An introduction to quantum spin liquids
Part I

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From Hubbard to Heisenberg

- Zero temperature $T = 0$
- Correlated electrons on the lattice

The starting point is the Hubbard model:

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + h.c. + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow}$$

At half-filling (i.e., $N_e = N_s$) for $U \gg t$, an insulating state exists

For $U/t \to \infty$, by perturbation theory, we obtain the Heisenberg model:

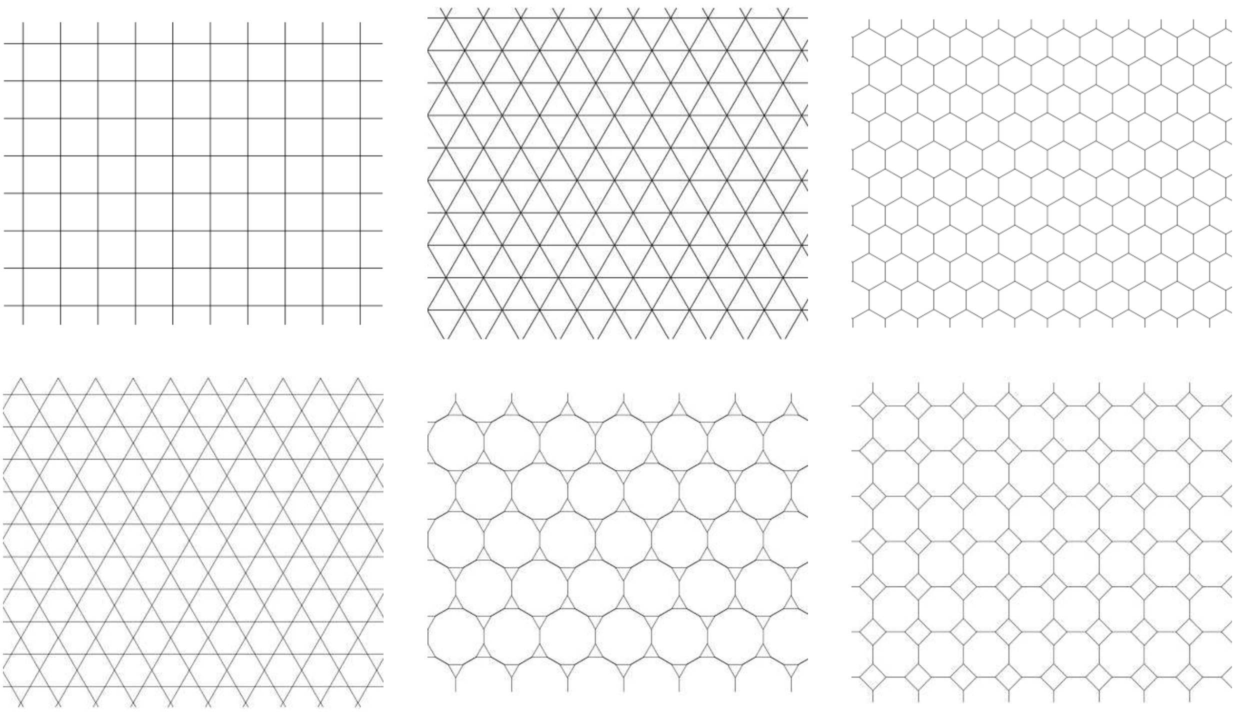
$$\mathcal{H} = \sum_{i,j} J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{i,j,k,l} (P_{i,j,k,l} + h.c.) + \dots$$

- Spin SU(2) symmetric models

> Here, I will discuss **spin models** (frozen charge degrees of freedom)
> Spin liquids in the Hubbard model (with also charge fluctuations)
> are possible, but much harder to detect

Some example for the lattice structure

Two-dimensional lattices



Simple considerations for classical spins

We want to find the lowest-energy spin configuration for classical spins
Consider the case of Bravais lattices (i.e., one site per unit cell)

$$E[\{\mathbf{S}_i\}] = \frac{1}{2} \sum_i \sum_r J(r) \mathbf{S}_i \cdot \mathbf{S}_{i+r}$$

with the *local* constraint $\mathbf{S}_i^2 = 1$
By Fourier transform:

$$E = \frac{1}{2} \sum_k J(k) \mathbf{S}_k \cdot \mathbf{S}_{-k}$$

Look for solutions with the *global* constraint: $\sum_i \mathbf{S}_i^2 = N \longrightarrow \sum_k \mathbf{S}_k \cdot \mathbf{S}_{-k} = N$

Assume $J(k)$ minimized for $k = k_0$

Take $\mathbf{S}_k = 0$ for all k's except for $k = \pm k_0$

$$\mathbf{S}_{k_0} = \frac{\sqrt{N}}{2} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix} \qquad \mathbf{S}_{-k_0} = \mathbf{S}^*_{k_0} = \frac{\sqrt{N}}{2} \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix}$$

Simple considerations for classical spins

$$\mathbf{S}_i = \frac{1}{\sqrt{N}} \left(\mathbf{S}_{k_0} e^{i k_0 r_i} + h.c. \right) = \{\cos(k_0 r_i), \sin(k_0 r_i), 0\}$$

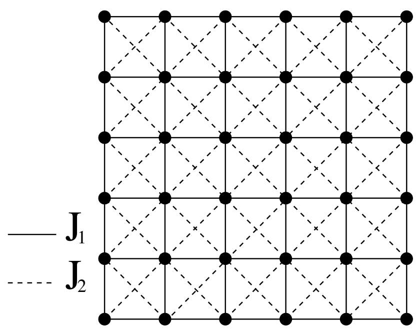
The *local* constraint is automatically satisfied!

Spiral configuration (in general non-collinear – coplanar)

Example: Classical $J_1 - J_2$ model on the square lattice

$J(k) = 2J_1 (\cos k_x + \cos k_y) + 4J_2 \cos k_x \cos k_y$

- For $J_2/J_1 < 1/2$, $k_0 = (\pi, \pi)$
- For $J_2/J_1 > 1/2$, $k_0 = (\pi, 0)$ or $(0, \pi)$
  The two sublattices are decoupled
  (free angle between spins in A and B sublattices)
- For $J_2/J_1 = 1/2$, $k_0 = (\pi, k_y)$ or (k_x, π)
  highly-degenerate ground state:
  $\mathcal{H} = \text{const.} + \sum_{\text{plaquettes}} (\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2$



Quantum fluctuations

In order to include the quantum fluctuations, perform a $1/S$ expansion

$$\mathcal{H} = \sum_{i,j} J_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j$$

- Let us denote by $\theta_j = k_0 \cdot r_j$
- Make a rotation around the z axis

$$\begin{cases} \tilde{S}_j^x = \cos\theta_j S_j^x + \sin\theta_j S_j^y \\ \tilde{S}_j^y = -\sin\theta_j S_j^x + \cos\theta_j S_j^y \\ \tilde{S}_j^z = S_j^z \end{cases}$$

- Perform the Holstein-Primakoff transformations:

$$\begin{cases} \tilde{S}_j^x = S - a_j^\dagger a_j \\ \tilde{S}_j^y \simeq \sqrt{\frac{S}{2}} \left(a_j^\dagger + a_j \right) \\ \tilde{S}_j^z \simeq i\sqrt{\frac{S}{2}} \left(a_j^\dagger - a_j \right) \end{cases}$$

Quantum fluctuations

At the leading order in $1/S$, we obtain:

$$\mathcal{H}_{\rm sw} = {\rm E}_{\rm cl} + \frac{S}{2} \sum_k \left\{ A_k a_k^\dagger a_k + \frac{B_k}{2} \left(a_k^\dagger a_{-k}^\dagger + a_{-k} a_k \right) \right\}$$

Where:

$$\mathrm{E}_{\rm cl} = \frac{1}{2} N S^2 J_{k_0}$$

$$\begin{cases} A_k = J_k + \frac{1}{2}(J_{k+k_0} + J_{k-k_0}) - 2J_{k_0} \\ B_k = \frac{1}{2}(J_{k+k_0} + J_{k-k_0}) - J_k \end{cases}$$

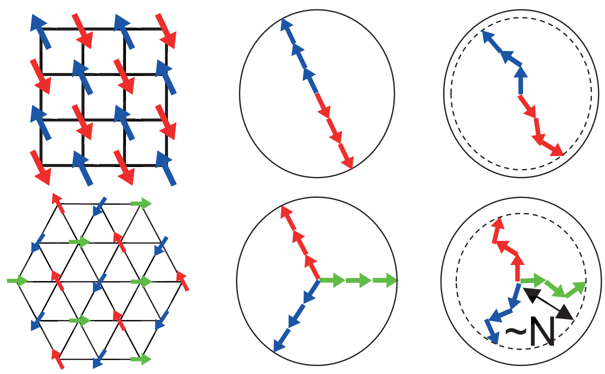
By performing a Bogoliubov transformation:

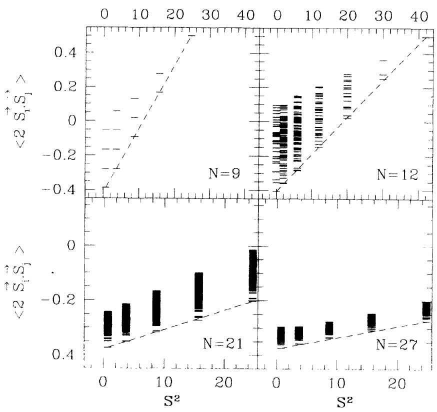
$$\mathcal{H}_{sw} = \mathrm{E}_{\rm cl} + \sum_k \omega_k (\alpha_k^\dagger \alpha_k + \tfrac{1}{2})$$

- Zero-point quantum fluctuations
- Leading-order corrections to the magnetization $\langle \tilde{S}_j^x \rangle = S - \langle a_j^\dagger a_j \rangle$

“Renormalization” of the classical state

The classical ground state is “dressed” by quantum fluctuations





- The lattice breaks up into sublattices
- Each sublattice keeps an extensive magnetization

- Spontaneously broken SU(2) symmetry
  Goldstone theorem
  Gapless spin waves ($S = 1$)

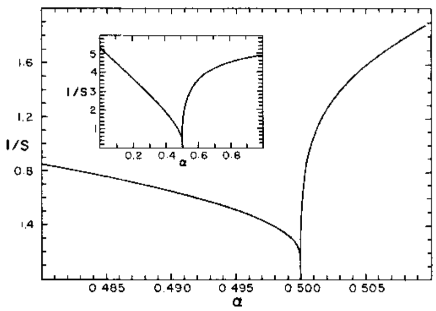
Anderson, Phys. Rev. **86**, 694 (1952)

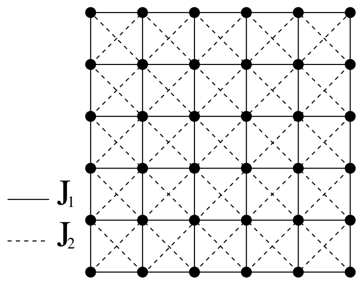
Bernu, Lhuillier, and Pierre, Phys. Rev. Lett. **69**, 2590 (1992)

Bernu, Lecheminant, Lhuillier, and Pierre, Phys. Rev. B **50**, 10048 (1994)

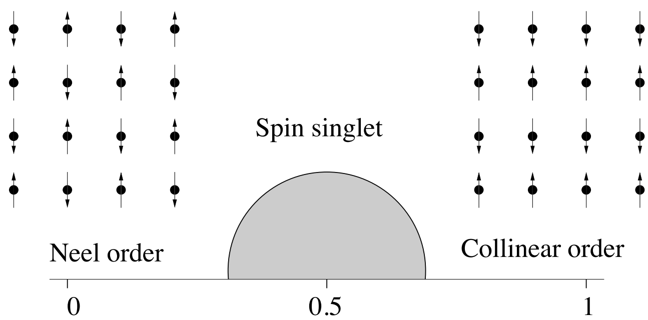
Absence of magnetic order in the strongly frustrated regime

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





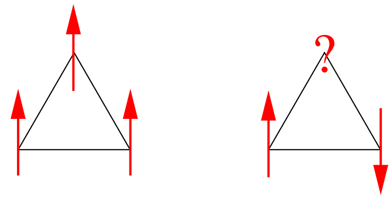
Chandra and Doucot, Phys. Rev. B **38**, 9335 (1988)



Mechanisms to destroy the long-range order

We have to stay away from the classical limit

- Small value of the spin S, e.g., $S = 1/2$ or $S = 1$
- Frustration of the super-exchange interactions
  (not all terms of the energy can be optimized simultaneously)



- Low spatial dimensionality
  In $D = 1$ there is no magnetic order, given the Mermin-Wagner theorem
  (not possible to break a continuous symmetry in D=1, even at $T = 0$)
  $D = 2$ is the "best" choice
- [Large continuous rotation symmetry group, e.g., SU(2), SU(N) or Sp(2N)]

Arovas and Auerbach, Phys. Rev. B **38**, 316 (1988); Arovas and Auerbach, Phys. Rev. Lett. **61**, 617 (1988)

Read and Sachdev, Phys. Rev. Lett. **66**, 1773 (1991); Read and Sachdev, Nucl. Phys. **B316**, 609 (1989)

A SL is a state without long-range magnetic order

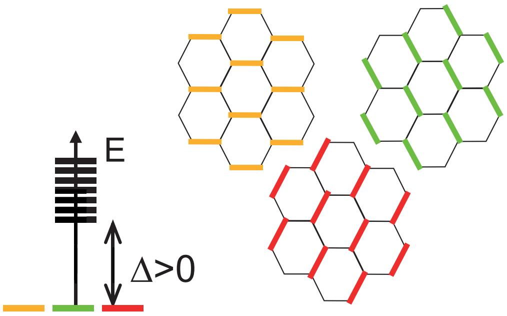
A spin liquid is a state without magnetic order
the structure factor $S(q)$ does not diverge, whatever the q is

$$S(q) = \frac{1}{N} \langle \Psi_0 | \left| \sum_j \mathbf{S}_j e^{iqr_j} \right|^2 | \Psi_0 \rangle = \frac{1}{N} \sum_{j,k} \langle \Psi_0 | \mathbf{S}_j \cdot \mathbf{S}_k | \Psi_0 \rangle e^{iq(r_j - r_k)}$$

$$S(q) = \begin{cases} O(1) & \text{for all q's} \quad \rightarrow \text{short-range correlations} \\ S(q_0) \propto N & \text{for} q = q_0 \quad \rightarrow \text{long-range order} \end{cases}$$

- Can be checked by using Neutron scattering
- Mermin-Wagner theorem implies that *any* 2D Heisenberg model at $T > 0$ is a SL according to this definition

A SL is a state without long-range magnetic order

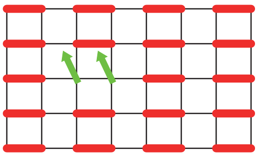


$J_1 - J_2$ Heisenberg model on the hexagonal lattice

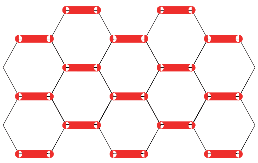
Fouet, Sindzingre, and Lhuillier, Eur. Phys. J. B **20**, 241 (2001)

Properties:

- Short-range spin-spin correlations
- Spontaneous breakdown of some lattice symmetries → ground-state degeneracy
- Gapped $S = 1$ excitations ("magnons" or "triplons")

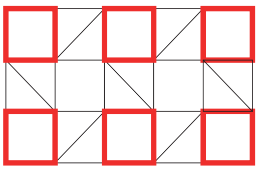


Valence-bond crystals, examples in 2D from numerical calculations



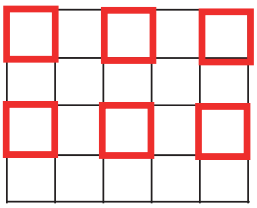
$J_1 - J_2$ model

Fouet, Sindzingre, and Lhuillier, EPJB (2001)



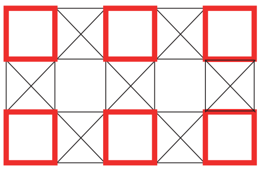
Shastry-Sutherland lattice

Koga and Kawakami, PRL (2000)



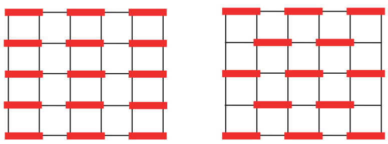
$J_1 - J_2 - J_3$ model

Mambrini, Lauchli, Poilblanc, and Mila, PRB (2006)



Heisenberg model on the Checkerboard lattice

Fouet, Mambrini, Sindzingre, and Lhuillier, PRB (2003)



Heisenberg model with a 4-spin ring exchange

Lauchli, Domenge, Lhuillier, Sindzingre, and Troyer, PRL (2005)

+ **others...**

Spin liquid: a second definition

A spin liquid is a state without any spontaneously broken (local) symmetry

- This definition rules out magnetically ordered states that break spin SU(2) symmetry (also NEMATIC states)
- This definition rules out valence-bond crystals that break some lattice symmetries

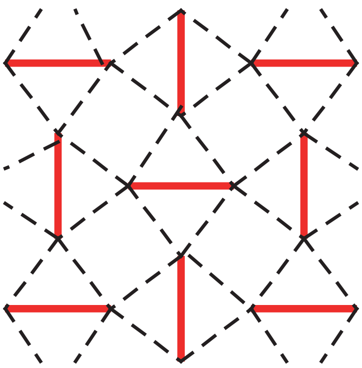
Remark I: "local" means that there is a *physical* order parameter that can be measured by some local probe

Remark II: within this definition we also rule out CHIRAL SLs that break time-reversal symmetries

Wen, Wilczek, and Zee, Phys. Rev. B **39**, 11413 (1989)

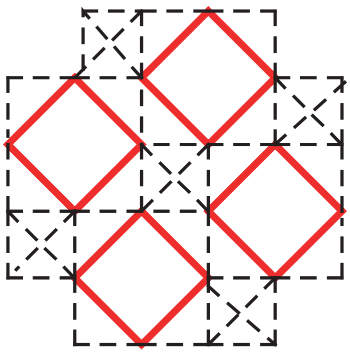
Quantum paramagnets

There are few examples of magnetic insulators without any broken symmetry



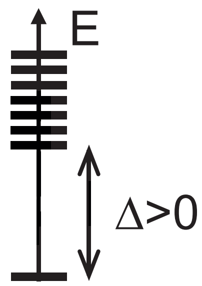
$SrCu_2(BO_3)_2$

Kageyama et al., Phys. Rev. Lett. **82**, 3168 (1999)



CaV_4O_9

Taniguchi et al., J. Phys. Soc. Jpn. **64**, 2758 (1995)

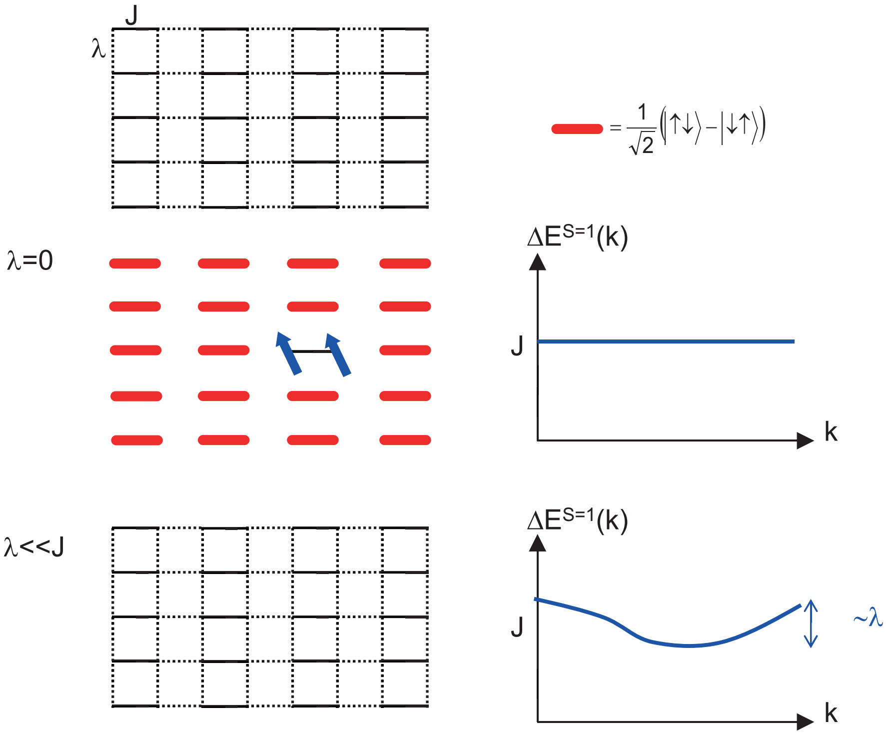


Non-degenerate ground state

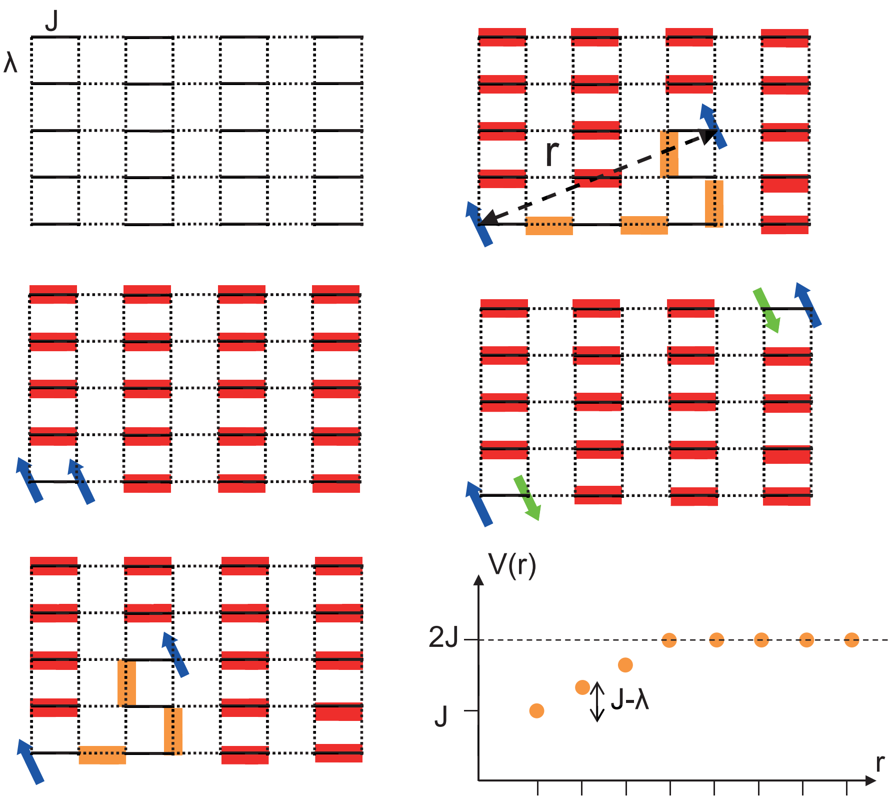
Properties:

- No broken symmetries
- Even number of spin-1/2 in the unit cell
- Adiabatically connected to the (trivial) limit of decoupled blocks
- No phase transition between $T = 0$ and $T = \infty$
  $\rightarrow$ "simple" quantum paramagnet at $T = 0$

Quantum paramagnets:excitation spectrum



Quantum paramagnets and VBCs are not fractionalized



The Lieb-Schultz-Mattis et al. theorem

A system with half-odd-integer spin in the unit cell cannot have a gap and a unique ground state

Valid in the thermodynamic limit for periodic boundary conditions and
$L_1 \times L_2 \times \cdots L_D = odd$

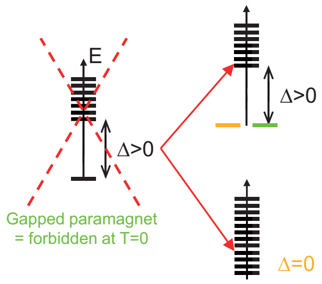
- The original theorem by Lieb, Schultz, and Mattis refers to 1D

Lieb, Schultz, Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); see also, Affleck and Lieb, Lett. Math. Phys. **12**, 57 (1986)

- Since then, several attempts to generalize it in 2D

Affleck, Phys. Rev. B **37**, 5186 (1988); Bonesteel, Phys. Rev. B **40**, 8954 (1989);

Oshikawa, Phys. Rev. Lett. **84**, 1535 (2000); Hastings, Phys. Rev. B **69**, 104431 (2004)



Case 1) Ground-state degeneracy
a) Valence-bond crystal
b) Resonating-valence bond SL
(gapped but with a topological degeneracy)
Case 2) Gapless spectrum
a) Continuous broken symmetry (magnetic order)
b) Resonating-valence bond SL
(gapless, i.e., critical state)

Proof of the Lieb-Shultz-Mattis theorem for the Heisenberg chain

- Consider the Heisenberg model on a chain:

$$\mathcal{H} = \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

with periodic boundary conditions ($\mathbf{S}_{N+1} \equiv \mathbf{S}_1$), even N, and half-odd integer spins

Theorem:
There exists an excited state with an energy that vanishes as $N \to \infty$

- $|\Psi_0\rangle$ is the ground state of $\mathcal{H}$ with energy E_0.
- Assume that $|\Psi_0\rangle$ is a singlet ("almost" always the case)
- Consider the twist operator $\mathcal{O} = \exp\{\frac{2\pi i}{N} \sum_{j=1}^{N} j S_j^z\}$
- Denote $|\Psi_1\rangle = \mathcal{O}|\Psi_0\rangle$

Then:

(1) $\langle \Psi_1 | \Psi_0 \rangle = 0$
(2) $\lim_{N\to\infty} [\langle \Psi_1 | \mathcal{H} | \Psi_1 \rangle - E_0] = 0$

Proof of the Lieb-Shultz-Mattis theorem in 1D

Consider the translation operator $\mathcal{T}$:

$$\mathcal{T}\mathbf{S}_j\mathcal{T}^{-1} = \mathbf{S}_{j+1} \qquad \mathcal{T}\mathbf{S}_N\mathcal{T}^{-1} = \mathbf{S}_1$$

$$[\mathcal{H},\mathcal{T}] = 0 \qquad \mathcal{T}|\Psi_0\rangle = e^{ik_0}|\Psi_0\rangle$$

$\langle\Psi_0|\Psi_1\rangle = \langle\Psi_0|\mathcal{O}|\Psi_0\rangle = \langle\Psi_0|\mathcal{T}\mathcal{O}\mathcal{T}^{-1}|\Psi_0\rangle$

$\mathcal{T}\mathcal{O}\mathcal{T}^{-1} = \mathcal{O}\exp\left(2\pi i S_1^z\right)\exp\left(-\frac{2\pi i}{N}S^z_{\text{tot}}\right)$

Then, $\exp\left(-\frac{2\pi i}{N}S^z_{\text{tot}}\right)|\Psi_0\rangle = |\Psi_0\rangle$, since $|\Psi_0\rangle$ is a singlet.

$$\exp\left(2\pi i S_1^z\right) = \begin{cases} +1 & S = 0,1,2,\cdots \\ -1 & S = 1/2, 3/2, 5/2, \cdots \end{cases}$$

- Therefore, for half-odd integer spin: $\langle\Psi_0|\Psi_1\rangle = -\langle\Psi_0|\Psi_1\rangle$

$\langle\Psi_1|\mathcal{H}|\Psi_1\rangle = E_0 + \langle\Psi_0|\{\cos(\frac{2\pi}{N}) - 1\}\sum_{j=1}^N (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y)|\Psi_0\rangle$

$\langle\Psi_0|(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y)|\Psi_0\rangle \leq S^2$

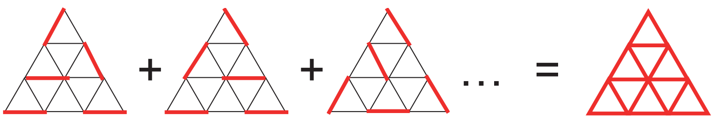
- We obtain an upper-bound for the energy: $\langle\Psi_1|\mathcal{H}|\Psi_1\rangle - E_0 \leq \frac{2\pi^2 J S^2}{N} + O(N^{-3})$

The short-range RVB picture

- Anderson's idea: the short-range resonating-valence bond (RVB) state:

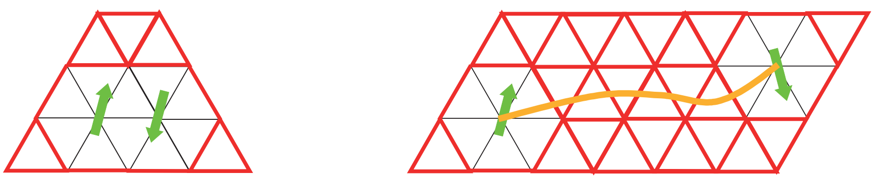
  Anderson, Mater. Res. Bull. **8**, 153 (1973)

  Linear superposition of many (an exponential number) of valence-bond configurations

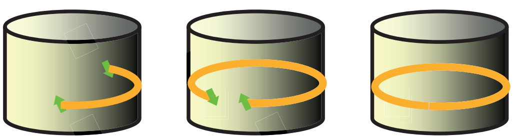


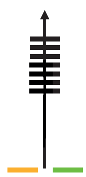
Spatially uniform state

- Spin excitations? No dimer order → we may have deconfined spinons



- Spinon fractionalization and topological degeneracy





Distinct ground states that are not connected by any local operator

Wen, Phys. Rev. B **44**, 2664 (1991); Oshikawa and Senthil, Phys. Rev. Lett. **96**, 060601 (2006)

Spin liquid: a third definition

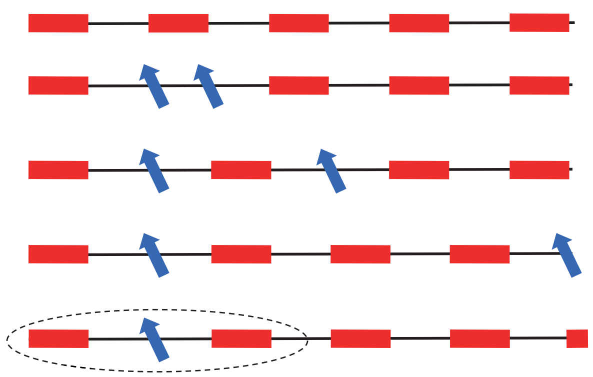
A spin liquid is a state without any spontaneously broken (local) symmetry, with a half-odd-integer spin in the unit cell

- This definition rules out magnetically ordered states that break spin SU(2) symmetry (also NEMATIC states)
- This definition rules out valence-bond crystals that break some lattice symmetries
- This definition rules out quantum paramagnets that have an even number of spin-half per unit cell

A spin liquid sustains fractional (spin-1/2) excitations

What is fractionalization?

- Majumdar-Gosh chain (1D): $\mathcal{H} = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J}{2} \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}$
- The exact ground state is known (two-fold degenerate), perfect dimerization



The "initial" $S = 1$ excitation can decay into two spatially separated spin-1/2 excitations (spinons)

Finite-energy state with an isolated spinon (the other is far apart) domain wall between two dimerization patterns

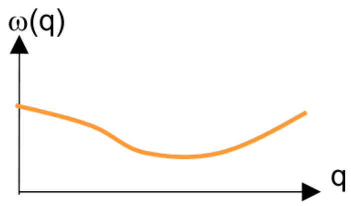
- A spinon is a neutral spin-1/2 excitation, "one-half" of a $S = 1$ spin flip. (it has the same spin as the electron, but no charge)
- Spinons can only be created by pairs in finite systems. The question is to understand whether they can propagate at large distances, as two elementary particles

Inelastic neutron scattering: spinon continuum

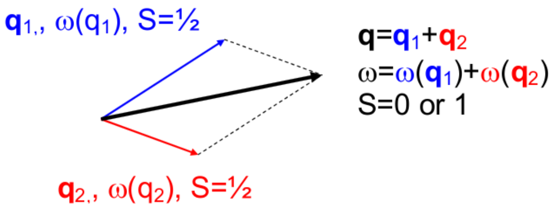
The inelastic neutron scattering is a probe for the dynamical structure factor

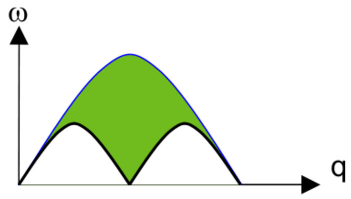
$$S(q,\omega) = \int dt \langle \Psi_0 | S^-_{-q}(t) S^+_q(0) | \Psi_0 \rangle e^{-i\omega t}$$

- The elementary excitations are spin-1 magnons: $S(q,\omega)$ has a single-particle pole at $\omega = \omega(q)$



- The spin-flip decays into two spin-1/2 excitations $S(q,\omega)$ exhibits a two-particle continuum

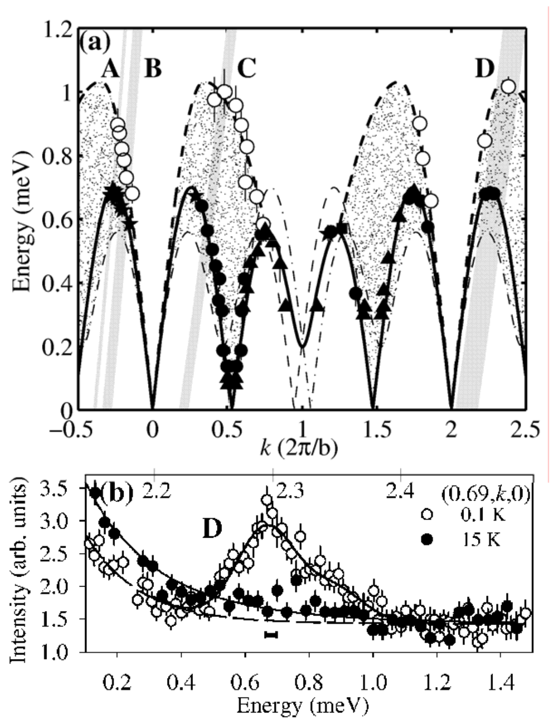




Inelastic neutron scattering: spinon continuum

Neutron scattering on Cs_2CuCl_4

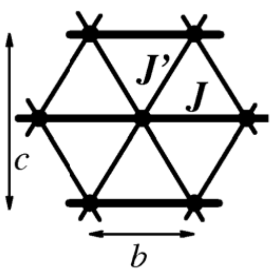
Coldea, Tennant, Tsvelik, and Tylczynski, Phys. Rev. Lett. **86**, 1335 (2001)



Almost decoupled layers

Strongly-anisotropic triangular lattice

$J' \simeq 0.33J$: **quasi-1D**



An introduction to quantum spin liquids
Part II

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Istituto Officina dei Materiali

1. Mean-field approaches to spin liquids
   - Non-standard mean-field approaches to spin-liquid phases
   - Fermionic representation of a spin-1/2
   - Projective symmetry group (PSG)

2. Beyond the mean-field approaches
   - "Low-energy" gauge fluctuations
   - Variational Monte Carlo for fermions

3. Numerical results
   - An example: the Heisenberg model on the Kagome lattice

Standard mean-field approach

Consider the spin-1/2 Heisenberg model on a generic lattice

$$\mathcal{H} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

In a standard mean-field approach, each spin couples to an effective field generated by the surrounding spins:

$$\mathcal{H}_{\rm MF} = \sum_{ij} J_{ij} \left\{ \langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle \right\}$$

However, by definition, spin liquids have a zero magnetization:

$$\langle \mathbf{S}_i \rangle = 0$$

How can we construct a mean-field approach for such disordered states?

We need to construct a theory in which all classical order parameters are vanishing

Halving the spin operator

- The first step is to decompose the pin operator in terms of spin-1/2 quasi-particles creation and annihilation operators.
- One possibility is to write:

$$S_i^\mu = \frac{1}{2} c_{i,\alpha}^\dagger \sigma_{\alpha,\beta}^\mu c_{i,\beta}$$

$\sigma_{\alpha,\beta}^\mu$ are the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$c_{i,\alpha}^\dagger$ ($c_{i,\beta}$) creates (destroys) a quasi-particle with spin-1/2
These may have various statistics, e.g., bosonic or fermionic

At this stage, splitting the original spin operator in two pieces is just a formal trick.
Whether or not these quasi-particles are true elementary excitations is THE question

Fermionic representation of a spin-1/2

- A faithful representation of spin-1/2 is given by:

$$
\begin{aligned}
S_i^z &= \frac{1}{2}\left(c_{i,\uparrow}^\dagger c_{i,\uparrow} - c_{i,\downarrow}^\dagger c_{i,\downarrow}\right) \\
S_i^+ &= c_{i,\uparrow}^\dagger c_{i,\downarrow} \\
S_i^- &= c_{i,\downarrow}^\dagger c_{i,\uparrow}
\end{aligned}
$$

$\{c_{i,\alpha}, c_{j,\beta}^\dagger\} = \delta_{ij}\delta_{\alpha\beta}$
$\{c_{i,\alpha}, c_{j,\beta}\} = 0$
$c_{i,\uparrow}^\dagger$ (or $c_{i,\downarrow}^\dagger$) changes S_i^z by 1/2 (or $-1/2$) and creates a "spinon"

- For a model with one spin per site, we must impose the constraints:

$$c_{i,\uparrow}^\dagger c_{i,\uparrow} + c_{i,\downarrow}^\dagger c_{i,\downarrow} = 1 \qquad c_{i,\uparrow} c_{i,\downarrow} = 0$$

- Compact notation by using a 2×2 matrix:

$$\Psi_i = \begin{bmatrix} c_{i,\uparrow} & c_{i,\downarrow}^\dagger \\ c_{i,\downarrow} & -c_{i,\uparrow}^\dagger \end{bmatrix} \qquad S_i^\mu = -\frac{1}{4}\mathrm{Tr}\left[\sigma^\mu \Psi_i \Psi_i^\dagger\right] \qquad G_i^\mu = \frac{1}{4}\mathrm{Tr}\left[\sigma^\mu \Psi_i^\dagger \Psi_i\right] = 0$$

Local redundancy and "gauge" transformations

$$S_i^\mu = -\frac{1}{4}\mathrm{Tr}\left[\sigma^\mu \Psi_i \Psi_i^\dagger\right]$$

$$\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{16}\sum_\mu \mathrm{Tr}\left[\sigma^\mu \Psi_i \Psi_i^\dagger\right] \mathrm{Tr}\left[\sigma^\mu \Psi_j \Psi_j^\dagger\right] = \frac{1}{8}\mathrm{Tr}\left[\Psi_i \Psi_i^\dagger \Psi_j \Psi_j^\dagger\right]$$

- Spin rotations are left rotations:

$$\Psi_i \to R_i \Psi_i$$

The Heisenberg Hamiltonian is invariant under global rotations

- The spin operator is invariant upon local SU(2) "gauge" transformations, right rotations:

$$\Psi_i \to \Psi_i W_i$$

$$\mathbf{S}_i \to \mathbf{S}_i$$

There is a huge redundancy in this representation

Affleck, Zou, Hsu, and Anderson, Phys. Rev. B **38**, 745 (1988)

Mean-field approximation

- We transformed a spin model into a model of interacting fermions (subject to the constraint of one-fermion per site)
- The first approximation to treat this problem is to consider a mean-field decoupling:

$$\Psi_i^\dagger \Psi_j \Psi_j^\dagger \Psi_i \to \langle \Psi_i^\dagger \Psi_j \rangle \Psi_j^\dagger \Psi_i + \Psi_i^\dagger \Psi_j \langle \Psi_j^\dagger \Psi_i \rangle - \langle \Psi_i^\dagger \Psi_j \rangle \langle \Psi_j^\dagger \Psi_i \rangle$$

We define the mean-field 2×2 matrix

$$U_{ij}^0 = \frac{J_{ij}}{4} \langle \Psi_i^\dagger \Psi_j \rangle = \frac{J_{ij}}{4} \begin{bmatrix} \langle c_{i,\uparrow}^\dagger c_{j,\uparrow} + c_{i,\downarrow}^\dagger c_{j,\downarrow} \rangle & \langle c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + c_{j,\uparrow}^\dagger c_{i,\downarrow}^\dagger \rangle \\ \langle c_{i,\downarrow} c_{j,\uparrow} + c_{j,\downarrow} c_{i,\uparrow} \rangle & -\langle c_{j,\downarrow}^\dagger c_{i,\downarrow} + c_{j,\uparrow}^\dagger c_{i,\downarrow} \rangle \end{bmatrix} = \begin{bmatrix} \chi_{ij} & \eta_{ij}^* \\ \eta_{ij} & -\chi_{ij}^* \end{bmatrix}$$

- $\chi_{ij} = \chi_{ji}^*$ is the spinon hopping
- $\eta_{ij} = \eta_{ji}$ is the spinon pairing

Mean-field approximation

The mean-field Hamiltonian has a BCS-like form:

$$\mathcal{H}_{MF} = \sum_{ij} \chi_{ij} (c_{j,\uparrow}^\dagger c_{i,\downarrow} + c_{j,\downarrow}^\dagger c_{i,\downarrow}) + \eta_{ij} (c_{j,\uparrow}^\dagger c_{i,\downarrow}^\dagger + c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger) + h.c.$$

$$+ \sum_i \lambda_i \, (c_{i,\uparrow}^\dagger c_{i,\uparrow} + c_{i,\downarrow}^\dagger c_{i,\downarrow} - 1) + \sum_i \zeta_i \; c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger + h.c.$$

- $\{\chi_{ij}, \eta_{ij}, \lambda_i, \zeta_i\}$ define the mean-field Ansatz
- At the mean-field level:
  - χ_{ij} and η_{ij} are fixed numbers
  - Constraints are satisfied only in average

At the mean-field level, spinons are free.
Beyond this approximation, they will interact with each other
Do they remain asymptotically free (at low energies)?

Redundancy of the mean-field approximation

- Let $|\Phi_{MF}(U_{ij}^0)\rangle$ be the ground state of the mean-field Hamiltonian (with a given Ansatz for the mean-field U_{ij}^0)
- $|\Phi_{MF}(U_{ij}^0)\rangle$ cannot be a valid wave function for the spin model (its Hilbert space is wrong, it has not one fermion per site!)
- Let us consider an arbitrary *site-dependent* SU(2) matrix W_i (gauge transformation)

$$\Psi_i \to \Psi_i W_i$$

Leaves the spin unchanged $\mathbf{S}_i \to \mathbf{S}_i$.

$$U_{ij}^0 \to W_i^\dagger U_{ij}^0 W_j$$

- Therefore, U_{ij}^0 and $W_i^\dagger U_{ij}^0 W_j$ define the same physical state (the same physical state can be represented by many different Ansätze U_{ij}^0)

$$\langle 0| \prod_i c_{i,\alpha_i} |\Phi_{MF}(U_{ij}^0)\rangle = \langle 0| \prod_i c_{i,\alpha_i} |\Phi_{MF}(W_i^\dagger U_{ij}^0 W_j)\rangle$$

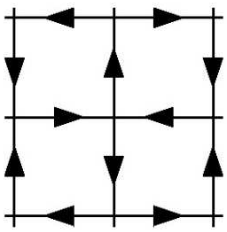
An example of the redundancy on the square lattice

- The staggered flux state is defined by

Affleck and Marston, Phys. Rev. B **37**, 3774 (1988)

$$j \in A \begin{cases} \chi_{j,j+x} = e^{i\Phi_0/4} \\ \chi_{j,j+y} = e^{-i\Phi_0/4} \end{cases}$$

$$j \in B \begin{cases} \chi_{j,j+x} = e^{-i\Phi_0/4} \\ \chi_{j,j+y} = e^{i\Phi_0/4} \end{cases}$$



- The d-wave "superconductor" state is defined by

Baskaran, Zou, and Anderson, Solid State Commun. **63**, 973 (1987)

$$\begin{cases} \chi_{j,j+x} = 1 \\ \chi_{j,j+y} = 1 \\ \eta_{j,j+x} = \Delta \\ \eta_{j,j+y} = -\Delta \end{cases}$$

- For $\Delta = \tan(\Phi_0/4)$, these two mean-field states become the same state after projection
- The mean-field spectrum is the same for the two states (it is invariant under SU(2) transformations)

Projective symmetry group (PSG)

- Ansätze that differ by a gauge transformation describe the same physical state
- This redundancy has important consequences on the structure of the fluctuations above the mean-field Ansatz
- A non-fully-symmetric mean-field Ansatz U^0_{ij} (that e.g. breaks translational symmetry) may correspond to a fully-symmetric physical state

  Let us define a generic lattice symmetry (translations, rotations, reflections) by T:

$$TU^0_{ij} = U_{T(i)T(j)} \neq U_{ij}$$

  but still the physical state may have all lattice symmetries.
  Indeed, we can still play with gauge transformations.
- To have a fully-symmetric physical state, a gauge transformation G_i must exist, such that

$$G_i^\dagger T U^0_{ij} G_j = G_i^\dagger U^0_{T(i)T(j)} G_j \equiv U^0_{ij}$$

$\{T, G\}$ define the PSG:
for each lattice symmetry T, there is an associated gauge symmetry G

Wen's conjecture on quantum order

- In general, the PSG is not trivial
  (the set of gauge transformations G associated to lattice symmetries T is non-trivial)
- Distinct spin liquids have the same lattice symmetries (i.e., they are totally symmetric), but different PSGs
- Wen proposed to use the PSG to characterize quantum order in spin liquids
- As in the Landau's theory for classical orders, where symmetries define various phases, the PSG can be used to classify spin liquids
  (the PSG of an Ansatz is a universal property of the Ansatz)

Although Ansätze for different spin liquids have the same symmetry, the Ansätze are invariant under different PSG. Namely different sets of gauge transformations associated to lattice symmetries

Wen, Phys. Rev. B **65**, 165113 (2002)

"Low-energy" gauge fluctuations

- The SU(2) gauge structure

$$\Psi_i \to \Psi_i W_i$$

is a "high-energy" gauge structure that only depends upon our choice on how to represent the spin operator [e.g., for the bosonic representation, it is U(1)]

- What are the "relevant" gauge fluctuations above a given mean-field Ansatz U^0_{ij}?
- Wen's conjecture: the relevant "low-energy" gauge fluctuations are determined completely from the PSG
- There is an important subgroup of the PSG: the invariant gauge group (IGG). The IGG of a mean-field Ansatz is defined by the set of all pure gauge transformations that leaves the mean-field Ansatz U^0_{ij} invariant:

$$\mathcal{G}_i^\dagger U^0_{ij} \mathcal{G}_j = U^0_{ij}$$

The IGG determines the "low-energy" gauge fluctuations above the mean-field state

"Low-energy" gauge fluctuations

- Consider an Ansatz U^0_{ij} for the mean-field state
- Assume that the IGG is U(1):

$$\mathcal{G}_j = e^{i\theta_j \sigma^z} \qquad \mathcal{G}_i^\dagger U^0_{ij} \mathcal{G}_j = U^0_{ij}$$

- Consider now some fluctuations above the mean field:

$$U_{ij} = U^0_{ij} e^{iA_{ij}\sigma^z}$$

- It is possible to show that A_{ij} is a gauge field:

$$\Psi_j \to \Psi_j e^{i\theta\sigma^z} \qquad A_{ij} \to A_{ij} + \theta_i - \theta_j$$

According to the symmetry of the IGG, we can have Z_2, U(1), SU(2)... spin liquids

- In U(1) spin liquids, the spinon pairing can be gauged away

the mean-field Ansatz U^0_{ij} may contain spinon hopping only

- In Z_2 spin liquids, the spinon pairing cannot be gauged away

the SU(2) or U(1) gauge structure is lowered to Z_2 through the Anderson-Higgs mechanism

The PSG + IGG allow us to classify spin liquid phases

- Consider the square lattice and a Z_2 IGG, e.g. $\mathcal{G}_i = \pm \mathbb{I}$
- Consider the case where only translations T_x and T_y are considered
  Only two Z_2 spin liquids are possible:

$$\begin{cases} G_i(T_x) = \mathbb{I} & G_i(T_y) = \mathbb{I} \quad \to \quad U^0_{i,i+m} = U^0_m \\ G_i(T_x) = (-1)^{i_y} \mathbb{I} & G_i(T_y) = \mathbb{I} \quad \to \quad U^0_{i,i+m} = (-1)^{m_y i_x} U^0_m \end{cases}$$

- The case with also point-group and time-reversal symmetries is much more complicated
  Two classes of Z_2 spin liquids are possible:

$$\begin{aligned} G_i(T_x) &= \mathbb{I} & G_i(T_y) &= \mathbb{I} \\ G_i(P_x) &= \epsilon^{i_x}_{xpx} \epsilon^{i_y}_{xpy} g_{P_x} & G_i(P_y) &= \epsilon^{i_x}_{xpy} \epsilon^{i_y}_{xpx} g_{P_y} \\ G_i(P_{xy}) &= g_{P_{xy}} & G_i(T) &= \epsilon^i_t g_T \end{aligned}$$

$$\begin{aligned} G_i(T_x) &= (-1)^{i_y} \mathbb{I} & G_i(T_y) &= \mathbb{I} \\ G_i(P_x) &= \epsilon^{i_x}_{xpx} \epsilon^{i_y}_{xpy} g_{P_x} & G_i(P_y) &= \epsilon^{i_x}_{xpy} \epsilon^{i_y}_{xpx} g_{P_y} \\ G_i(P_{xy}) &= (-1)^{i_x i_y} g_{P_{xy}} & G_i(T) &= \epsilon^i_t g_T \end{aligned}$$

In total, 272 possibilities
At most 196 different Z_2 spin liquids!

$$g_{Pxy} = \tau^0, \quad g_{P_x} = \tau^0, \quad g_{P_y} = \tau^0, \quad g_T = \tau^0; \qquad (67)$$
$$g_{Pxy} = \tau^0, \quad g_{P_x} = i\tau^3, \quad g_{P_y} = i\tau^3, \quad g_T = \tau^0; \qquad (68)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = \tau^0, \quad g_{P_y} = \tau^0, \quad g_T = \tau^0; \qquad (69)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = i\tau^3, \quad g_{P_y} = \tau^3, \quad g_T = \tau^0; \qquad (70)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^1, \quad g_T = \tau^0; \qquad (71)$$
$$g_{Pxy} = \tau^0, \quad g_{P_x} = \tau^0, \quad g_{P_y} = \tau^0, \quad g_T = i\tau^3; \qquad (72)$$
$$g_{Pxy} = \tau^0, \quad g_{P_x} = i\tau^3, \quad g_{P_y} = i\tau^3, \quad g_T = i\tau^3; \qquad (73)$$
$$g_{Pxy} = \tau^0, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^1, \quad g_T = i\tau^3; \qquad (74)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = \tau^0, \quad g_{P_y} = \tau^0, \quad g_T = i\tau^3; \qquad (75)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = i\tau^3, \quad g_{P_y} = i\tau^3, \quad g_T = i\tau^3; \qquad (76)$$
$$g_{Pxy} = i\tau^3, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^1, \quad g_T = i\tau^3; \qquad (77)$$
$$g_{Pxy} = i\tau^1, \quad g_{P_x} = \tau^0, \quad g_{P_y} = \tau^0, \quad g_T = i\tau^3; \qquad (78)$$
$$g_{Pxy} = i\tau^1, \quad g_{P_x} = i\tau^3, \quad g_{P_y} = i\tau^3, \quad g_T = i\tau^3; \qquad (79)$$
$$g_{Pxy} = i\tau^1, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^1, \quad g_T = i\tau^3; \qquad (80)$$
$$g_{Pxy} = i\tau^1, \quad g_{P_x} = i\tau^2, \quad g_{P_y} = i\tau^2, \quad g_T = i\tau^3; \qquad (81)$$
$$g_{Pxy} = i\tau^{12}, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^2, \quad g_T = \tau^0; \qquad (82)$$
$$g_{Pxy} = i\tau^{12}, \quad g_{P_x} = i\tau^1, \quad g_{P_y} = i\tau^2, \quad g_T = i\tau^3; \qquad (83)$$

Wen, Phys. Rev. B **65**, 165113 (2002)

Fluctuations above the mean field and gauge fields

- Some results about lattice gauge theory (coupled to matter)
  may be used to discuss the stability/instability of a given mean-field Ansatz
- What is known about U(1) gauge theories?
  Monopoles proliferate → confinement
  Polyakov, Nucl. Phys. B **120**, 429 (1977)

  Spinons are glued in pairs by strong gauge fluctuations and are not physical excitations
- Deconfinement may be possible in presence of gapless matter field
  The so-called U(1) spin liquid
  Hermele et al., Phys. Rev. B **70**, 214437 (2004)
- In presence of a charge-2 field (i.e., spinon pairing) the U(1) symmetry
  can be lowered to Z_2 → deconfinement
  Fradkin and Shenker, Phys. Rev. D **19**, 3682 (1979)
- For example in D=2:
  - Z_2 gauge field (gapped) + gapped spinons may be a stable deconfined phase
    short-range RVB physics — Read and Sachdev, Phys. Rev. Lett. **66**, 1773 (1991)
  - U(1) gauge field (gapless) + gapped spinons should lead to an instability
    towards confinement and valence-bond order — Read and Sachdev, Phys. Rev. Lett. **62**, 1694 (1989)

Variational Monte Carlo for fermions

- The exact projection on the subspace with one spin per site can be treated within the variational Monte Carlo approach (part of the gauge fluctuations are considered!)

$$|\Phi\rangle = \mathcal{P}|\Phi_{MF}(U^0_{ij})\rangle$$

- The variational energy

$$E(\Phi) = \frac{\langle\Phi|\mathcal{H}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \sum_x P(x) \frac{\langle x|\mathcal{H}|\Phi\rangle}{\langle x|\Phi\rangle}$$

$P(x) \propto |\langle x|\Phi\rangle|^2$ and $|x\rangle$ is the (Ising) basis in which spins are distributed in the lattice

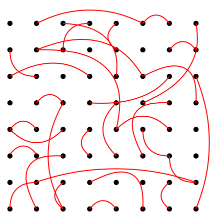
- $E(\Phi)$ can be sampled by using "classical" Monte Carlo, since $P(x) \geq 0$
- $\langle x|\Phi\rangle$ is a determinant
- The ratio of to determinants (needed in the Metropolis acceptance ratio) can be computed very efficiently, i.e., O(N), when few spins are updated
- The algorithm scales polinomially, i.e., O(N^3) to have almost independent spin configurations

The projected wave function

- The mean-field wave function has a BCS-like form

$$|\Phi_{MF}\rangle = \exp\left\{\frac{1}{2}\sum_{i,j} f_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}\right\}|0\rangle$$

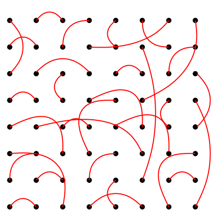
It is a linear superposition of all singlet configurations (that may overlap)

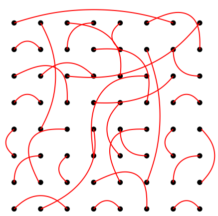


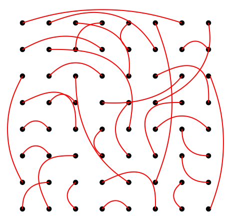
$+ \ldots$

- After projection, only non-overlapping singlets survive: the resonating valence-bond (RVB) wave function

Anderson, Science **235**, 1196 (1987)







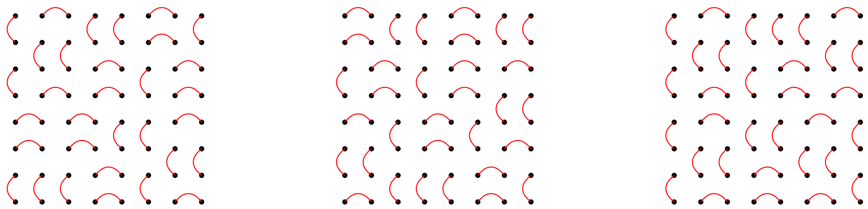
$+ \ldots$

The projected wave function

- The mean-field wave function has a BCS-like form

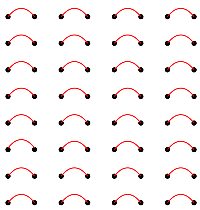
$$|\Phi_{MF}\rangle = \exp\left\{\frac{1}{2}\sum_{i,j} f_{i,j} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow}\right\}|0\rangle$$

- Depending on the pairing function $f_{i,j}$, different RVB states may be obtained...



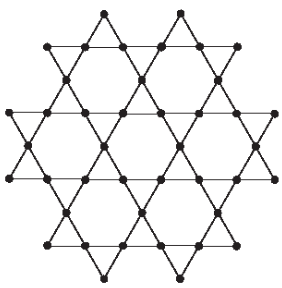
$+ \dots$

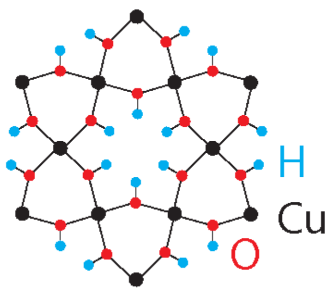
- ...even with valence-bond order (valence-bond crystals)



The Heisenberg model on the Kagome lattice

$$\mathcal{H} = J\sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle\langle ij\rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \mathrm{DM} + \mathrm{distortions} + \mathrm{3D\ couplings} + \dots$$





- No magnetic order down to 50mK (despite $T_{CW} \simeq 200$K)
- Spin susceptibility rises with $T \to 0$ but then saturates below 0.5K
- Specific heat $C_v \propto T$ below 0.5K
- No sign of spin gap in dynamical Neutron scattering measurements

Mendels *et al.*, PRL 98, 077204 (2007)

Helton *et al.*, PRL 98, 107204 (2007)

Bert *et al.*, PRB 76, 132411 (2007)

Some of the previous results

Nearest-neighbor Heisenberg model on the Kagome lattice

Author	GS proposed	Energy/site	Method used
P.A. Lee	$U(1)$ gapless SL	$-0.42866(1)J$	Fermionic VMC
Singh	36-site HVBC	$-0.433(1)J$	Series expansion
Vidal	36-site HVBC	$-0.43221\ J$	MERA
Poilblanc	12- or 36-site VBC		QDM
Lhuillier	Chiral gapped SL		SBMF
White	Z_2 gapped SL	$-0.4379(3)J$	DMRG
Schollwoeck	Z_2 gapped SL	$-0.4386(5)J$	DMRG

Ran, Hermele, Lee, and Wen, PRL **98**, 117205 (2007)

Yan, Huse, and White, Science **332**, 1173 (2011)

Schwinger fermion approach for projected wave functions

$$S_i^\mu = \frac{1}{2} c_{i,\alpha}^\dagger \sigma_{\alpha,\beta}^\mu c_{i,\beta}$$

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j,\alpha,\beta} J_{ij} \left(c_{i,\alpha}^\dagger c_{j,\alpha} c_{j,\beta}^\dagger c_{i,\beta} + \frac{1}{2} c_{i,\alpha}^\dagger c_{i,\alpha} c_{j,\beta}^\dagger c_{j,\beta} \right)$$

$$c_{i,\alpha}^\dagger c_{i,\alpha} = 1 \qquad c_{i,\alpha} c_{i,\beta} \epsilon_{\alpha\beta} = 0$$

- At the mean-field level:

$$\mathcal{H}_{\rm MF} = \sum_{i,j,\alpha} (\chi_{ij} + \mu \delta_{ij}) c_{i,\alpha}^\dagger c_{j,\alpha} + \sum_{i,j} \{ (\eta_{ij} + \zeta \delta_{ij}) c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + h.c. \}$$

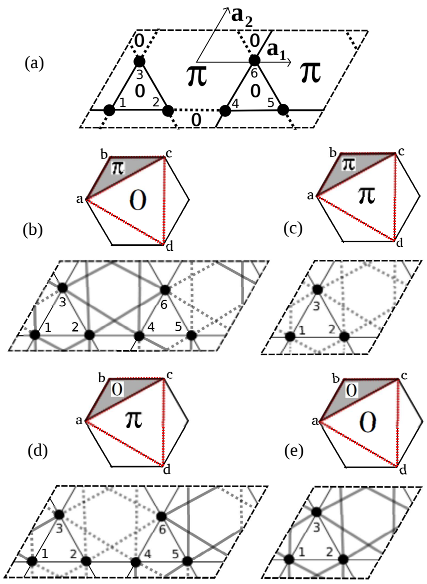
$$\langle c_{i,\alpha}^\dagger c_{i,\alpha} \rangle = 1 \qquad \langle c_{i,\alpha} c_{i,\beta} \rangle \epsilon_{\alpha\beta} = 0$$

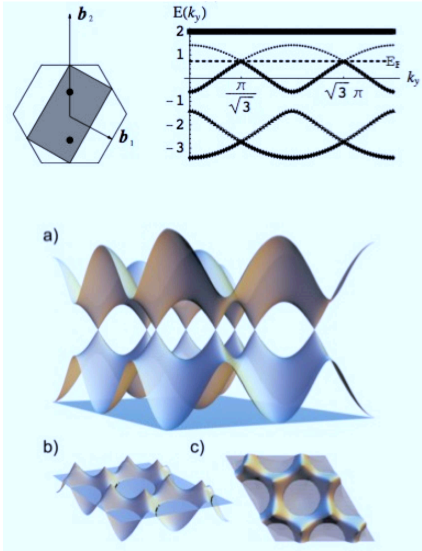
- Then, we reintroduce the constraint of one-fermion per site:

$$|\Phi(\chi_{ij}, \eta_{ij}, \mu)\rangle = \mathcal{P}_G |\Phi_{\rm MF}(\chi_{ij}, \eta_{ij}, \mu, \zeta)\rangle$$

$$\mathcal{P}_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$$

Results with projected wave functions





- The U(1) gapless (Dirac) spin liquid is a good variational Ansatz

Ran, Hermele, Lee, and Wen, PRL **98**, 117205 (2007)

- It is stable for dimerization

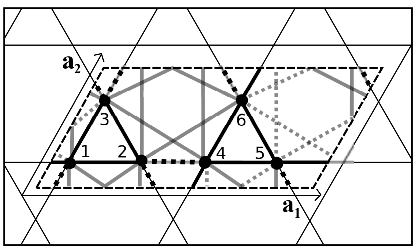
Iqbal, Becca, and Poilblanc, PRB 83, 100404 (2011); New Journal of Phys., to appear

Can we have a Z_2 gapped spin liquid (DMRG)?

Projective symmetry-group (PSG) analysis

Lu, Ran, and Lee, PRB **83**, 224413 (2011)

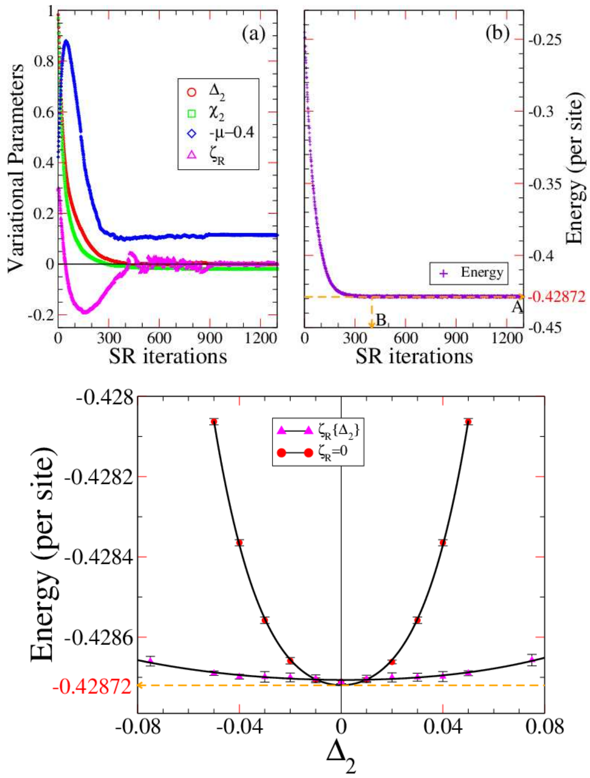
$$U^0_{ij} = \begin{pmatrix} \chi_{ij} & \eta^*_{ij} \\ \eta_{ij} & -\chi^*_{ij} \end{pmatrix}$$



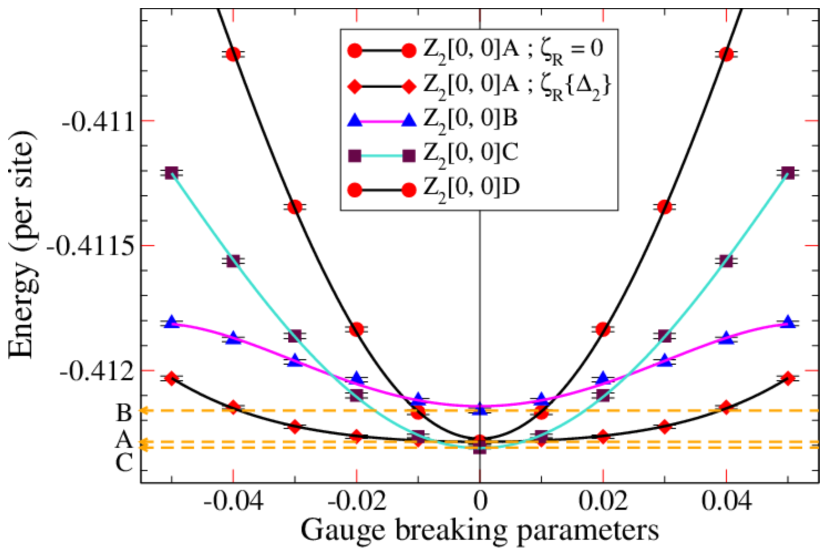
No.	η_{12}	Λ_s	u_α	u_β	u_γ	$\tilde{u}_\gamma$	Label	Gapped?
1	+1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	$Z_2[0,0]A$	Yes
2	−1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	0	$\mathbb{Z}_2[0,\pi]\beta$	**Yes**
3	+1	0	τ^2,τ^3	0	0	0	$Z_2[\pi,\pi]A$	No
4	−1	0	τ^2,τ^3	0	0	τ^2,τ^3	$Z_2[\pi,0]A$	No
5	+1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^3	$Z_2[0,0]B$	Yes
6	−1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^2	$Z_2[0,\pi]\alpha$	No
7	+1	0	0	τ^2,τ^3	0	0	–	–
8	−1	0	0	τ^2,τ^3	0	0	–	–
9	+1	0	0	0	τ^2,τ^3	0	–	–
10	−1	0	0	0	τ^2,τ^3	0	–	–
11	+1	0	0	τ^2	τ^2	0	–	–
12	−1	0	0	τ^2	τ^2	0	–	–
13	+1	τ^3	τ^3	τ^2,τ^3	τ^3	τ^3	$Z_2[0,0]D$	Yes
14	−1	τ^3	τ^3	τ^2,τ^3	τ^3	0	$Z_2[0,\pi]\gamma$	No
15	+1	τ^3	τ^3	τ^3	τ^2,τ^3	τ^3	$Z_2[0,0]C$	Yes
16	−1	τ^3	τ^3	τ^3	τ^2,τ^3	0	$Z_2[0,\pi]\delta$	No
17	+1	0	τ^2	τ^3	0	0	$Z_2[\pi,\pi]B$	No
18	−1	0	τ^2	τ^3	0	τ^3	$Z_2[\pi,0]B$	No
19	+1	0	τ^2	0	τ^2	0	$Z_2[\pi,\pi]C$	No
20	−1	0	τ^2	0	τ^2	τ^3	$Z_2[\pi,0]C$	No

Only ONE gapped SL connected with the U(1) Dirac SL: The $Z_2[0,\pi]\beta$ spin liquid
FOUR gapped SL connected with the Uniform U(1) SL: $Z_2[0,0]$A, B, C, and D

The Dirac U(1) SL is stable against opening a gap...



...and also the Uniform U(1) spin liquid is stable



The gapless U(1) Dirac SL is very stable

- Against dimerization
- For breaking the gauge structure down to Z_2

The gapless uniform U(1) SL is stable against Z_2 SLs