Title: Fractionalized Charge Excitations in a Spin Liquid on Partially-Filled

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Abstract: <span>Electron charge may fractionalize in a quantum spin liquid Mott insulator. We study the Mott transition from a metal to a cluster Mott insulator in the 1/4- and 1/8-filled pyrochlore lattice systems. Such Mott transitions can arise due to charge localization in clusters or in tetrahedron units, driven by the nearest-neighbor repulsion. The resulting cluster Mott insulator is a quantum spin liquid with spinon Fermi surface, but at the same time a novel fractionalized charge liquid with charge excitations carrying half the electron charge. There exist two emergent U(1) gauge fields or "photons" that mediate interactions between spinons and charge excitations, and between fractionalized charge excitations themselves, respectively. In particular, it is suggested that the emergent photons associated with the fractionalized charge excitations can be measured in X-ray scattering experiments. This and other experimental signatures of the quantum spin and fractionalized charge liquid state are discussed in light of candidate materials with partially-filled bands on pyrochlore lattices. â€œFractionalized Charge Excitations in a Spin Liquid on Partially-Filled Pyrochlore Latticeâ€• Electron charge may fractionalize in a quantum spin liquid Mott insulator. We study the Mott transition from a metal to a cluster Mott insulator in the 1/4- and 1/8-filled pyrochlore lattice systems. Such Mott transitions can arise due to charge localization in clusters or in tetrahedron units, driven by the nearest-neighbor repulsion. The resulting cluster Mott insulator is a quantum spin liquid with spinon Fermi surface, but at the same time a novel fractionalized charge liquid with charge excitations carrying half the electron charge. There exist two emergent U(1) gauge fields or "photons" that mediate interactions between spinons and charge excitations, and between fractionalized charge excitations themselves, respectively. In particular, it is suggested that the emergent photons associated with the fractionalized charge excitations can be measured in X-ray scattering experiments. This and other experimental signatures of the quantum spin and fractionalized charge liquid state are discussed in light of candidate materials with partially-filled bands on pyrochlore lattices.

Fractionalized charge excitations in a spin liquid on a partially-filled pyrochlore lattice

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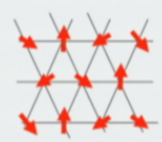
in collaboration with Hae-Young Kee and Yong Baek Kim

arXiv:1402.5425

Triangular lattice Hubbard model at half filling

$$H = -t \sum_{\langle ij \rangle, \sigma} c^\dagger_{i\sigma} c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Expected phase diagram

Fermi liquid metal	U(1) quantum spin liquid with spinon Fermi surface	120-degree magnetic order	U/t
Mott transition	such a regime is supported by various numerical studies		

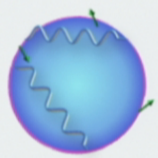
- Weak Mott insulator spin liquids (can be understood perturbatively)

  from insulating side, small charge gap, perturbation in t/U generates competing exchanges that frustrates 120 state, leading to a QSL phase.

$$H_{\text{pert}} = \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + K \sum_{1234} (P_{1234} + P_{1234}^{-1}) + \cdots$$

long-range exchange — 4-site ring exchange — Motrunich 2005

- This QSL and Mott xtion can be described by a slave rotor formalism



$$c_{i\sigma} = e^{-i\theta_i} f_{i\sigma}$$

$e^{-i\theta_i}$: charge-q_e spin-0 boson

$f_{i\sigma}$: charge-0 spin-1/2 fermion

Fermi liquid: rotor is condensed, and U(1) gauge field is higgsed

QSL Mott insulator: rotor is gapped, low energy effective theory of QSL: spinon Fermi surface coupled with a fluctuating internal U(1) gauge theory (also see Mandal's talk on non-Fermi liquid renormalization group.)

S.S. Lee, 2008

Even though the QSL has fractionalized spin excitation, the charge sector is trivial and is characterized by local gapped charge-q_e excitations.

My goal of this talk

- Provide a possible example of quantum spin liquid whose charge excitations are also fractionalized.
- Introduce a (slave-particle) formalism to describe this phase and the related Mott transition.
- Suggest a meaningful physical quantity to measure in a real experiment.

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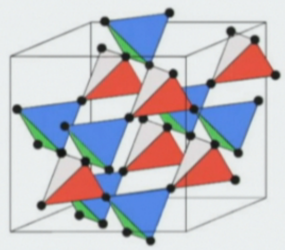
- The model is an extended Hubbard model defined on a pyrochlore lattice

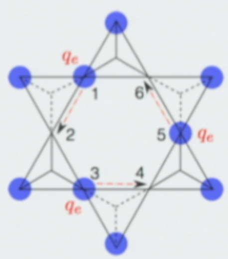
$$H = -t \sum_{\langle ij \rangle, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + V \sum_{\langle ij \rangle} n_i n_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



- The electron filling is 1/4 (or 1/8), i.e. two electrons per tetrahedron

- Hubbard U does not cause Mott localization. U is set to be large.

- Nearest-neighbor repulsion V can cause Mott localization with 2 electrons per tetrahedron when V >> t.



electrons are localized inside the tetrahedra cluster, not on a lattice site.

We expect: t>>V, Fermi liquid metal
t<<V, (**cluster**) Mott insulator

Slave particle formalism/description

- To describe mott transition, first rewrite the Hubbard model using slave-rotor formalism

$$c_{i\sigma} = e^{-i\theta_i} f_{i\sigma}$$

with a Hilbert space constraint $L_i^z = (\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}) - \frac{1}{2}$,

- The Hubbard model is reformulated as two coupled spinon and rotor Hamiltonians

$$H_{\mathrm{sp}} = -\sum_{\langle ij\rangle,\sigma} t_{ij}^{\mathrm{eff}}(f_{i\sigma}^\dagger f_{j\sigma} + h.c.) - \sum_{i,\sigma}(\mu + h_i) f_{i\sigma}^\dagger f_{i\sigma}$$

$$H_{\mathrm{ch}} = -\sum_{\langle ij\rangle} J_{ij}^{\mathrm{eff}}(e^{i\theta_i - i\theta_j} + h.c.) + V\sum_{\langle ij\rangle} L_i^z L_j^z$$

$$+3V\sum_i L_i^z + \sum_i h_i(L_i^z + \frac{1}{2}) + \frac{U}{2}\sum_i (L_i^z)^2.$$

with $t_{ij}^{\mathrm{eff}} = t\langle e^{i\theta_i - i\theta_j}\rangle \equiv |t_{ij}^{\mathrm{eff}}| e^{ia_{ij}}, J_{ij}^{\mathrm{eff}} = t\sum_\sigma \langle f_{i\sigma}^\dagger f_{j\sigma}\rangle \equiv |J_{ij}^{\mathrm{eff}}| e^{-ia_{ij}}$

- Spinon and rotor Hamiltonians are invariant under a U(1) gauge transforma

$$f_{i\sigma}^\dagger \to f_{i\sigma}^\dagger e^{-i\chi_i}, \theta_i \to \theta_i + \chi_i \text{ and } a_{ij} \to a_{ij} + \chi_i - \chi_j.$$

Charge sector

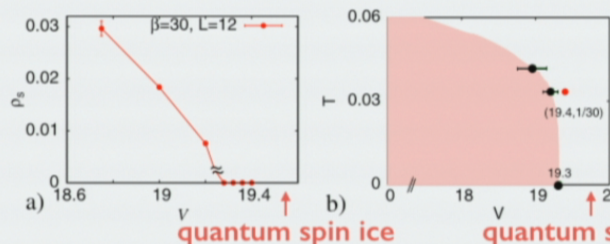
While spinons form spinon Fermi surface, the charge sector is also non-trivial !

$$H_{\rm ch} = -\sum_{\langle ij\rangle} J_{ij}^{\rm eff}(e^{i\theta_i - i\theta_j} + h.c.) + V\sum_{\langle ij\rangle} L_i^z L_j^z + \frac{U}{2}\sum_i (L_i^z)^2$$

in large U limit, $L_i^z = \begin{cases} +\frac{1}{2}, & n_i = 1, \\ -\frac{1}{2}, & n_i = 0. \end{cases}$ and identify $e^{\pm i\theta} = L^{\pm}$

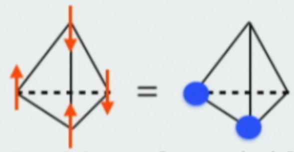
Charge sector is nothing but a "spin-1/2 XXZ model" in term of *L's* in the large U limit !

- Quantum Monte Carlo of XXZ model (Isakov etc 2008)



When V>>J, we obtain quantum spin ice state, which is a U(1) QSL.

Quantum spin ice in L = quantum charge ice in charge sector

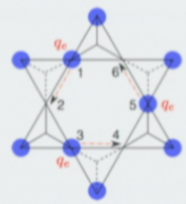


2up 2down spin ice rule = 2occupied 2empty charge ice rule

$$H_{\mathrm{ch}} = -\sum_{\langle ij \rangle} J_{ij}^{\mathrm{eff}}(e^{i\theta_i - i\theta_j} + h.c.) + V \sum_{\langle ij \rangle} L_i^z L_j^z$$

and identify $e^{\pm i\theta} = L^{\pm}$

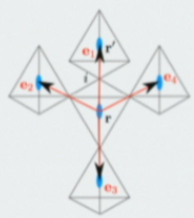
We can see the low-energy physics from perturbation theory in J/V.



Third order perturbation in *J/V* generates ring hopping around a hexagon that acts on the **highly degenerate** ice manifold. (Hermele 2004)

$$H_{\mathrm{C,eff}} = -J_{\mathrm{ring}} \sum_{\mathrm{hexagon}} \cos(\theta_1 - \theta_2 + \theta_3 - \theta_4 + \theta_5 - \theta_6)$$

Mapping to lattice U(1) gauge theory after identifying the vector gauge field



$e^{i\theta_i} \sim e^{iA_{\mathbf{rr}'}}$ r, r' are centers of tetrahedra

$$H_{\mathrm{eff}} = -K \sum_{\mathrm{hexagon}} cos(\nabla \times A)$$ "magnetic field" term

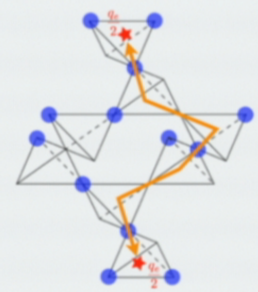
hexagons on the dual diamond lattice formed by the center of the tetrahedra

Charge fractionalization

From the properties of quantum spin ice, we can identify the corresponding properties for quantum charge ice in the charge sector !

- Low-energy physics of QCI is described by an emergent (compact) quantum electrodynamics in 3+1D, showing an **extra U(1) gauge structure** in the charge sector.

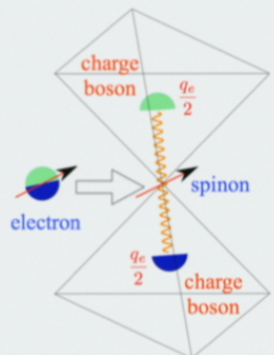
or



- Just as spin quantum number fractionalization in a QSI, charge excitation in QCI is also fractionalized, carrying a $q_e/2$ electric charge.

To capture the further charge fractionalization, we modify the slave particle description to

$$c^\dagger_{i\sigma} = e^{i\theta_i} f^\dagger_{i\sigma} \quad \Longrightarrow \quad c^\dagger_{i\sigma} = \Phi^\dagger_{\mathbf{r}} \Phi_{\mathbf{r}'} l^+_{\mathbf{r}\mathbf{r}'} f^\dagger_{i\sigma}.$$



Cartoon of electron fractionalization in the Mott regime

Here, charge rotor excitation fractionalizes into two charge bosons, each carries half the charge quantum number.

The charge sector becomes

$$H_{\text{ch}} = -J^{\text{eff}} \sum_{\mathbf{r},\mu\neq\nu} \Phi^\dagger_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_\mu} \Phi_{\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_\nu} l^{-\eta_{\mathbf{r}}}_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_\mu} l^{+\eta_{\mathbf{r}}}_{\mathbf{r},\mathbf{r}+\eta_{\mathbf{r}}\mathbf{e}_\nu} + \frac{V}{2} \sum_{\mathbf{r}} (Q^{\text{ch}}_{\mathbf{r}})^2,$$

This describes the hopping of charge bosons which minimally couples to the $U(1)_{\text{ch}}$ gauge field ($l_{\mathbf{r}\mathbf{r}'}$) on the dual diamond lattice (i.e. centers of the tetrahedra)

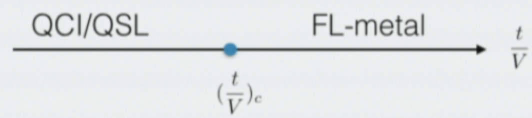
Mott transition

Mott transition occurs when the charge boson condenses

$$\text{metal:} \quad \langle \Phi \rangle \neq 0$$

$$\text{QCI/QSL:} \quad \langle \Phi \rangle = 0$$

Phase diagram



When the charge bosons are condensed, the $U(1)_{ch}$ gauge field is gapped from the Higgs' mechanism. The charge fractionalization is then destroyed. The charge rotor is also condensed from which the $U(1)_{sp}$ gauge field picks up a mass. The spinon and charge rotor are then combined back into a full electron in the Fermi liquid metal phase.

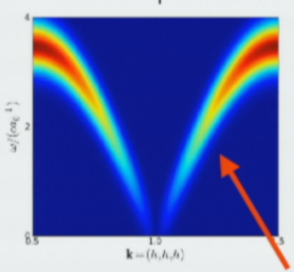
How to detect the QCI phase?

- (Inelastic) X-ray scattering **directly** measures $U(1)_{ch}$ gauge field correlation in the QCI phase

$$\mathrm{Im}[E^{\alpha}_{-\mathbf{k},-\omega} E^{\beta}_{\mathbf{k},\omega}] \propto [\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{\mathbf{k}^2}]\, \omega\, \delta(\omega - v|\mathbf{k}|),$$

$$\mathbf{E}_{\mathbf{r}+\frac{1}{2}\mathbf{e}_\mu} \equiv L^z_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu} \frac{\mathbf{e}_\mu}{|\mathbf{e}_\mu|} = (n_{\mathbf{r}+\frac{1}{2}\mathbf{e}_\mu} - \frac{1}{2}) \frac{\mathbf{e}_\mu}{|\mathbf{e}_\mu|}$$

low-temperature



O. Benton *et al*, 2012

emergent gauge photon spectrum

$I(\omega) \sim \omega$

for $T_{qc}<T<V$

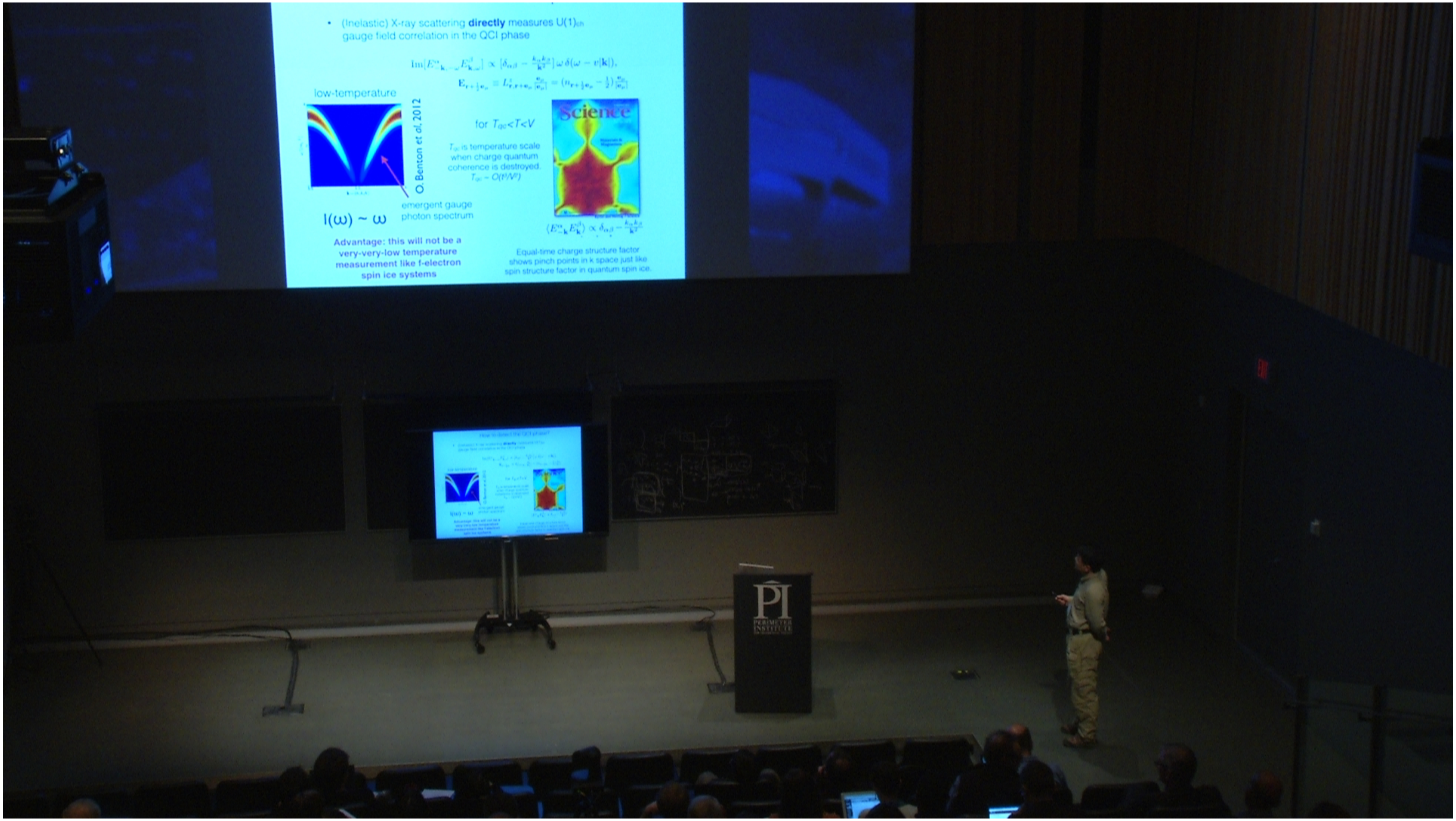
T_{qc} is temperature scale when charge quantum coherence is destroyed. $T_{qc} \sim O(t^3/V^2)$

Byron den Hertog / Science

$$\langle E^{\alpha}_{-\mathbf{k}} E^{\beta}_{\mathbf{k}} \rangle \propto \delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{\mathbf{k}^2}$$

Advantage: this will not be a very-very-low temperature measurement like f-electron spin ice systems

Equal-time charge structure factor shows pinch points in k space just like spin structure factor in quantum spin ice.


(Inelastic) X-ray scattering directly measures U(1)ch gauge field correlation in the QCI phase
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Science
emergent gauge photon spectrum
I(ω) ~ ω
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Pyrochlore systems with fractional electron filling

VOLUME 93, NUMBER 12 PHYSICAL REVIEW LETTERS week ending 17 SEPTEMBER 2004

Transition from Mott Insulator to Superconductor in $GaNb_4Se_8$ and $GaTa_4Se_8$ under High Pressure

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$GaTa_4Se_8$ (with $Ta^{3.25+}$:$d^{1.75}$)

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LiV_2O_4 Spinel as a Heavy-Mass Fermi Liquid: Anomalous Transport and Role of Geometrical Frustration

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(Received 27 January 2000)

LiV_2O_4 (with $V^{3.5+}$:$d^{1.5}$)

and many others

Summary

- We propose an interesting exotic **cluster** Mott insulator with both spin and charge quantum number fractionalizations.
- We develop a slave-particle formalism to describe this exotic phase and the Mott transition.
- We suggest some physical quantity to measure the internal gauge structure.