Fully symmetric and non-fractionalized Mott insulators at fractional site-filling

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PRL 2013 (kagome), 1207.0498...[PNAS] (honeycomb)

Collaborators







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Kagome magnetization plateaus



Wang, Tokunaga, He, Yamaura, Matsuo, Kindo, Phys. Rev. B 84, 220407(R) (2011)

Magnetization plateau ↔ boson Mott insulator

Describe plateaus via bosons:

<N>=3

(N) = 2

<N>= |

<N>=0

SF

J/V

μ/٧

3

2

MI N=3

MI

MI

N = 1

N=2

 $2/3 S^{z}=1 magnetization \leftrightarrow 1/3 boson occupancy$

at density n=1/3 boson/site,

no definite-occupancy Mott insulator

Can make n=1/3 insulator by **breaking symmetry**

any alternative?



J_/V

Ultracold atoms on kagome

Must n=1/3 bosonic insulators *break symmetry*?



Gyu-Boong Jo, Phys. Rev. Lett. 108, 045305 (2012)

Free fermions, square lattice

Metallic or insulating? Band theory:

f ≡ number of particles per unit cell = number of filled bands

Non-integer $f \rightarrow$ partially-filled bands \rightarrow metal



Free fermions, square lattice

Metallic or insulating? Band theory:

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Half site-filled square lattice:

 $f = 1/2 \rightarrow$ always metallic



Free fermions, kagome lattice

t3



 $t_2 = t_3 = 0$



But t_2 , t_3 open gap:

1/3 site-filling (*f*=1) can be insulating

Free fermions, honeycomb (graphene) lattice

Graphene: gapless Dirac cones





Free fermions, honeycomb (graphene) lattice

Graphene: gapless Dirac cones





protected by lattice symmetry:

Half site-filled honeycomb lattice (*f*=1) always metallic

Interacting bosons / fermions

Lieb-Schultz-Mattis-Hastings-Oshikawa theorems:

Non-integer f:



always gapless / degenerate

insulators trigger conventional or topological order

| <u>Integer</u> <i>f</i> = 1 : | | |
|--------------------------------------|-----------|-----------------|
| | kagome: | honeycomb: |
| free fermions: | insulator | always metallic |
| interacting particles: | ? | ? |

interacting featureless insulators?



Yan et al, Science (2011)

How to identify fractionalization?

Half-filled (*f*=1) honeycomb:

Gapped + fully-symmetric



Fractionalization

implication holds when featureless insulators forbidden

e.g. non-integer **f**

f = 1 kagome, honeycomb:

featureless insulators?

Bosons (cold atoms, magnetized spins, paired electrons)

Trying to make a featureless Bose insulator

Honeycomb at half site-filling:

- Trivial n=1 Mott insulator -> wrong filling
- Put 1 boson in some sites or
- Smear bosons across unit cell
 - -> breaks lattice symmetry





- Smear bosons across overlapping regions -> likely superfluid
- Put 1 fractionalized 1/2-quasiparticle per site -> fractionalization

Route #1 (kagome): Band to Mott

given a band insulator



can construct an analogous featureless boson insulator

Wannier orbital permanent wavefunction



insulating, symmetric, **f**=1 (1/3 site-filling)

Featureless Insulators?

• **f**=1 kagome: yes -- Wannier Permanent. PRL 2013



f=1 honeycomb: band insulator prohibited
 → no Wanniers



• Route #2: use a localized symmetric orbital





Candidate featureless Boson insulator



Hexagon-orbital operators

(R on Bravais lattice)



$$|\Psi_{\bigcirc}\rangle = \prod_{\mathbf{R}} B_{\mathbf{R}}^{\dagger} |0\rangle$$

site-filling of 1/2 on honeycomb 1/3 on kagome Establishing $|\Psi_{\bigcirc}\rangle$ is featureless, insulating $|\Psi_{\bigcirc}\rangle = \prod B_{\mathbf{R}}^{\dagger}|0\rangle$ highly entangled state

must explicitly check for superfluidity, symmetry-breaking, fractionalization

Compute within classical statistical mechanics model that maps to $|\Psi_{\bigcirc}\rangle$

Like *plasma analogy* for Laughlin's 1/m FQHE states:

 $|\Psi_{\bigcirc}
angle$ defines **2D** classical partition function, of self-avoiding closed loops on Bravais triangular lattice



$\mathbf{Z} \equiv \langle \Psi_{\bigcirc} | \Psi_{\bigcirc} \rangle$

 $=\sum m^{L_{\text{total}}}$ loop configs



m = 1/3





States for continuous m loop models



m=1/3

States for continuous m loop models

Shift to hexagon-center site $a_{\mathbf{R}}^{\dagger}$



smooth evolution?

Loop model correlators:



Loop model correlators: decay exponentially



Helicity modulus: vanishes, no transition



Helicity modulus: vanishes, no transition



No lattice symmetry breaking



 $|\Psi_{igodot}
angle$ is featureless

• Mott insulator with inherent quantum fluctuations



- $|\Psi_{\bigcirc}\rangle$ is positive \rightarrow arises from unfrustrated *H*?
- Construction generalizes to symmorphic lattices fully-symmetric orbital at each unit cell

Symmorphic Lattice Symmetry Groups

Point group and translations split: no glides or screws

Fully-symmetric orbital for each unit cell Non-symmorphic:



Non-symmorphic lattices at *f*=1 prohibit featureless insulators Nat Phys 9, 299 (2013) & arxiv:1212.2944

Hexagon construction & classical Bravais lattice loop model

generalize to all symmorphic lattices

Project out multiple occupancy \rightarrow

hardcore bosons = onsite paired electrons

$$b_{i}^{\dagger} \longleftrightarrow c_{i,\uparrow}^{\dagger} c_{i,\downarrow}^{\dagger}$$

$$|\Psi_{\text{spinful electrons}}\rangle = \prod_{R} \sum_{j \in \mathcal{O}_{R}} c_{j,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} |0\rangle$$

Featureless insulator? check via dimer model

Density correlator via dimer model mapping

Site occupancy $\{n_i\}$ amplitudes map to classical dimer model on *depleted dice lattice*

 $\mathbf{R}-j$ dimer selects b_j^{\dagger} from hexagon $B_{\mathbf{R}}^{\dagger}$

Kasteleyn algorithm: bipartite dimer coverings

→ determinant (Monte Carlo)







Spin-singlet electron featureless insulator

$$\Psi_{\text{spinful electrons}}\rangle = \prod_{R} \sum_{j \in \mathcal{O}_{R}} c_{j,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger} |0\rangle$$

1/2 electron of each spin / site: **f**=1

Pairing is short ranged → insulator (cooper pairs aren't condensed)

Featureless, SU(2)-symmetric, fully-gapped spinful electron state

How to identify fractionalization?

Half-filled (*f*=1) Honeycomb Hubbard model (generic interactions):

Gapped + fully-symmetric



Fractionalization

How to identify fractionalization?

Half-filled (*f*=1) Honeycomb Hubbard model (generic interactions):



Future directions: SU(2) spin-1/2 paramagnetic state? Parent Hamiltonian for honeycomb state? Simple one? Featureless (fully symmetric, non-fractionalized) bosonic Mott insulators:

- 1. If band gap (kagome): *Band to Mott*
- 2. On honeycomb at half site-filling (despite no band insulator)
- 3. Construction generalizes to symmorphic lattices
- 4. Hard core bosons

 \rightarrow **f** = 1 featureless SU(2)-singlet electron insulator

Then, absence of order does not imply fractionalization

PRL 2013 (kagome), 1207.0498...[PNAS] (honeycomb)