Beyond the Kitaev model: slave-particle, gauge fields, and fractional excitations

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Current Trends in Frustrated Magnetism
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ma per seguir virtute e conoscenza

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

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:

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

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 spin operator in terms of spin-1/2 quasi-particles creation and annihilation operators.
- One possibility is to write:

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

$\sigma_{\alpha,\beta}^\mu$ 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:

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

$\{c_{i,\alpha}, c_{j,\beta}^\dagger\} = \delta_{ij}\delta_{\alpha\beta}$
$\{c_{i,\alpha}, c_{j,\beta}\} = 0$
$c_{i,\uparrow}^\dagger$ (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:

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

- Compact notation by using a 2×2 matrix:

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

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

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

- 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

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

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

Mean-field approximation

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

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

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

- $\{\chi_{ij}, \eta_{ij}, \mu_i \, , \zeta_i \, \}$ 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 $|\Phi_{MF}(U^0_{ij})\rangle$ be the ground state of the mean-field Hamiltonian (with a given Ansatz for the mean-field U^0_{ij})
- $|\Phi_{MF}(U^0_{ij})\rangle$ 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 $\mathbf{S}_i \to \mathbf{S}_i$.

$$U^0_{ij} \to W_i^\dagger U^0_{ij} W_j$$

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

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

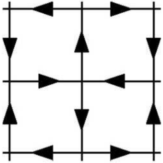
An example of the redundancy on the square lattice

- 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:

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

  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

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

$\{T, G\}$ 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_{ij}^0 for the mean-field state
- Assume that the IGG is U(1):

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

- Consider now some fluctuations above the mean field:

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

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

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

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_{ij}^0 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:

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

- The case with also point-group and time-reversal symmetries is much more complicated

  Two classes of Z_2 spin liquids are possible:

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

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

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

In total, 272 possibilities

At most 196 different Z_2 spin liquids!

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 $\longrightarrow$ 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 $\longrightarrow$ 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!)

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

- 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

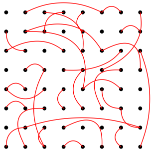
- $E(\Phi)$ can be sampled by using "classical" Monte Carlo, since $P(x) \geq 0$
- $\langle x|\Phi\rangle$ is a determinant
- The ratio of to determinants (needed in the Metropolis acceptance ratio) can be computed very efficiently, i.e., O(N), when few spins are updated
- The algorithm scales polinomially,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

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

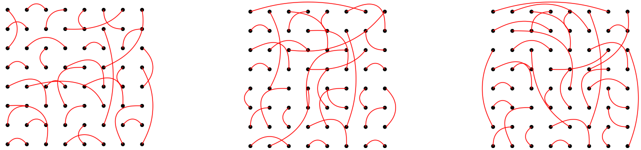
It is a linear superposition of all singlet configurations (that may overlap)



$+ \ldots$

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

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



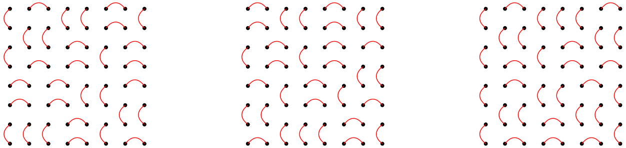
$+ \ldots$

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...



$+ \ldots$

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