spins
- nearest-neighbor Ising interactions
- easy axes depend on bond

(blue bond has easy axis parallel to *x*)

Kitaev, *Ann. Phys.* **321** (2006) 2-111.
Image adapted from Jinsheng Wen, Shun-Li Yu, Shiyan Li, Weiqiang Yu, Jian-Xin Li, *npj Quantum Mater.* **4** (2019) 12.

Kitaev model Hamiltonian



Kitaev coupling constant

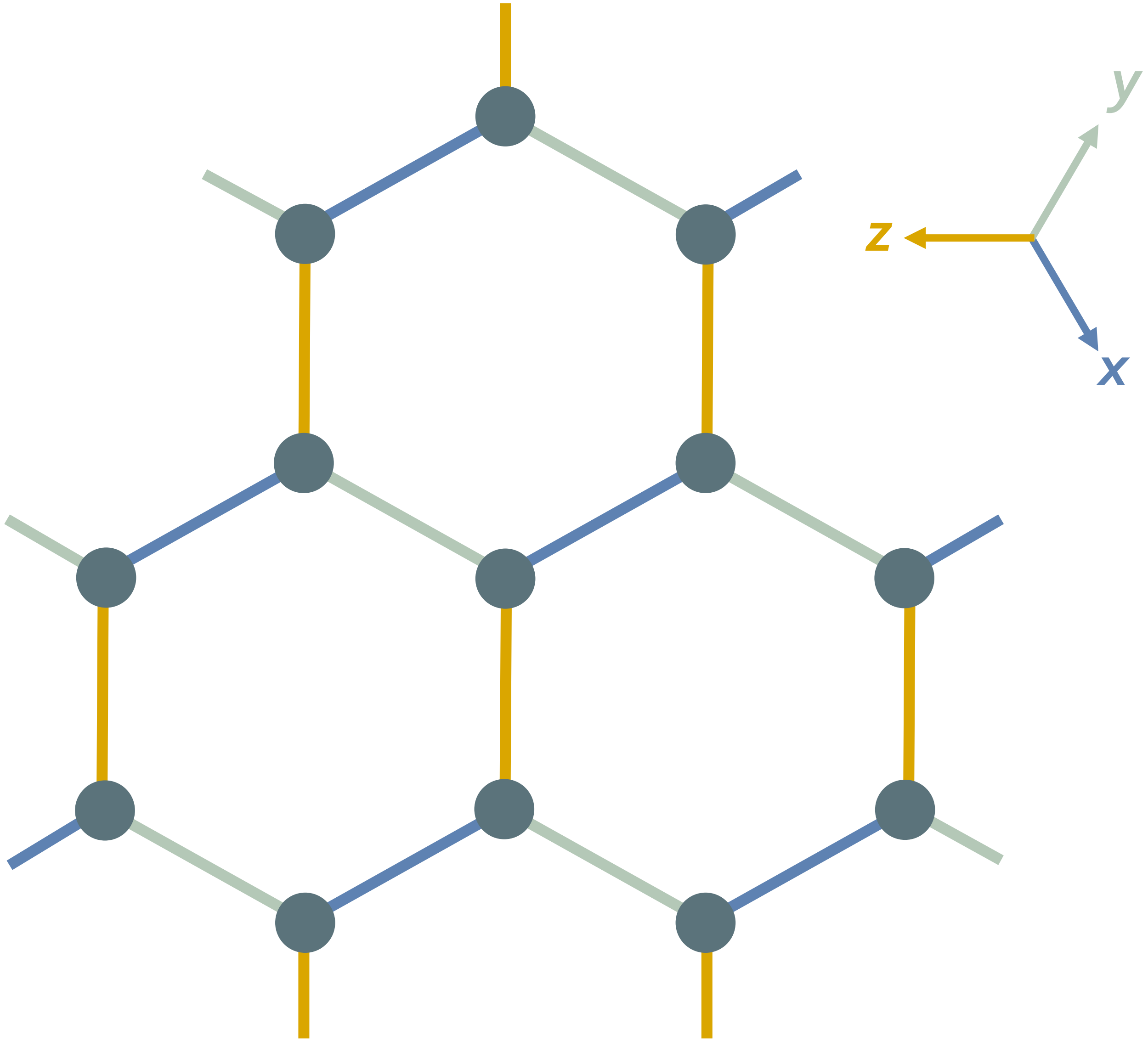
$$H = -\sum_{\langle ij \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma$$

site- and bond-indexed spins

γ = x, y, z type bonds

Kitaev, *Ann. Phys.* **321** (2006) 2-111.
Image adapted from Jinsheng Wen, Shun-Li Yu, Shiyan Li, Weiqiang Yu, Jian-Xin Li, *npj Quantum Mater.* **4** (2019) 12.

Kitaev model in the classical limit



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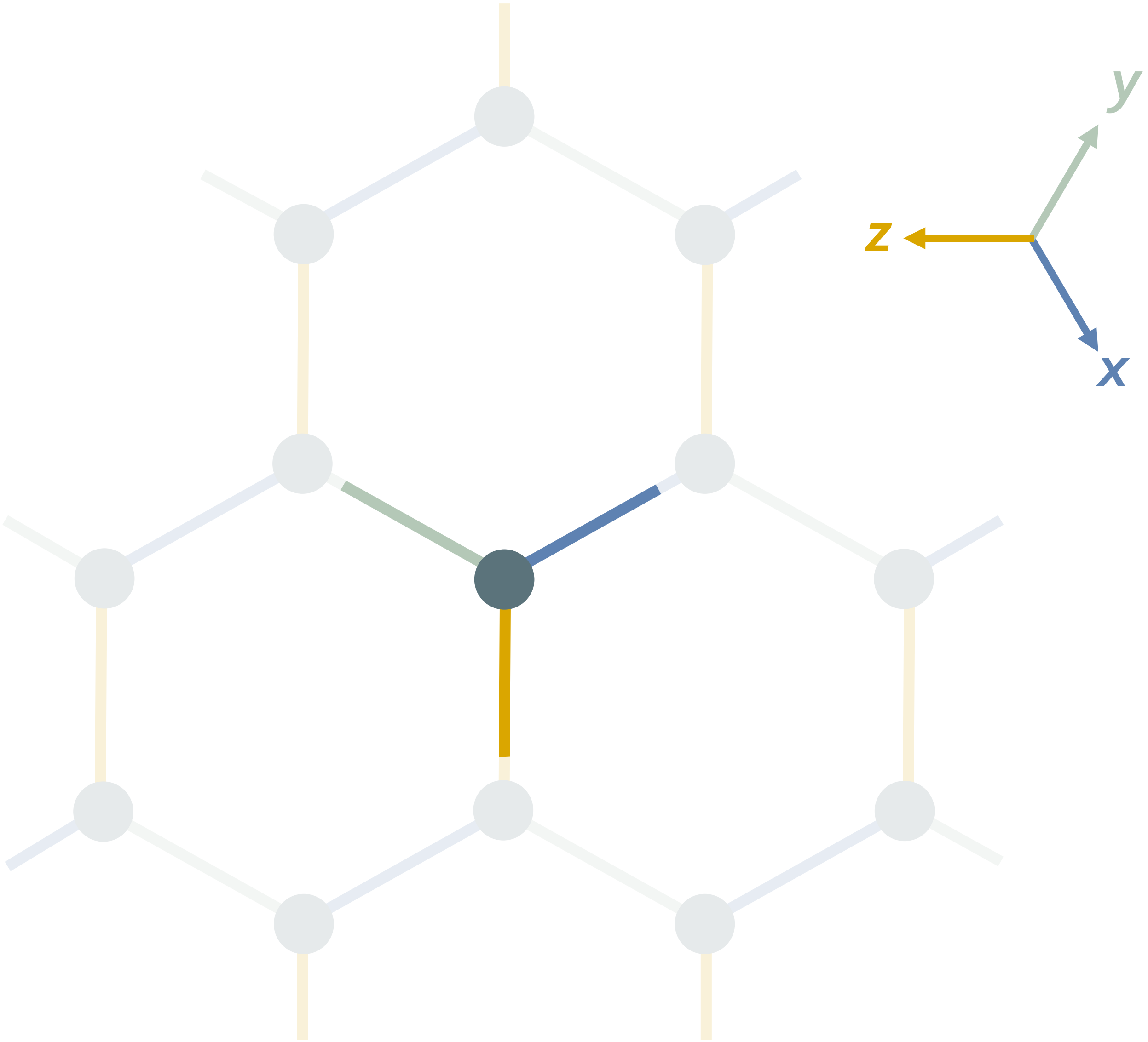
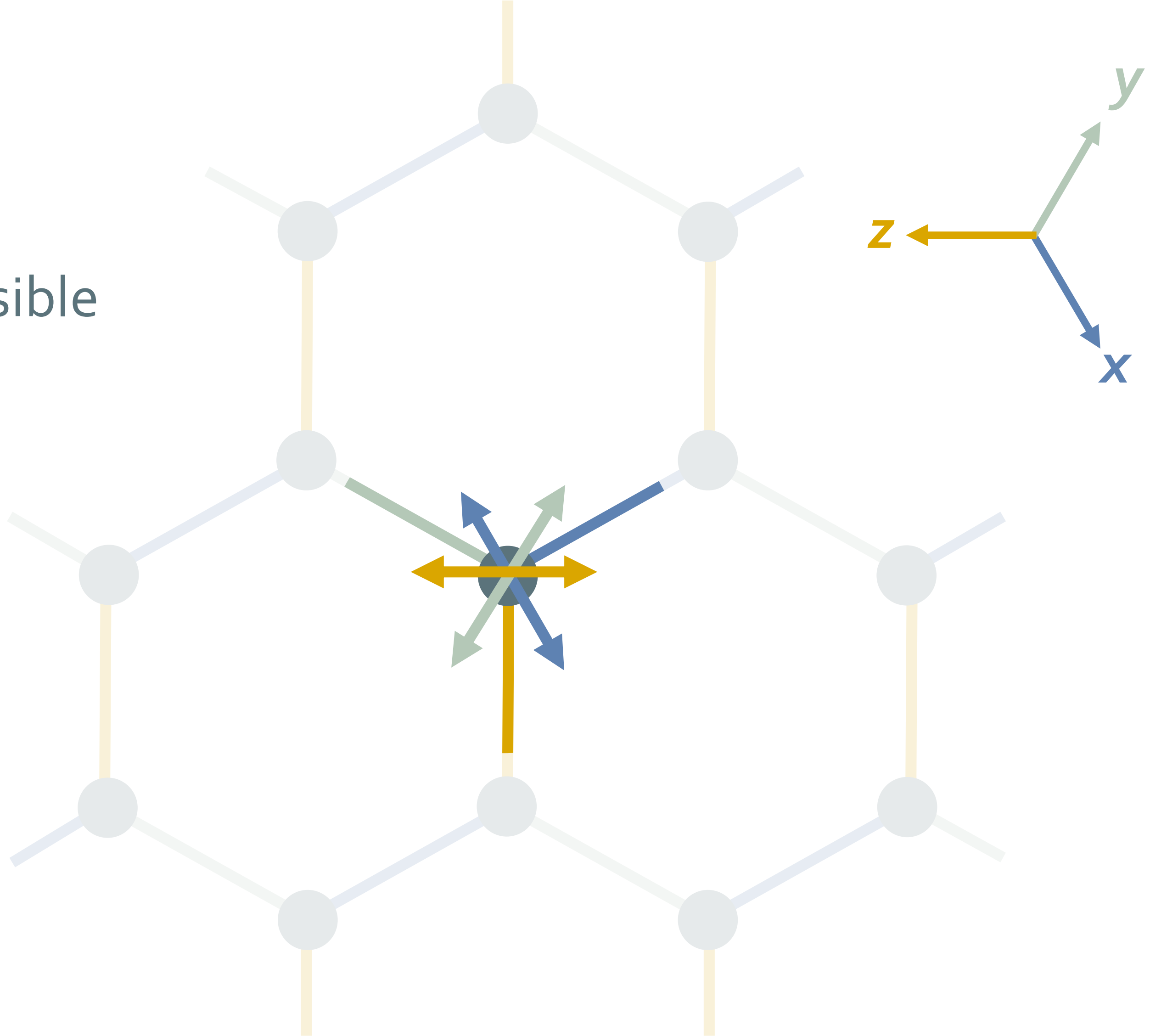


Kitaev, *Ann. Phys.* **321** (2006) 2-111.

Kitaev model in the classical limit

each site has 6 possible spin directions

- 3 easy axes
- Ising spins



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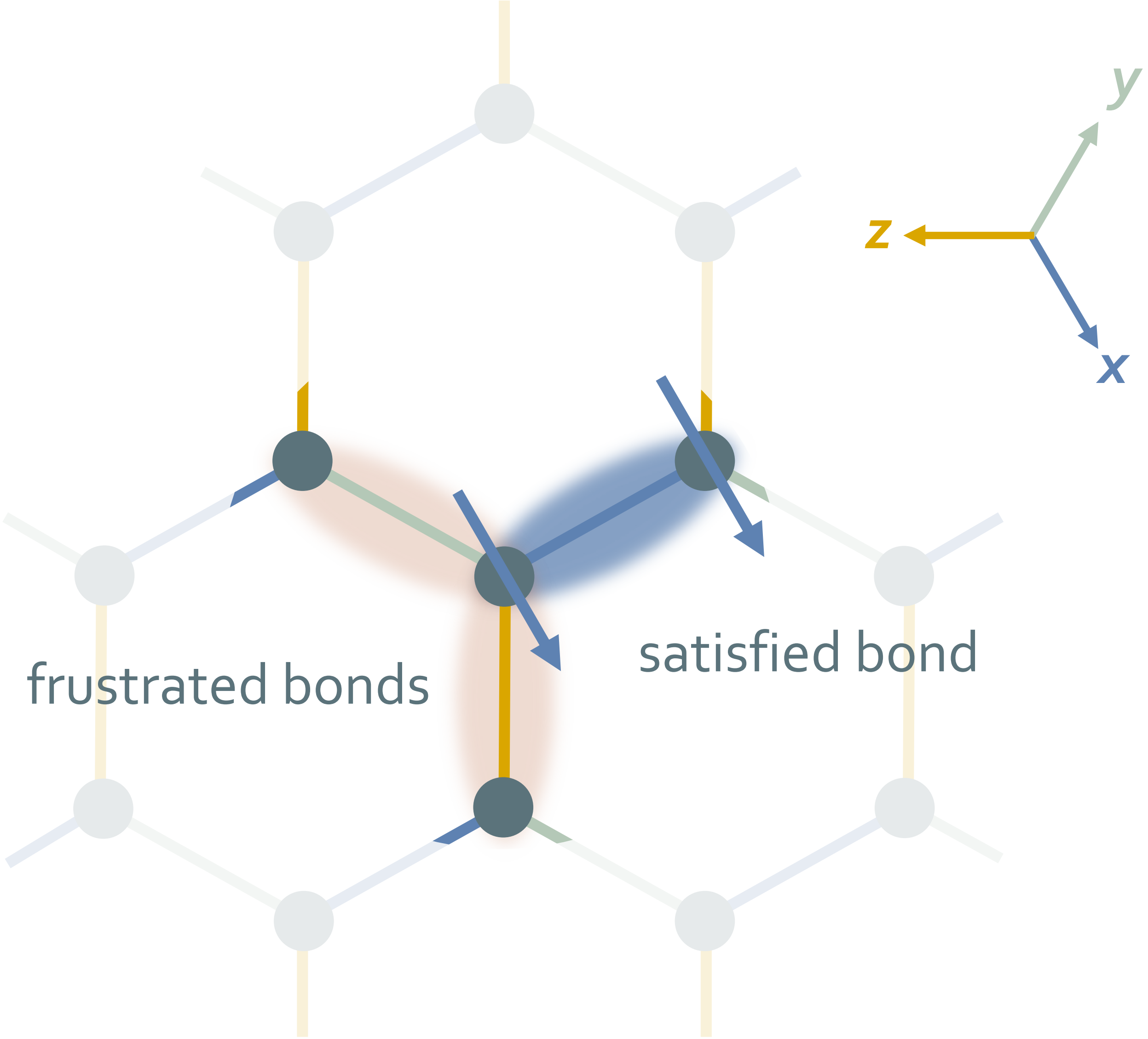

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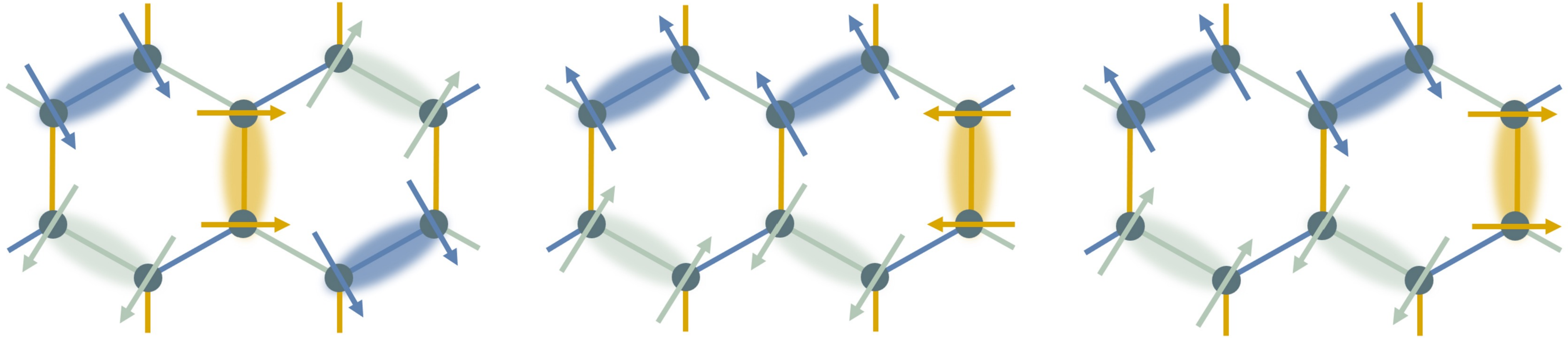
Ground state degeneracy in (classical) Kitaev model

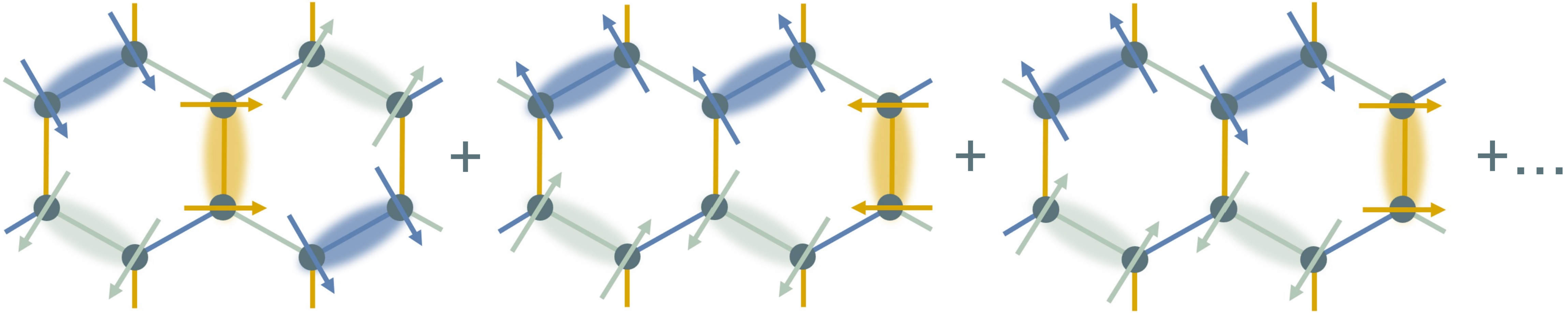
number of ways to distribute satisfied bonds across honeycomb × 2 spin alignments



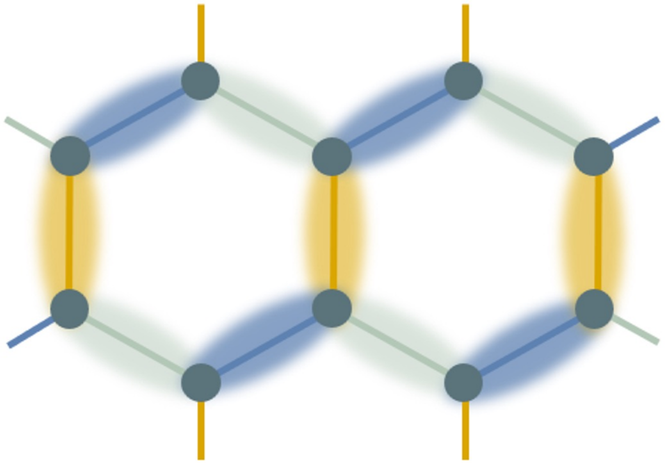
Kitaev, *Ann. Phys.* **321** (2006) 2-111.

Quantum effects in Kitaev model

adding in quantum mechanical effects:



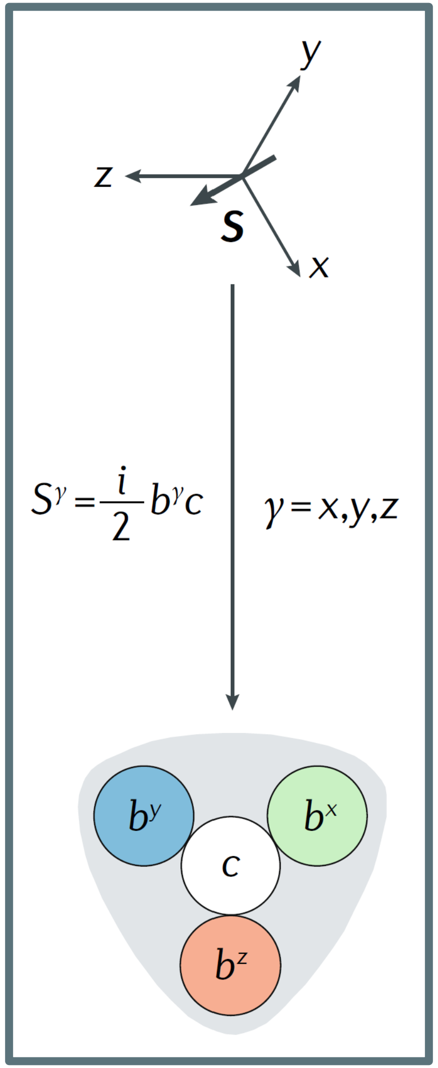
highly entangled superposition of states within classical ground state manifold



1/3 satisfied bonds
2/3 frustrated bonds

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

Kitaev QSL excitations



exact solution of Kitaev model has QSL ground state

$$H = -\sum_{\langle ij \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma$$

Kitaev Hamiltonian

$$H = -\frac{1}{4}\sum_{\langle ij \rangle_\gamma} K_\gamma b_i^\gamma b_j^\gamma c_i c_j$$

fractionalize spin operators into 4 Majorana operators (three localized, one itinerant)

Majorana fermions:

- particles that are their own antiparticle
- obey non-Abelian statistics
- application in topological quantum computing

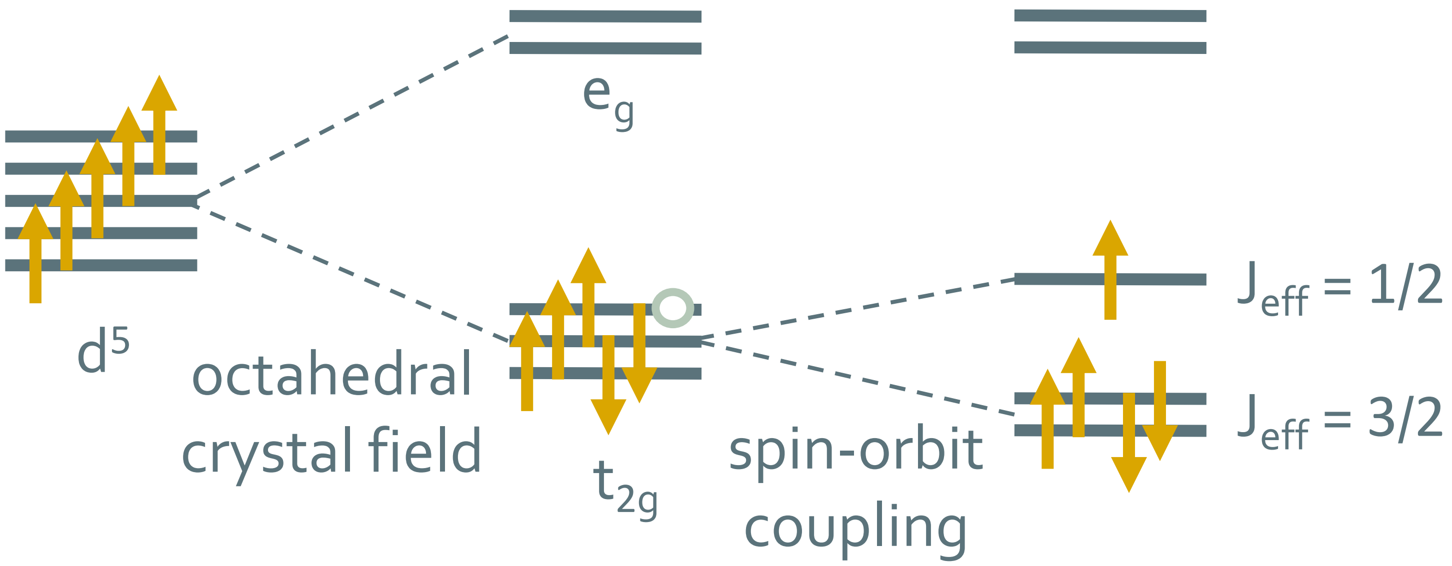
Kitaev, *Ann. Phys.* **321** (2006) 2-111.
Image from Jinsheng Wen, Shun-Li Yu, Shiyan Li, Weiqiang Yu, Jian-Xin Li, *npj Quantum Mater.* **4** (2019) 12.

Ingredients for Kitaev QSL materials

honeycomb network with bond-dependent Ising-type exchange interactions

↓

anisotropy requires moments with
orbital components



+ U: $J_{eff} = 1/2$ Mott insulator

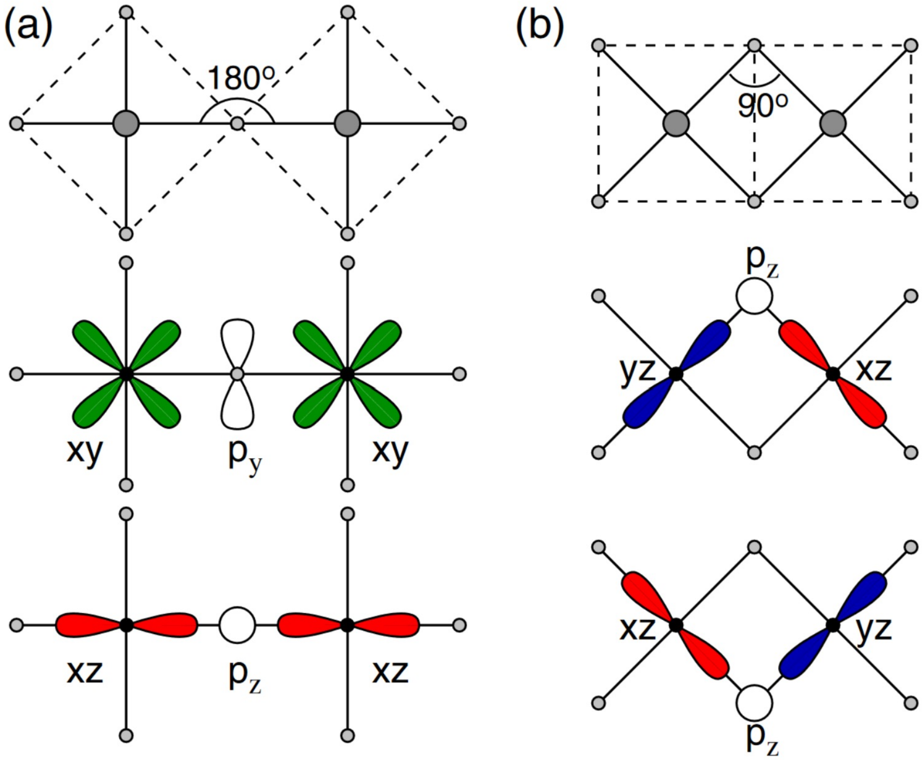
Wen, Yu, Li, Yu, Li, *npj Quantum Mater.* ***4*** (2019) 12.
Clark, Abdeldaim, *Annu. Rev. Mater. Res.* **51** (2021) 495-519.
Jackeli, Khaliullin, *Phys. Rev. Lett.* **102** (2009) 017205.

“Engineering” Kitaev QSL materials

Jackeli + Khaliullin: Kitaev QSL from $J_{eff} = 1/2$ Mott insulator

corner-sharing octahedra

super-exchange interaction between $J_{eff} = 1/2$ moments dominated by isotropic Heisenberg term

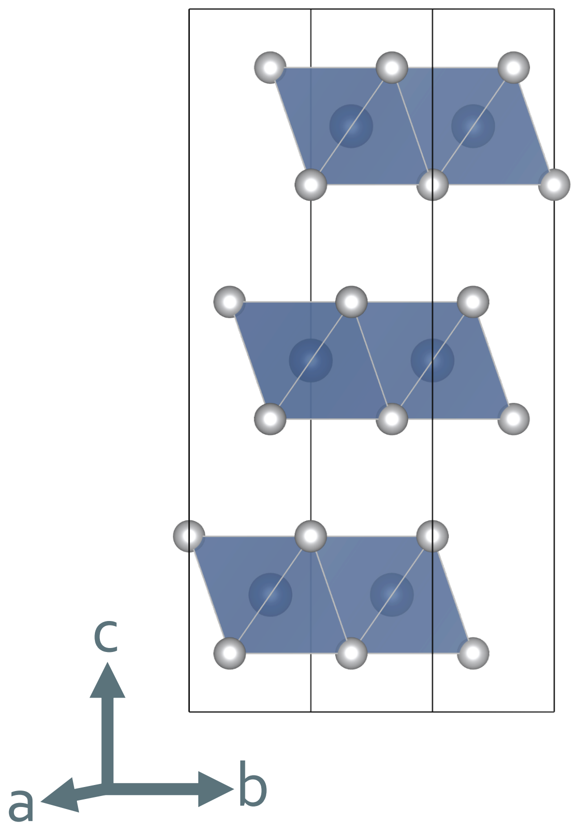


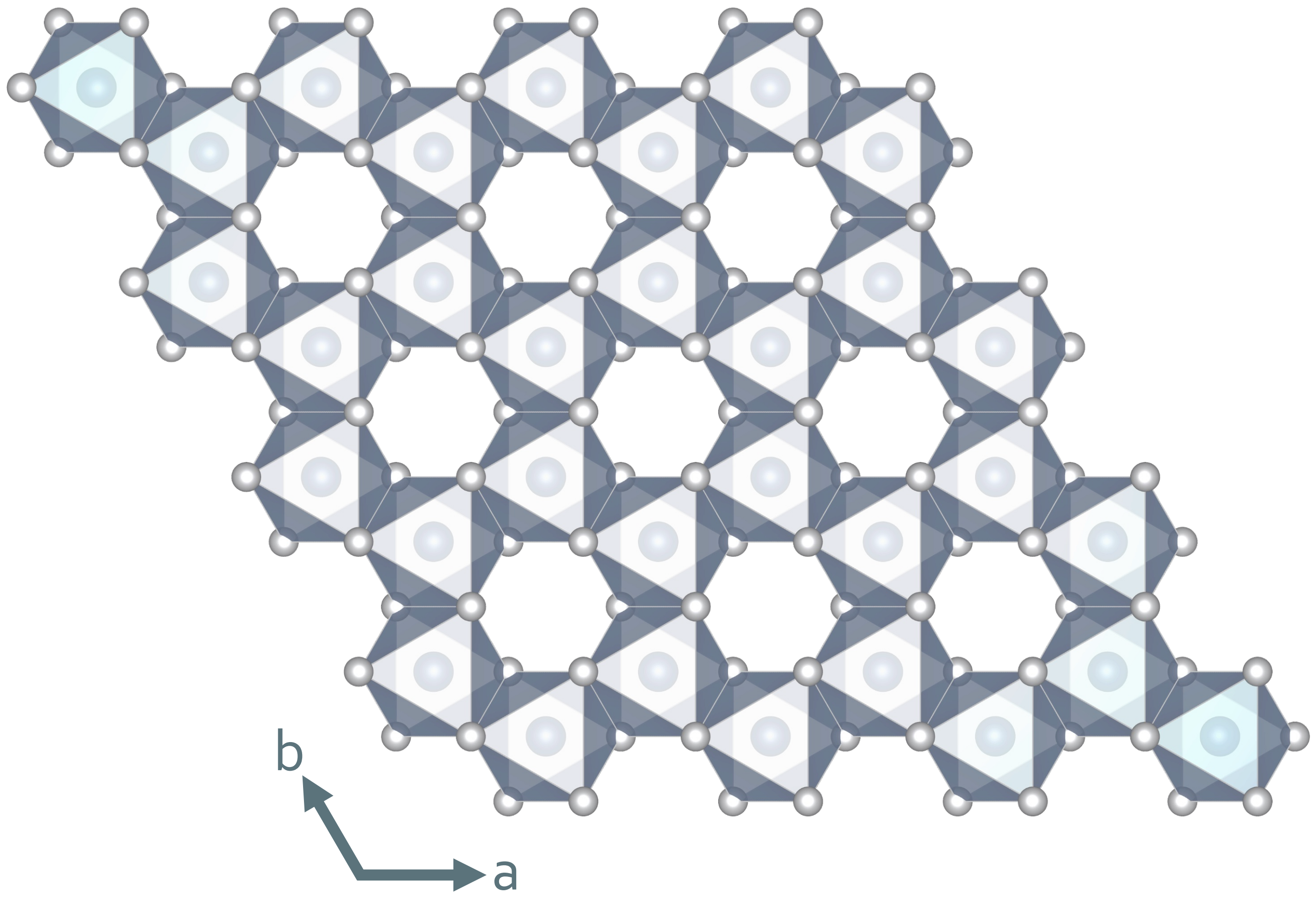
edge-sharing octahedra

interference between super-exchange paths suppresses Heisenberg term

Jackeli, Khaliullin, *Phys. Rev. Lett.* **102** (2009) 017205.
Wen, Yu, Li, Yu, Li, *npj Quantum Mater.* **4** (2019) 12.
Clark, Abdeldaim, *Annu. Rev. Mater. Res.* **51** (2021) 495-519.

α-$RuCl_3$

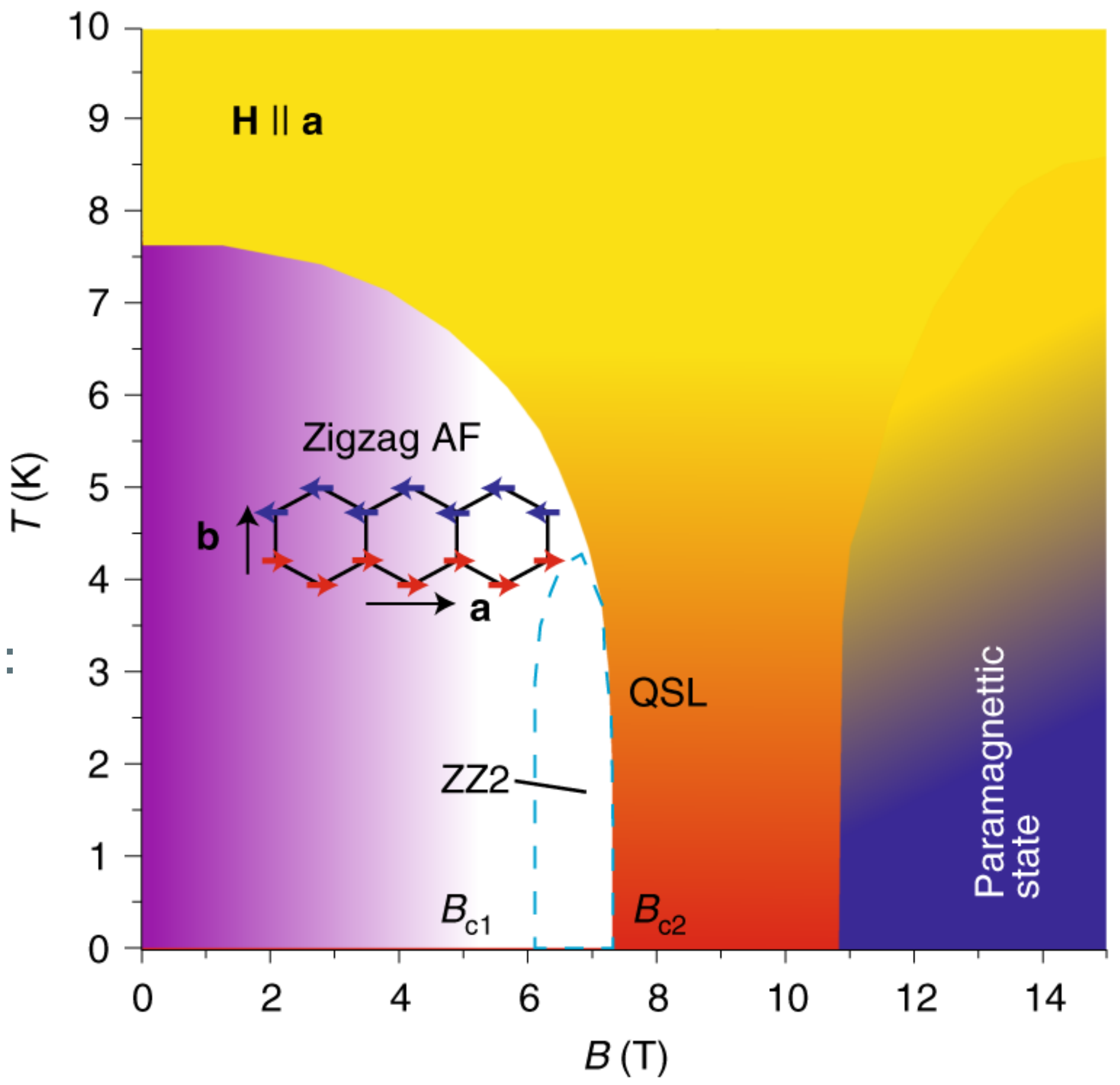




Stroganov, Ovchinnikov. *Ser. Fiz. Khim.* **12** (1957) 152.

Proximate Kitaev QSL candidate α-$RuCl_3$

ground state:
zigzag AFM

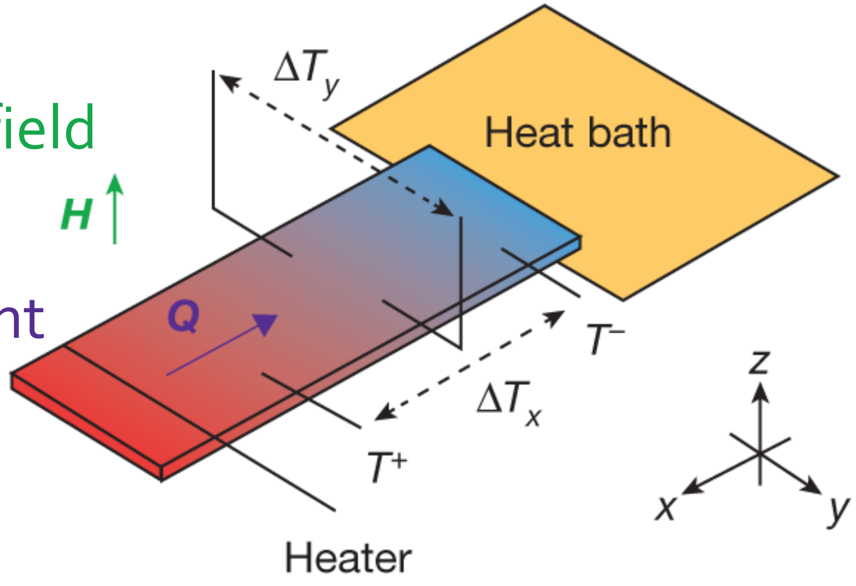


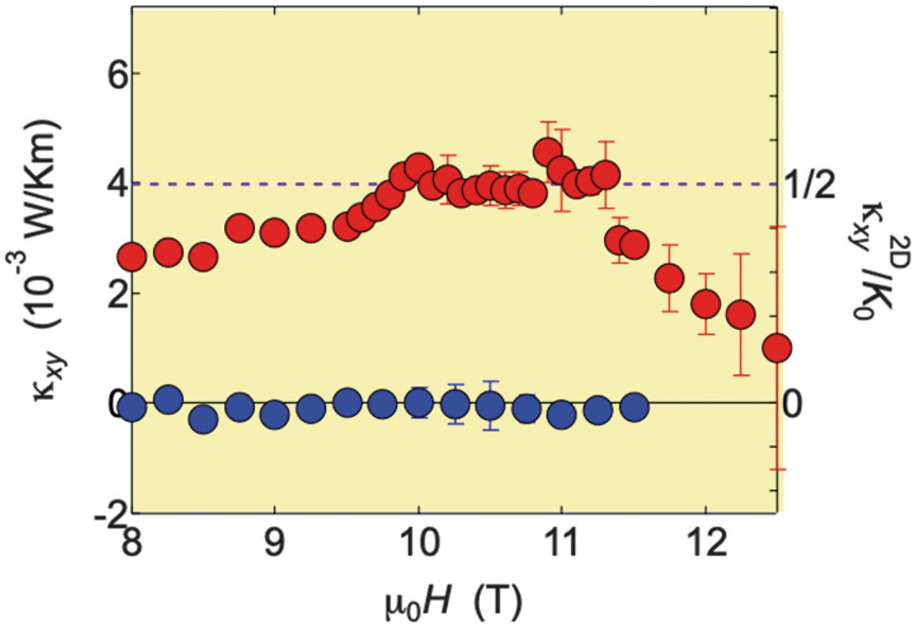
intermediate KQSL state?

Czajka, Gao, Hirschberger, Lampen-Kelley, Banerjee, Yan, Mandrus, Nagler, Ong, *Nat. Phys.* **17** (2021) 915-919.

Quantized thermal Hall conductivity in α-$RuCl_3$

thermal Hall effect





thermal transport to detect charge-neutral Majorana fermions

quantized thermal Hall conductivity indicative of Majorana edge modes?

Image of thermal Hall effect from DOI: 10.1038/s41586-019-1375-0
Yokoi, Ma, Kasahara, Shibauchi, Kurita, Tanaka, Nasu, Motome, Hickey, Trebst, Matsuda, *Science* **373** (2021) 568-572.
Kasahara, Ohnishi, Mizukami, Tanaka, Ma, Sugii, Kurita, Tanaka, Nasu, Motome, Shibauchi, Matsuda, *Nature* **559** (2018) 227-231.
Broholm, Cava, Kivelson, Nocera, Norman, Senthil, *Science* **367** (2020) eaayo668.

Summary

Quantum spin liquid

- no long-range ordering of spins even at 0 K

Kitaev model

- QSL ground state
- honeycomb network with bond-dependent Ising exchange

α-$RuCl_3$

- ground state: zigzag AFM
- proximate KQSL in intermediate magnetic field

Thank you