Quantum spin liquids in frustrated magnets

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[R. V. Mishmash, J. R. Garrison, **SB**, and C. Xu, PRL **111**, 157203 (2013)]
[**SB**, M. Serbyn, T. Senthil, and P. A. Lee, PRB **86**, 224409 (2012)]

Outline

- Ordinary liquids and quantum (spin) liquids
- Quantum spin liquids: Theory
- Experimental realizations
- Spin-1/2 QSL state for organic candidate materials
- Spin-1 liquid in recently discovered Ni compound

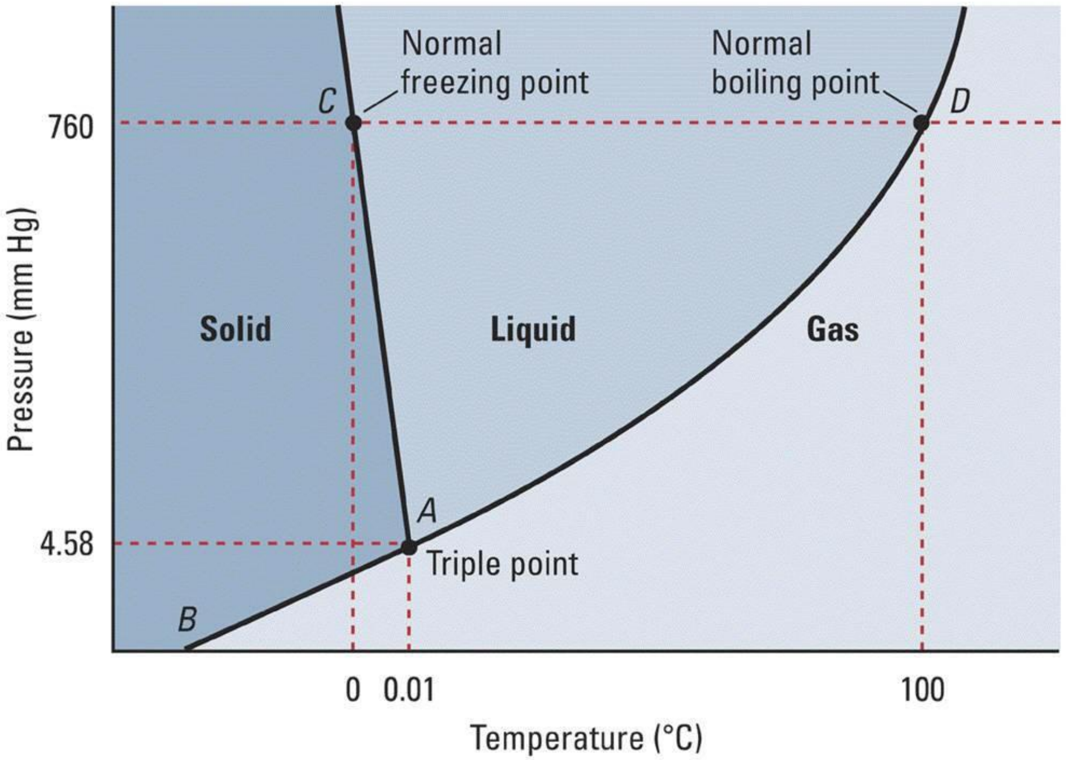
Liquids ? or solids ?

Solids

- Described by local order parameters and symmetry breaking
- Rich structure; classification: 230 space groups in 3D; 17 in 2D

Liquids (water)

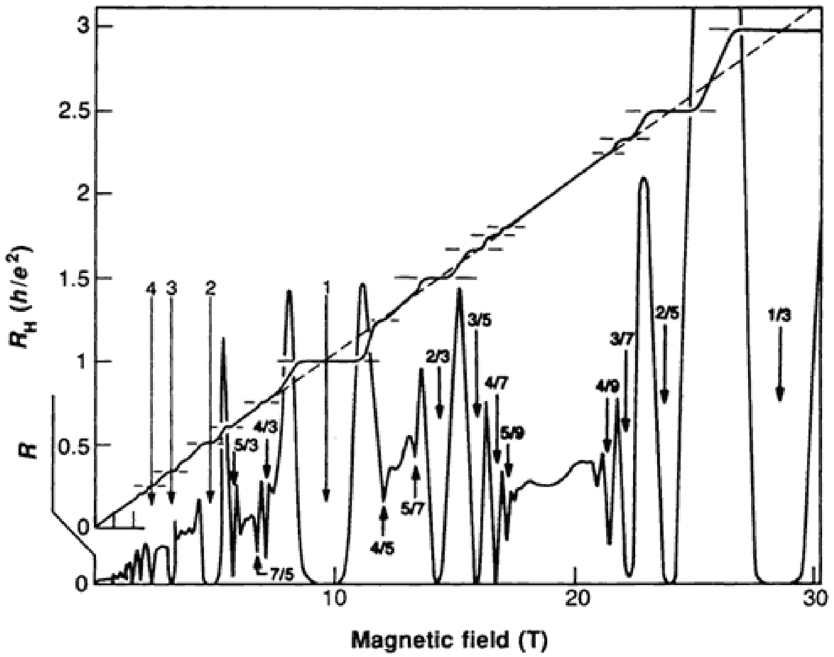
- Unbroken space symmetries
- Characterized by short distance correlations, dynamical properties
- Much more subtle to classify than solids
- Crossover between different phases



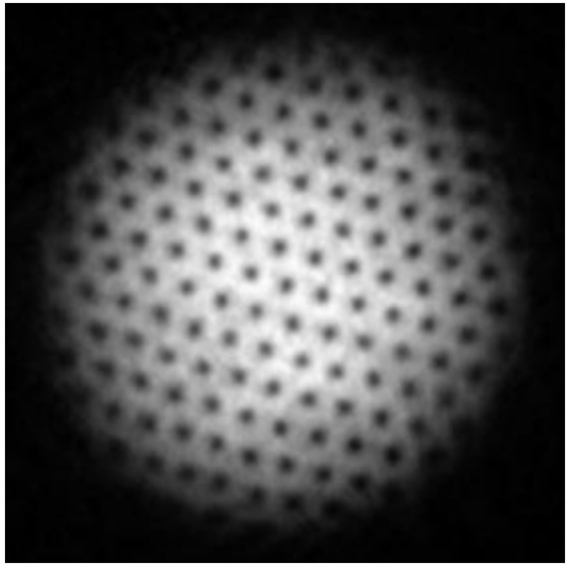
Quantum liquids

- No (or only partial) symmetry breaking at T=0
- No local order parameter
- Prominent examples:

Quantum Hall effect



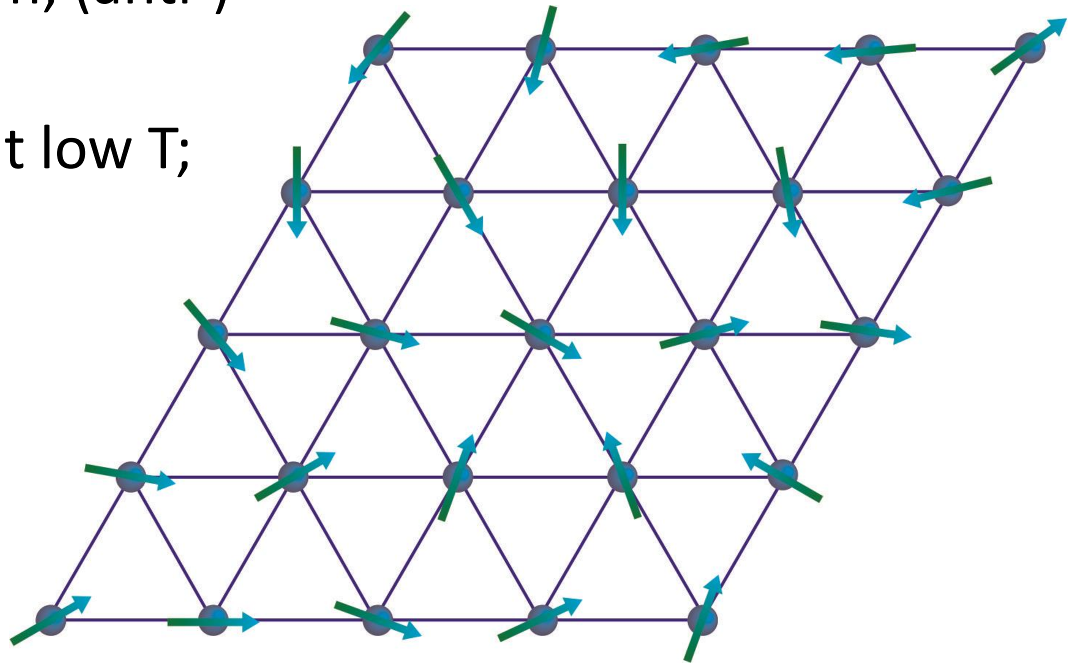
Superfluidity



Similar phases in magnetic systems

Phases:

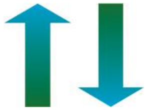
- **Spin gas**: independent spins point in random directions; high-T paramagnetic phase.
- **Spin solid**: Freezing of spins to a regular pattern; (anti-) ferromagnetic phase.
- **Spin liquid?** Interacting and fluctuating spins at low T; no ordering and no symmetry breaking



Geometric frustration

$$H = J S_i^z S_j^z \,, \ J > 0$$

- Three Ising spins with anti-ferromagnetic interaction: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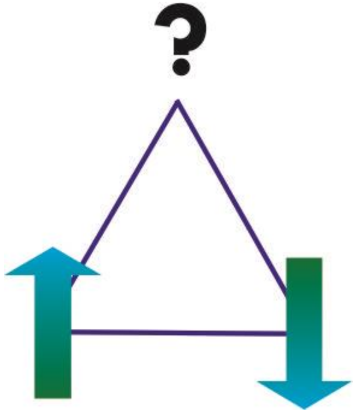
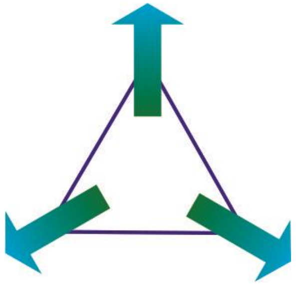


→Degeneracy of classical ground state.

Triangular Ising lattice [Wannier 1950].

- Heisenberg spins (classical):

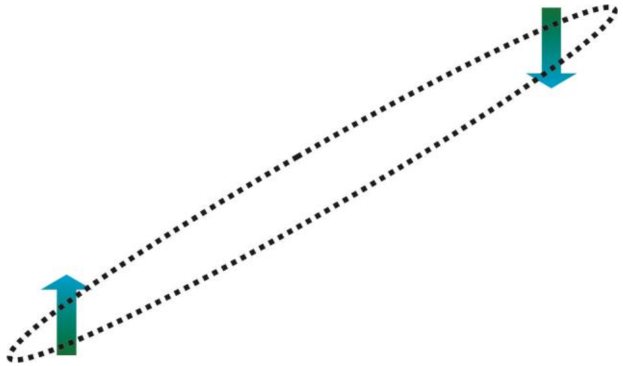


→More complicated interactions?
→Quantum spins?

Quantum spin liquids: Theory

- Absence of lattice symmetry breaking at T=0 (negative definition)
- Certainly happens in 1D spin models.

  What about 2D? Neel order or disorder GS?
- Long-range entanglement [Levin, Wen 06]; state that cannot be approximated by any finite-region product wave function.

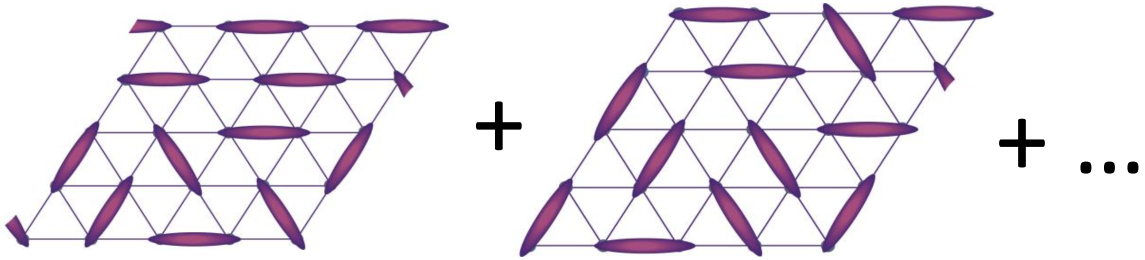


Resonating valence bonds

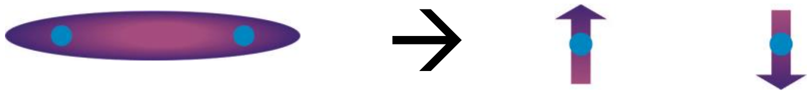
- Valence bond singlet: $|\mathrm{VB}\rangle = \frac{1}{\sqrt{2}}[|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle]$ =  $\langle \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \rangle = -3/4$

  Neel:  $\langle \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \rangle = -1/4$

- Anderson 1973: Quantum superposition of valence bond states may beat Neel order



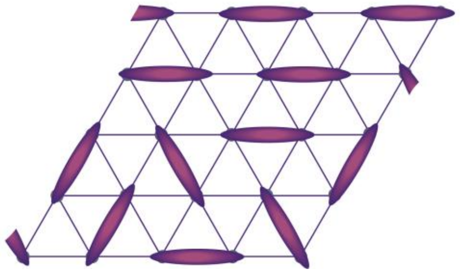
- Spinon excitation (spin-1/2); broken valence bond (ΔE = J/2)



- Anderson 1987: High-temperature superconductivity can naturally emerge from RVB states

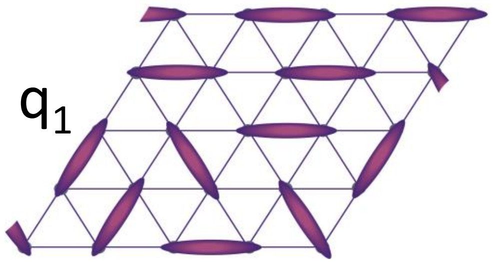
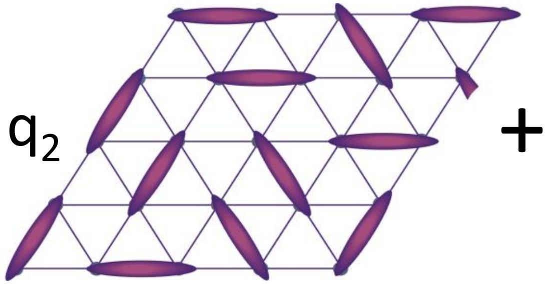
Types of valence bond states

- Valence bond solids



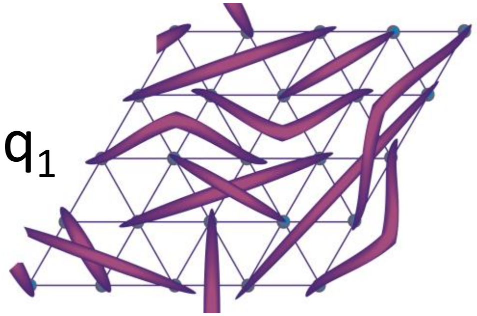
→ Lattice symmetry breaking
→ Product state of valence bonds
→ No long-range entanglement

- Liquid of “short” valence bonds

q_1  $+ \; q_2$  $+ \ldots$

→ No lattice symmetry breaking
→ Long-range entangled
→ Gapped (S=1/2) spinon excitation
→ Spinless vortex excitation (visons)
→ Topological order; group cohomology classification [Chen,Gu,Wen 12]

- Liquid of “long” valence bonds

q_1  $+ \ldots$

→ No lattice symmetry breaking
→ Long-range entangled
→ Low-energy spinon excitations
→ Algebraic dimer-dimer correlations
→ Classification more subtle (open)

Gutzwiller construction of RVB states

- A priori very hard to make the RVB picture quantitative
- Take simple long-range entangled state – the Fermi gas: $|FS\rangle = \prod_{\epsilon_k<\mu} c^\dagger_{k\downarrow} c^\dagger_{k\uparrow} |0\rangle$

$$P_G\, |FS\rangle = q_1 |\uparrow,\downarrow,\downarrow,\uparrow,\ldots\rangle + q_2 |\downarrow,0,\uparrow,\downarrow,\ldots\rangle + q_3 |\downarrow,\uparrow,\uparrow\downarrow,\downarrow,\ldots\rangle + \ldots$$

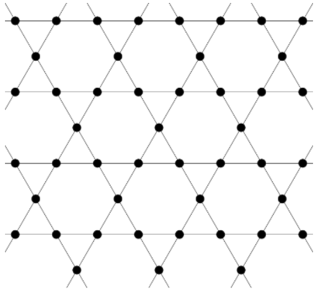
- Projection (P_G) can efficiently be done (for Fermions) using Monte Carlo tec.
- Liquid character not destroyed by projection ? [Grover, Vishwanath 11]
- Auxiliary degree of freedom (slave particles) $c_{j\sigma}$ → parton construction
- Emergent local symmetry in the parton Hilbert space

Parton construction

- Choose slave particles (bosons, fermions, number of flavors…)
- Example: spin-1/2, two fermionic flavors: $S_a = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} f_\alpha^\dagger (\sigma^{\alpha\beta})_a f_\beta$
- Local SU(2) symmetry: $f_\sigma \mapsto f_\sigma \, e^{i\beta_1} \cos\beta_2 + \sigma f_{\bar{\sigma}}^\dagger \, e^{i\beta_3} \sin\beta_2$
- Emergent gauge fields in the parton mean field description
- Symmetry generally broken via Higgs mechanism → U(1), Z_2 spin liquids
- Microscopic spin wave function obtained by projection

Physical realizations of QSL

- Fancy stuff. Does it have anything to do with physical reality?
- Most anti-ferromagnets seem to order at low T.
- In recent years, a number of experimental QSL candidate materials were discovered
  - Kagome lattice ($ZnCu_3(OH)_6Cl_2$)
    - Herbertsmithite [Nocera 05; Y. Lee 12]
    - Kapellasite [Wills 08; Fak 12];



  - Triangular lattice spin-1/2. organics: k-ET, dMIT; $Ba_3CuSb_2O_9$ [Balicas 11, Nakasuji 12]
  - Triangular lattice spin-1 system: $Ba_3NiSb_2O_9$ (?)
  - 3D candidates: $Yb_2Ti_2O_7$, $Na_4Ir_3O_8$,… (pyrochlore, hyperkagome)

Organic candidate materials

- k-$(ET)_2Cu_2(CN)_3$ [Shimizu 03, Saito 05] and $Pd(dmit)_2$ [Yamashita 08]
- Nearly perfect (isotropic) triangular lattice, spin S=1/2
- Anti-ferro interaction J ≈ 250 K
- No ordering transition observed down to 32 mK
- Mott insulator, but pressure induced superconductivity (close to Mott transition)
- Low-temp: Finite spin susceptibility : $\chi_0 \simeq \mathrm{cst.}$

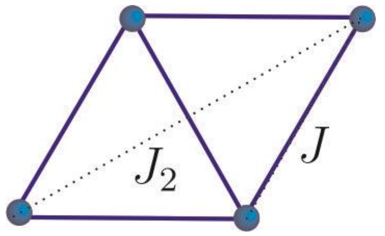
  Linear magnetic specific heat: $C_M \sim \gamma T$

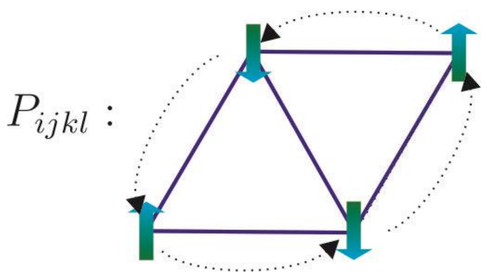
→ gapless QSL !?

Spin model & states

Microscopic triangular lattice spin-1/2 model:

$$H = J\sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j\rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + K/2 \sum_{\langle i,j,k,l\rangle} \{P_{ijkl} + \text{h.c.}\}$$





Hubbard model: K > 0

We check an extensive list of variational states…

[R. V. Mishmash, J. R. Garrison, **SB**, and C. Xu, PRL **111**, 157203 (2013)]

Two flavors of fermionic partons: $$S_a = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} f^\dagger_\alpha (\sigma^{\alpha\beta})_a f_\beta$$

- U(1) Fermi surface state [Lee&Lee 09]: $$H_0 = \sum_{\langle i,j \rangle,\sigma} f^\dagger_{i\sigma} f_{j\sigma}$$
- Pairing instabilities: $$H_0 = \sum_{\langle i,j \rangle,\sigma} f^\dagger_{i\sigma} f_{j\sigma} + \Delta_{ij} f_{i\uparrow} f_{j\downarrow} + \text{h.c.}$$

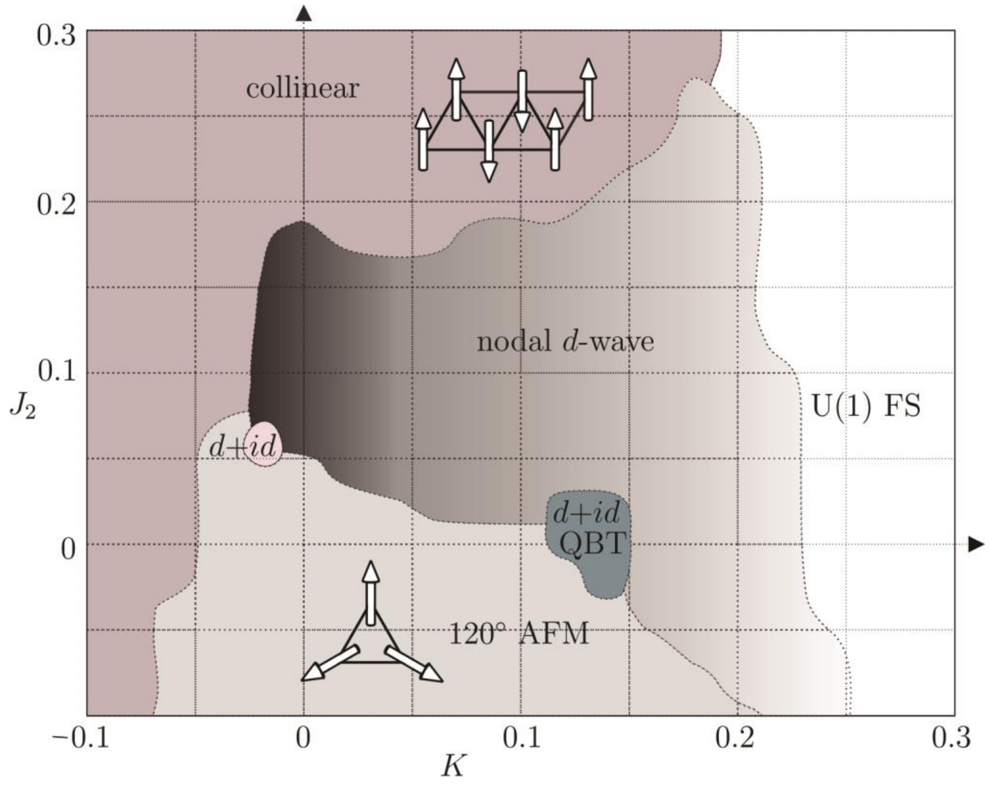
  Various pairing fields Δ:
  s-wave, d-wave, d+id-wave (singlet)
  p, p+ip, f-wave (triplet), finite-momentum pairing (amperean), …
- Symmetry-broken; ordered states: $$H_0 = \sum_{\langle i,j \rangle,\sigma} f^\dagger_{i\sigma} f_{j\sigma} - \sum_j \boldsymbol{S}_j \cdot \boldsymbol{h}_j$$ (spin-density wave)

(check various known ordering vectors, spiral states; in-plane spins only!)

$$e^{-\sum_{i,j} \gamma_{ij} S^z_i S^z_j} \prod_j |\sigma_j\rangle$$ (Huse-Elser type)

Variational phase diagram

$$H = \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + K/2 \sum_{\langle i,j,k,l \rangle} \{P_{ijkl} + \text{h.c.}\}$$



- Consistency checks
  - Neel state near J_2=K=0.
  - Collinear/columnar order as J_2>0.15 [Jolicoeur 90; Lecheminant 95].
  - Competitive nodal d-wave state when K>0, J_2>0 [Grover 10].
  - Gapless U(1) spin liquid as K>0.2 [Sheng 09, Block 11]
- New spin liquid with quadratic bands touching (d+id QBT):
  - Pure d+id pairing ($|\Delta| \to \infty$)
  - Z_2 liquid; no gauge fluctuations
  - Gapless spinon excitations at k=0
  - Finite spinon density of states: $C_M = \gamma T$

    $\chi_0 \simeq \text{cst.}$

Nickel (spin S=1) candidate

[Balicas et al., PRL 107, 197204 (2011)]:

- $Ba_3NiSb_2O_9$
- Pressure-induced structural transition; triangular plains of spin S=1; ("6H-B" phase)
- $\Theta_{cw} \approx 80$ K (AF)
- No ordering observed down to 350 mK
- Linear-T specific heat, constant spin susceptibility

→ gapless QSL !?

In a spin-1 magnet ?

Spin-1 parton construction

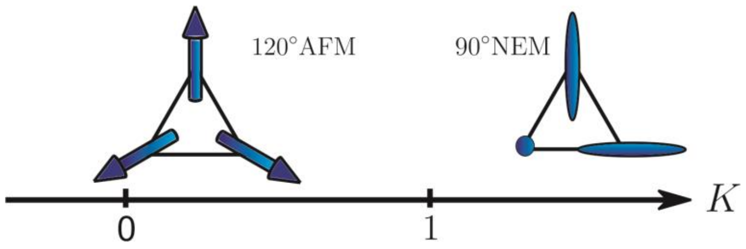
- Three fermionic partons for spin S = 1: $\boldsymbol{S} = i\boldsymbol{f}^\dagger \times \boldsymbol{f}$, $\boldsymbol{f} = (f_x, f_y, f_z)$
- Local U(1) symmetry: $\boldsymbol{f} \mapsto e^{i\alpha}\boldsymbol{f}$
- Projection to one fermion per site gives physical spin 1 state
- States:
  - U(1) Fermi surface state: $H_0 = \sum_{\langle i,j\rangle,\alpha} f_{i\alpha}^\dagger f_{j\alpha}$
  - Singlet pairing instabilities: $H_0 = \sum_{\langle i,j\rangle,\alpha} f_{i\alpha}^\dagger f_{j\alpha} + \Delta_{ij} f_{i\alpha} f_{j\alpha} + \mathrm{h.c.}$ (p+ip, f-wave)
  - Triplet pairing: $H_0 = \sum_{\langle i,j\rangle,\alpha} f_{i\alpha}^\dagger f_{j\alpha} + \sum_{\langle i,j\rangle} \Delta_{ij}^{xy} f_{ix} f_{jy} + \mathrm{h.c.}$ (s, d+id-wave)

→ Novel Z_2 QSL state, with an extended Fermi surface

[**SB**, M. Serbyn, T. Senthil, and P. A. Lee, PRB **86**, 224409 (2012)]; [Serbyn et al., 2011]

- Model with explicitly broken spin rotation symmetry:

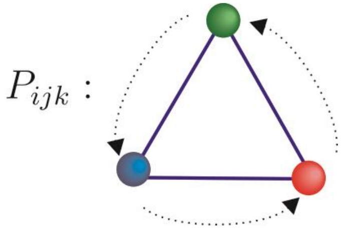
$$H = \sum_{\langle i,j \rangle} \{ \boldsymbol{S}_i \cdot \boldsymbol{S}_j + K (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 \} + D \sum_j (S_j^z)^2$$

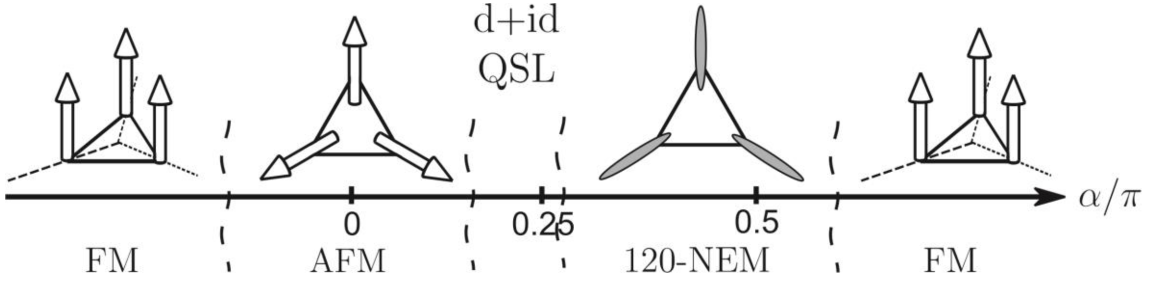


D=0 [Läuchli 06]

- SU(3) ring exchange model; spin-1 exchange op: $P_{ij} = \boldsymbol{S}_i \cdot \boldsymbol{S}_j + (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 - 1$

$$H = \cos\alpha \sum_{\langle i,j \rangle} P_{ij} + \sin\alpha \sum_{\langle i,j,k \rangle} \{ P_{ijk} + \text{h.c.} \}$$





Conclusion

- Spin-1/2:
  - We find highly competitive Z_2 spin liquid in a triangular-lattice Heisenberg model with realistically large ring-exchange term
  - The gapless QBT state is consistent with all current experimental observations
  - QBT has less issues than alternative U(1) state (theory)
- Spin-1:
  - Difficult to stabilize RVB spin liquids in triangular-lattice SU(2) Heisenberg models
  - Propose an SU(3) model that supports exotic Z_2 QSL with extended spinon Fermi surface
  - Further experiments on Ni-compound needed

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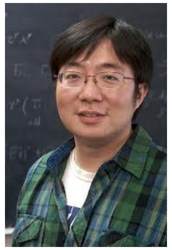


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Thank you!

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PRL 107, 197204 (2011) PHYSICAL REVIEW LETTERS week ending 4 NOVEMBER 2011

High-Pressure Sequence of $Ba_3NiSb_2O_9$ Structural Phases: New $S = 1$ Quantum Spin Liquids Based on Ni^{2+}

J. G. Cheng,[1] G. Li,[2] L. Balicas,[2] J. S. Zhou,[1] J. B. Goodenough,[1] Cenke Xu,[3] and H. D. Zhou[2,*]

6H-A

6H-B

3C