Kagome lattice structures with charge degrees of freedom

Aroon O’Brien
Max Planck Institute for the Physics of Complex Systems, Dresden

Frank Pollmann, University of California, Berkeley
Masaaki Nakamura, MPI-PKS, Dresden

Peter Fulde, MPI-PKS, Dresden, Asian Pacific Center for the Theoretical Physics, Pohang
Michael Schreiber, TU Chemnitz

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Outline

• Introduction-Frustration and Fractionalization
• A theoretical model of frustration
• Analysing the model
• Current approaches and Outlook
Fractionalization

• First theoretical model supporting fractional excitations-spin-charge separation in polyacetylene molecules [1,2]
• Ground state - idealized chain molecule:

A bond (= -2e) is removed from either ground state - we obtain two defects both with charge +e and spin 0 (spin charge-separation):

One excitation-decays into two collective excitations

Fractionalization

- Similarly - removed bond would with charge $-e$ would give rise to fractional charges with charge $e/2+!$

- Similarly - add/remove one charged particles on a frustrated lattice - gives two fractionally charged excitations

**One excitation-decays into two collective excitations**

- Fractionalization-observed experimentally in Fractional Quantum Hall Effect [3]

Geometric Frustration

• Fractional charges - arise also in theoretical models of geometrically frustrated systems [1]

• Occur in lattice structures where it is impossible to minimize the energy of all local interactions:

• Characterised by a macroscopic ground-state degeneracy - high density of low-lying excitations:

Geometric Frustration in nature

- Spinel minerals form **pyrochlore** structures:

  - $M_3H(XO_4)$ forms a **kagome lattice** structure:

  ```plaintext
  possible position of proton
  \[ \text{XO}_4 \text{ tetrahedron (downward)} \]
  \[ \text{XO}_4 \text{ tetrahedron (upward)} \]
  \( M = \text{Rb, Cs} \quad \text{X = S, Se} \)
  \text{M atoms are omitted for simplicity}
  ```
Fractionalised charges due to geometrical frustration

*What we know already…*

- There are models of 2D lattice structures supporting fractional excitations [5].
- These approaches so far yield fractional excitations that are confined [6].
- 3D lattices have been shown to support deconfined phases [7,8]

Fractionalised charges due to geometrical frustration

*What we would like to know…*!

- Kagome lattice models—can we investigate the dynamics of systems exhibiting charge fractionalization? Can we determine the **confinement/deconfinement** of the excitations?
- Do these fractionalized excitations exhibit **fractionalised statistics**? What are they?
- Can we use such models to **explain experimental observations** in real materials with such structures?
A model of fractionalization

- Consider a model of spinless fermions on the kagome lattice
- Extended Hubbard model with charge degrees of freedom

\[ H = -t \sum_{\langle i, j \rangle} (c_i^\dagger c_j + H.c.) + V \sum_{\langle i, j \rangle} n_i n_j \]

- Consider 1/3 filling
- At \( t=0, V>0 \), macroscopic number of ground states
A model of fractionalization

• **Strong correlation limit** (large nearest-neighbour repulsions $V$) -> **local constraint** of 1 particle per triangle on the lattice -> “triangle rule”

• Finite hopping of fractional charges in strongly correlated limit where $0 < |t| \ll V$

• Add one particle -> increase system energy by $2V$
A model of fractionalization

- One particle with charge $e$ is added to the system - it can decay into two defects each carrying the charge $e/2$ -> \textbf{2 fractional charges are created}

One excitation decays into two collective excitations
A model of fractionalization

• Large Hilbert space sizes -> limit numerical investigation

  Derive an effective model Hamiltonian encapsulating behaviour in the strong correlation limit

• Lowest order hopping process lifting degeneracy - particle hopping around hexagons:
A model of fractionalization

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + H.c.) + V \sum_{\langle i,j \rangle} n_i n_j$$

$$H_{\text{eff}} = -g \sum_{\langle \rangle} (|\text{sixed} \rangle \langle \text{sixed}| + H.c.)$$

Where $g = \frac{12t^3}{V^2}$
Effective model...

- Exact in the limit of infinitely large $V$
- Reduces drastically Hilbert space size

Example: No. of configurations for a 147-site cluster at 1/3 filling:

\[
\binom{147}{49} \approx 10^{39}
\]

No. of configurations for a 147-site cluster at 1/3 filling subject to the triangle rule:

\[
\approx 10^{11}
\]

- Has no fermionic sign problem!

\[
\langle \text{final} \| \cdots \rangle \langle \cdots | \text{initial} \rangle \rightarrow -1
\]
Effective model...

- Is equivalent to a hard-core bosonic model!
- Can be mapped to a Quantum Dimer Model!

-> kagome lattice model at 1/3 filling maps to honeycomb dimer covering
Mapping to Quantum Dimer Model
Mapping to Quantum Dimer Model
Mapping to Quantum Dimer Model
Mapping to Quantum Dimer Model
Mapping to Quantum Dimer Model
Quantum Dimer Mapping

- Mapping-effective Hamiltonian to ‘plaquette phase’ ($\mu=0$) of known system [8]:

$$H_{QDM} = \sum -g(|\begin{array}{c}\textcircled{1}\end{array}\rangle\langle\begin{array}{c}\textcircled{2}\end{array}| + H.c) + \mu(|\begin{array}{c}\textcircled{1}\end{array}\rangle\langle\begin{array}{c}\textcircled{2}\end{array}| + |\begin{array}{c}\textcircled{3}\end{array}\rangle\langle\begin{array}{c}\textcircled{4}\end{array}|)$$

- Numerically confirmed - exact diagonalisation gives ground-states energies
- Distance between defects $1/#$ flippable hexagons

Investigating dynamical properties...

- With a ‘doped system’-consider dynamical properties - add extra term to Hamiltonian

\[ H_{doped} = H_{eff} - t \sum_{i,j} P(c_i^\dagger c_j + H.c.) P \]

Original effective Hamiltonian

Projected hopping operator

Describes a system at 1/3 filling +/- one particle
Numerical Methods

• Model Hamiltonian basis transformation -> Lanczos recursion method [9]
• Analyse finite clusters from 25-75 sites
• Direct insight into system dynamics- from spectral function calculations

Spectral function - \( A(k, \omega) \) gives probability for adding (+) or removing (-) a particle with momentum \( k \) and energy \( \omega \) to the system…

\[
A(k, \omega) = A^-(k, \omega) + A^+(k, \omega)
\]

Density of states- sum over all \( k \) - space contributions:

\[
D(\omega) = \frac{1}{N_k} \sum_k A(k, \omega)
\]

How good is the model?

- Exact and effective models on a 27-site cluster are compared...

**Density of States - a comparison**

- Hole contribution
- Particle contribution
Density of states figures show that finite-size effects decrease markedly with system size:
Results

• Hole contribution is symmetric; the eigenspectrum for the 1/3 filled system in the presence of one hole defect is symmetric:

Hole contribution to the density of states

→ Underlying **bipartiteness** for the particle hopping in the presence of one hole defect!

→ A **gauge transformation** that changes the sign of each hopping process must exist...!
Results

Eigenspectrum symmetry

Bipartiteness

Bipartite hopping on kagome lattice

expressible in terms of a gauge transformation

Example - 2D Square Lattice

\[ |\tilde{b}_i\rangle = (-1)^{\sum_A n_i} |b_i\rangle \]

\[ \implies \tilde{H}_{hop} = -H_{hop} \]

\[ \implies \text{Eig}[H_{hop}] = \text{Eig}[-H_{hop}] \]
Results

• Large peak in particle contribution - at zero momentum- full spectral weight of flat band contained in a single delta peak:

→ GS wavefunction exact eigenfunction of the effective Hamiltonian, in the limit of \( t/V \to 0 \).

→ This can be shown analytically…

\[
|\tilde{\psi}^{N+1}\rangle = c_{k=0,\text{band 1}}^\dagger |\psi_0\rangle
\]

\[
H|\tilde{\psi}^{N+1}\rangle = (\epsilon(k = 0, \text{band 1}) + 2V + E_0)|\tilde{\psi}^{N+1}\rangle
\]
Do such models model real systems?

- Materials which may provide the answer…$\text{MH}_3(\text{XO}_4)_2$
- Here protons act as particles at 1/3 filling
Do such models model real systems?

- Model gives three possible charge-ordered states - material shows just two of these at different temperatures!
- Goal-to obtain a phase diagram of the model to compare with that of corresponding real materials
- Apply Random Phase Approximation to calculate charge susceptibilities; calculate spectral functions in the limit of small $V$
Conclusion and Outlook

• With exact diagonalisation on finite size clusters we are able to analyse the dynamics of kagome lattice models at specific fillings
  • Understand most prominent features of spectrum - what is the physical interpretation?
  • Compare -bosonic and fermionic dynamics
  • Effective model is bipartite in nature-how can we understand this through a gauge transformation?
  • QDM mapping -> we have a confined ground state- evidence of this in the spectral function results?

• RPA treatment of Hubbard model/spectral function calculations - hope to compare the results of our theoretical model with real materials

Thank you!
Fractionalization

- Fractional excitations exhibit fractional statistics [a]:

\[ \psi(1, 2) \rightarrow \psi'(1, 2) = e^{i\nu \Delta \varphi} \psi(1, 2) \]

3D -> fermionic/bosonic statistics

2D -> possibility of anyonic statistics!