Spinons in the S=1/2 Heisenberg antiferromagnet on kagome

Oleg Tchernyshyov
Johns Hopkins University
Papers

- **Zhihao Hao and Oleg Tchernyshyov:**
  - Spin-1/2 Heisenberg antiferromagnet on kagome: a $\mathbb{Z}_2$ spin liquid with fermionic spinons. arxiv:1301.3261
Spinons on kagome resemble strongly spinons of the Heisenberg model on the Delta/sawtooth chain. Both come in two flavors and have similar kinematics.
Spinons exhibit Fermi statistics: upon exchange of two spinons, the 2-spinon wavefunction changes sign.

They feel strong attraction in the $S=0$ channel mediated by the exchange interaction. This attraction binds two spinons into a small pair with a binding energy of $0.06J$. 
Long story

Many-body physics

We find a finite concentration of spinons in the ground state, one spinon per unit cell (3 sites). Their ground state is \textit{not} a Fermi sea (as in large-$N$ inspired approaches), for two reasons.

First, strong attraction in the $S=0$ channel (see 2-body physics).

Second, strong interaction with an emergent U(1) gauge field. Spinons carry the U(1) charge $+1$. They also have a small electric charge and couple to the real electric field.

Spin pairs are bosons with charge $+2$. Their condensation may create a $\mathbb{Z}_2$ spin liquid with vison excitations.
Spinons on kagome:
The gory details
Kagome lattice

lattice of corner-sharing triangles

\[ H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J}{2} \sum_{\triangle} \mathbf{S}^2_{\triangle} + \text{const.} \]
Single triangle of $s=1/2$

hw02, problem 4

$$H = J \left( \vec{s}_1 \cdot \vec{s}_2 + \vec{s}_2 \cdot \vec{s}_3 + \vec{s}_3 \cdot \vec{s}_1 \right) = \frac{1}{2} J \left[ \left( \vec{s}_1 + \vec{s}_2 + \vec{s}_3 \right)^2 - 3 \vec{s}_1^2 \right]$$

$$= \frac{1}{2} J \left( \vec{s}_{\text{tot}}^2 - 3 \cdot \frac{3}{4} \right)$$

$$\vec{s}_{\text{tot}} = \vec{s}_1 + \vec{s}_2 + \vec{s}_3$$

Since $S = \frac{1}{2}$, $S_{\text{tot}} = \left\{ \frac{3}{2}, \frac{1}{2} \right\}$

$$= \frac{3}{2} \quad E_{\frac{3}{2}} = \frac{1}{2} J \left( \frac{3}{2} \left( \frac{3}{2} + 1 \right) - \frac{9}{4} \right) = \frac{3}{4} J$$

$$\frac{1}{2} \quad E_{\frac{1}{2}} = \frac{1}{2} \left( \frac{1}{2} \left( \frac{1}{2} + 1 \right) - \frac{9}{4} \right) = -\frac{3}{4} J$$

$E = -\frac{3}{4} J$ is the energy of a spin singlet: the lowest energy state of the single triangle is made of a **singlet bond** and a **free unpaired spin**

$$\begin{align*}
\text{OS addition}
\end{align*}$$
Construct a ground state?

Place a valence bond on every triangle.

Every triangle minimizes its exchange energy and the entire lattice is in a state of lowest possible energy.
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No matter how hard we try, we always end up with a few defect triangles containing no valence bond.
Defects are inevitable!

- $N$ unit cells.
- $2N$ triangles (up and down).
- $3N$ sites.
- $3N/2$ valence bonds.
- $3N/2$ have valence bonds.
- $N/2$ triangles are empty.
- That is one in four triangles.

Focus on defect triangles

Defect triangles are sources of quantum fluctuations. Without them, the system would have valence bonds frozen in place.
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Quantum fluctuations of valence bonds near a defect triangle. No fluctuations away from the defects.
Look at defect triangles

Can’t study isolated defects on kagome. Instead, use the Husimi cactus: same local connectivity, but no loops apart from triangles.
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The dual lattice is a tree
Husimi cactus

(kagome in a hyperbolic plane)

Husimi cactus

(kagome in a hyperbolic plane)

A ground state.

A single defect triangle

The triangle without a bond is not in a stationary state. Nearby bonds fluctuate, those farther away remain static.
Ground state without defects

Ground state without defects

A ground state.

$S=1$ excitations
$S=1$ excitations

$H = \frac{5}{4} \quad -\frac{1}{2} \quad -\frac{1}{2}$
Displaced bonds are shown in blue.
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The free spin can freely travel along a particular line. It shifts bonds along its path (cf. the sawtooth chain).
It's a $\Delta$-sawtooth chain embedded in the Husimi cactus.

The rest of the lattice remains frozen in time.
Spin excitations on the cactus

- are spinons: quasiparticles with $S=1/2$;
- come in two flavors:
  - kinks are completely localized,
  - antikinks are able to move along a line, rearranging bonds along the way;
- resemble closely spinons on the $\Delta$/sawtooth chain.
Defect triangle revisited

The triangle without a bond is not in a stationary state.
State with a 3rd-neighbor singlet bond.
Long-range bond = spins $\bullet$ and $\bullet$ with total $S=0$. 
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Long-range bond = spins $\bullet$ and $\bullet$ with total $S=0$.

Consider a general state of the two spins, $|\alpha,\beta\rangle$. 
Spin 🔄 is able to move around.
Spin ● is able to move around.
So is spin $\bullet$. 
The spinons are antikinks traveling along three branches of the cactus.
We can now probe their exchange statistics.
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An important technical point

Arrows indicate a sign convention for singlet bonds.

\[ | \uparrow \cdot \downarrow \rangle - | \downarrow \cdot \uparrow \rangle \over \sqrt{2} \]
An important technical point

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An important technical point

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\[
\frac{|\uparrow \downarrow \downcirc \kdowarrown \upcirc \uparrow\rangle - |\downarrow \uparrow \upcirc \kdowarrown \downcirc \uparrow\rangle}{\sqrt{2}} = - \frac{|\upcirc \downarrow \downcirc \kdowarrown \uparrow \upcirc \rangle - |\downcirc \uparrow \upcirc \kdowarrown \downarrow \upcirc \rangle}{\sqrt{2}}
\]
Initial state

State with spinons exchanged
Initial state

State with spinons exchanged

Tuesday, April 23, 13
Spinon exchange flips one valence bond. That produces a minus sign.
Forget about the singlet signs and treat valence bonds as passive dimers. Then the extra minus sign must be assigned to the spinons themselves.
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In this sense, spinons are fermions.
On a more technical level

- Obtain an orthogonal basis (similar to the sawtooth chain).

- Find the ground state of two spinons with a given total spin $S$ and check the spatial wavefunction. Fermi statistics requires that
  - $\Psi(r_\bullet, r_\bullet) = +\Psi(r_\bullet, r_\bullet)$ for total $S=0$. ✔
  - $\Psi(r_\bullet, r_\bullet) = -\Psi(r_\bullet, r_\bullet)$ for total $S=1$. ✔

- Spinons are fermions.
Finite-size scaling of the ground-state energies

\( S=1 \): no bound state.

\( S=0 \): bound state with binding energy \( \Delta = 0.06J \) and radius \( \xi = 1.4 \) spacings of the dual lattice.
What about kagome?

- Antikinks are still fermions.
- 1 in 4 triangles contains a spinon pair,
- That translates to 1 spinon per unit cell.
Low-energy spin excitations

\[ S=0 \quad S=1 \]
Low-energy spin excitations

\[ S=0 \quad \text{and} \quad S=1 \]
Low-energy spin excitations

Away from the pair:

$S=0$ bond $\rightarrow S=1$ bond $\rightarrow$ kink + antikink. $E \approx 0.25J$. 
Low-energy spin excitations

Away from the pair:
\[ \text{S}=0 \text{ bond} \rightarrow \text{S}=1 \text{ bond} \rightarrow \text{kink + antikink. } E \approx 0.25J. \]

Near the pair:
\[ \text{S}=0 \text{ bond} \rightarrow \text{S}=1 \text{ bond} \rightarrow 2 \text{ antikinks. } E \approx 0.06J. \]
Inelastic neutron scattering just above the spin-gap threshold

Left: $I(Q)$ of inelastic neutron scattering just above the spin gap.
Right: same for isolated dimers of three different orientations.

Fractionalized excitations in the spin-liquid state of a kagome-lattice antiferromagnet

Tian-Heng Han1, Joel S. Helton2, Shaoyan Chu3, Daniel G. Nocera4, Jose A. Rodríguez-Rivera3,5, Collin Broholm3,6 & Young S. Lee1

Figure 1 | Inelastic neutron scattering from the spin excitations, plotted in reciprocal space. a–c, Measurements were made at T = 1.6 K on a single-crystal sample of ZnCu3(OH)6Cl2. The dynamic structure factor, \( S_{\text{mag}}(Q,\omega) \), is plotted for \( h\omega = 6 \text{ meV} \) (a) and \( h\omega = 2 \text{ meV} \) (b) with \( E_1 = 5.1 \text{ meV} \) and \( h\omega = 0.75 \text{ meV} \) (c) with \( E_2 = 3.0 \text{ meV} \). The background was measured with an empty sample holder and subtracted. The diffuse scattering is mostly magnetic in origin, because the phonon contribution to the signal is small (except near the (2, 2, 0)-type positions, where the fundamental Bragg peaks are strong). d, The magnetic part of the dynamic structure factor, \( S_{\text{mag}}(Q,\omega) \), integrated over \( 1 \leq h\omega \leq 9 \text{ meV} \). e, Calculation of the equal-time structure factor, \( S_{\text{tot}}(Q) \), for a model of uncorrelated nearest-neighbour dimers. The intensity corresponds to 1/8 of the total moment sum rule \( S(S + 1) \) for the spins on the kagome lattice. The data presented in a–c are expressed in barn sr\(^{-1}\) eV\(^{-1}\) per formula unit, as shown by the left colour bars. The data presented in parts d and e are dimensionless, with the scale given by the right colour bar. The Brillouin zone boundaries are drawn in the figure for clarity; they correspond to the conventional unit cell with parameters \( a = b = 6.83 \text{ Å} \), \( c = 14.05 \text{ Å} \), \( \alpha = \beta = 90^\circ \) and \( \gamma = 120^\circ \).
Figure 3 | The measured dynamic structure factor along specific directions in reciprocal space with comparison to the nearest-neighbour singlet model. a, $S_{\text{mag}}(Q, \omega)$ along the $(-2, 1 + K, 0)$ direction, indicated by the thick red line on the reciprocal space map in d. Three energy transfers, $h\omega = 2, 6$ and $10$ meV, are shown. b, $S_{\text{mag}}(Q, \omega)$ along the $(-2, 1 + K, 0)$ direction integrated over $1 \leq h\omega \leq 11$ meV. c, $S_{\text{mag}}(Q, \omega)$ along the $(0, K, 0)$ direction, indicated by the thick orange line on the reciprocal space map in d, integrated over $1 \leq h\omega \leq 7$ meV. The solid lines in b and c are the calculated equal-time structure factors for uncorrelated nearest-neighbour singlets multiplied by $|F(Q)|^2$. d, The trajectories in reciprocal space referred to in a–c. Error bars, 1 s.d.
Spin gap

- Our calculation: 0.06 to 0.10.
- less than 0.1, exact diagonalization*.
- 0.06 to 0.10, perturbation series†.
- 0.05 to 0.06, DMRG (Sheng).
- Steve White’s DMRG: 0.14 or so?

Spinons in $d=1$: \( \Delta / \)sawtooth chain

\[
H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = \frac{J}{2} \sum_{\triangle} \mathbf{S}_\triangle^2 + \text{const.}
\]

Ground state: every triangle has total spin 1/2.

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Spin excitations
Spin excitations
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Spin excitations
Spinons

- Serve as domain walls between the 2 vacua.
- Carry spin $S=1/2$.
- Kinks are localized in this model.
- Antikinks are mobile.
- Their quantum statistics is undefined: can’t exchange particles in 1 spatial dimension.
Energetics

\[ E_-(k) = 0. \]
\[ E_+(k) = \frac{3}{4} + \frac{1}{2} - \cos k \approx \frac{1}{4} + \frac{k^2}{2}. \]

\[ \Delta = \min (E_- + E_+) = \frac{1}{4}. \]
Virtual excitations
Virtual excitations

\[ \Delta = 0.250 \text{ in 1-band approximation.} \]
\[ \Delta = 0.219 \text{ in 2-band approximation.} \]
\[ \Delta = 0.215 \text{ exact diag (Kubo 1996).} \]

Fast convergence.
Not much room for improvement.