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

Gang Chen (UofT)

in collaboration with Hae-Young Kee and Yong Baek Kim

arXiv:1402.5425

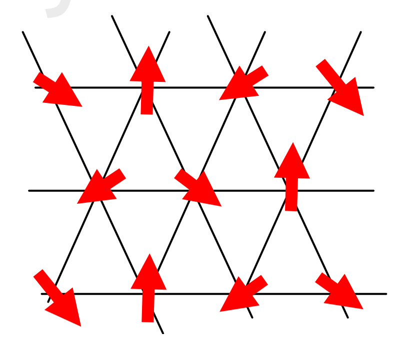
Triangular lattice Hubbard model at half filling

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

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

from insulating side, perturbation in t/U, competing exchanges

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

4-site ring exchange

Motrunich 2005

- A slave particle formalism/description

$$\underbrace{e^{-i\theta_i}}_{\substack{\text{charge-}q_e \\ \text{spin-0 boson}}} \quad \underbrace{f_{i\sigma}}_{\substack{\text{charge-0} \\ \text{spin-1/2 fermion}}}$$

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

charge-q_e
spin-0 boson

charge-0
spin-1/2 fermion

Fermi liquid: rotor is condensed

QSL Mott insulator: rotor is gapped

Low energy effective theory of QSL: spinon Fermi surface coupled with a fluctuating U(1) gauge theory

S.S. Lee, 2008

My goal of this talk

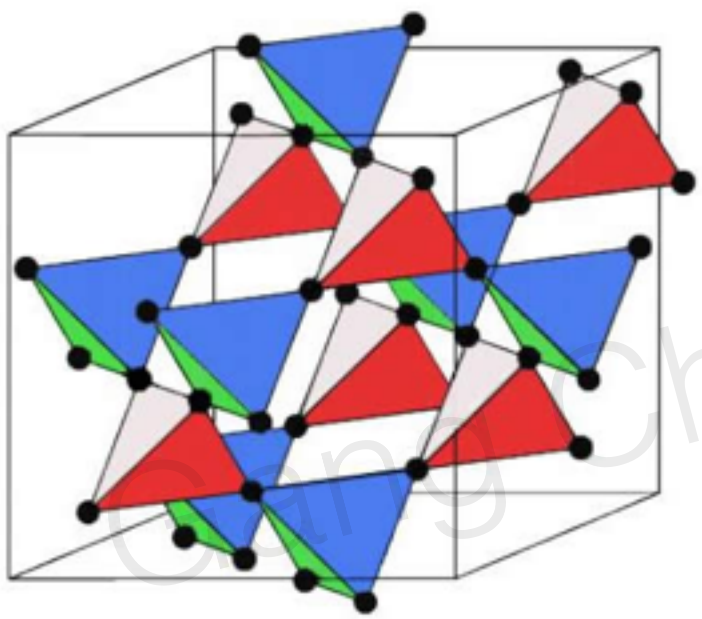
- Provide a possible example of quantum spin liquid whose charge excitations are also fractionalized.

- 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.

- The extended Hubbard model on a pyrochlore lattice

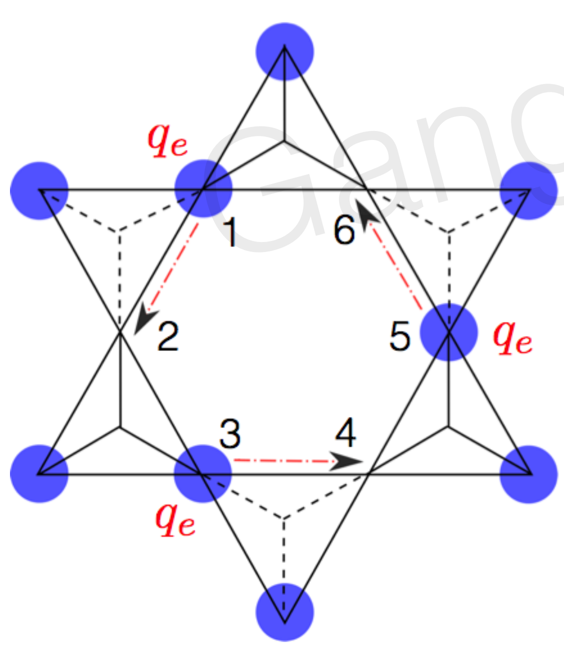
$$H = -t \sum_{\langle ij \rangle, \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + V \sum_{\langle ij \rangle} n_i n_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



- 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.



We expect: t>>V, Fermi liquid metal
t<<V, Mott insulator

Slave particle formalism/description

- First, rewrite the Hubbard model with 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

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

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

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

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

- U(1) gauge transformation (both spinon and charge rotor are involved)

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

Charge sector

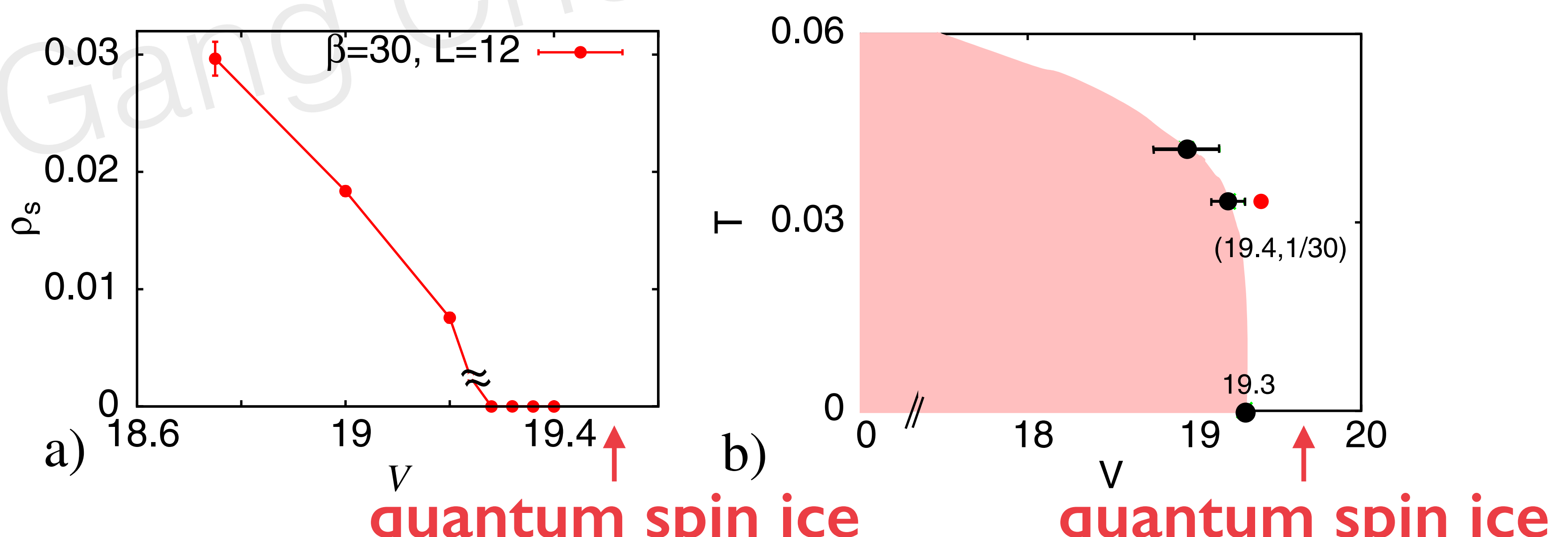
While spinons form spinon Fermi surface, the charge sector is also non-trivial !

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

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 (Isakov etc 2008)

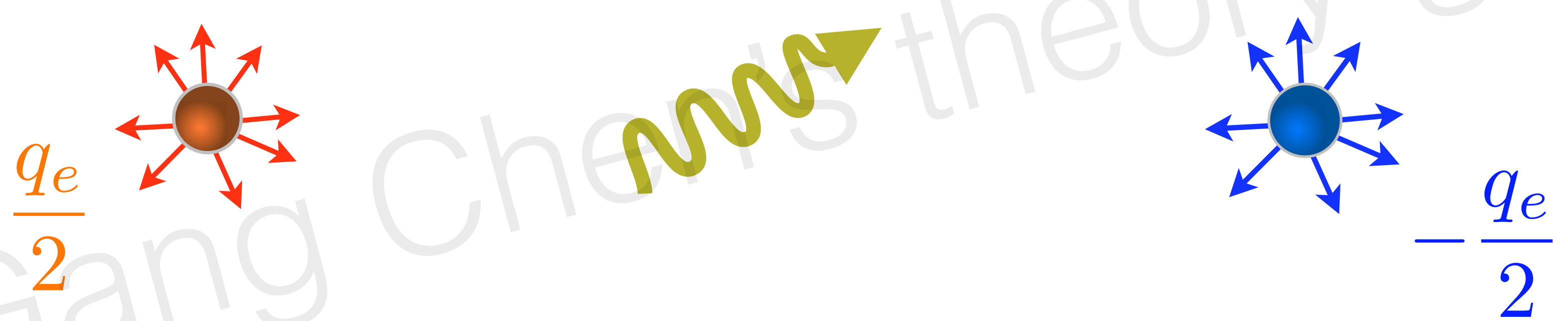


Charge fractionalization

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

Quantum spin ice in *L* = fractional charge liquid in charge sector

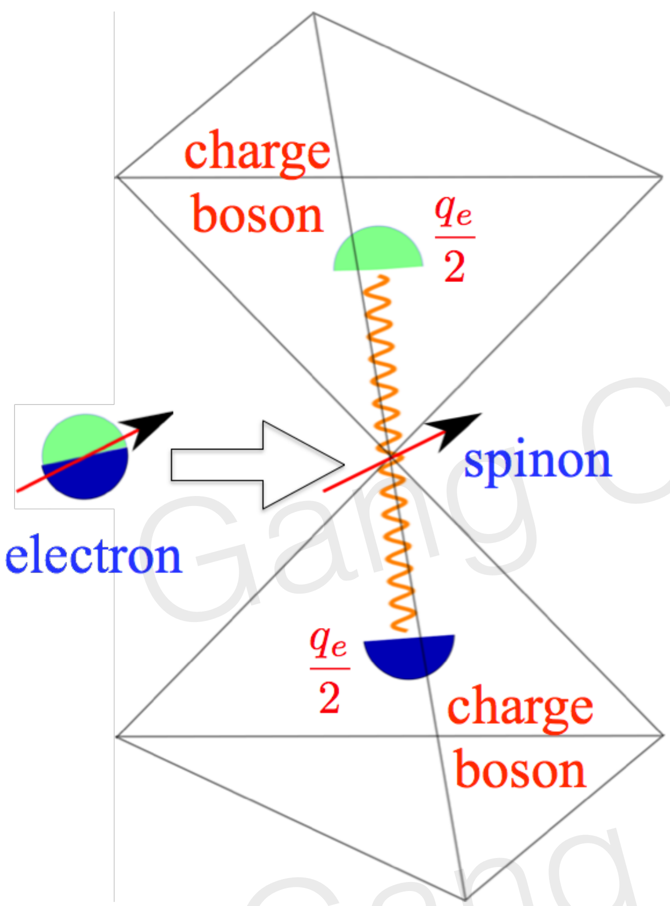
- Low-energy physics is described by an emergent (compact) quantum electrodynamics in 3+1D, indicating an **additional U(1) gauge structure** in the charge sector.



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

Slave particle description

$$c_{i\sigma}^{\dagger} = e^{i\theta_i} f_{i\sigma}^{\dagger} \quad \Longrightarrow \quad c_{i\sigma}^{\dagger} \;=\; \Phi_{\mathbf{r}}^{\dagger}\Phi_{\mathbf{r}'} l_{\mathbf{r}\mathbf{r}'}^{+} f_{i\sigma}^{\dagger}.$$



Cartoon of electron fractionalization in the Mott regime

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

The charge sector becomes

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

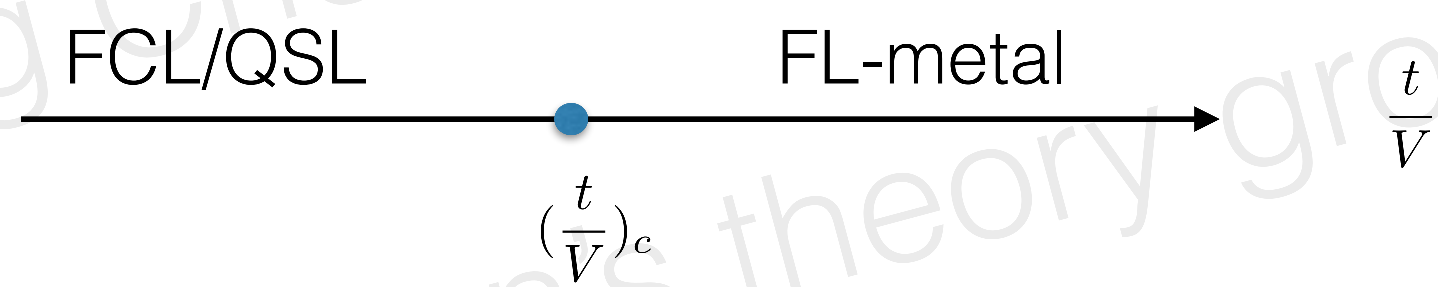
This describes the hopping of charge bosons which minimally couple to the U(1)$_{\text{ch}}$ gauge field (l) on the dual diamond lattice (i.e. centres of the tetrahedra)

Mott transition

Mott transition occurs when the charge boson condenses

metal: $\langle \Phi \rangle \neq 0$

FCL/QSL: $\langle \Phi \rangle = 0$

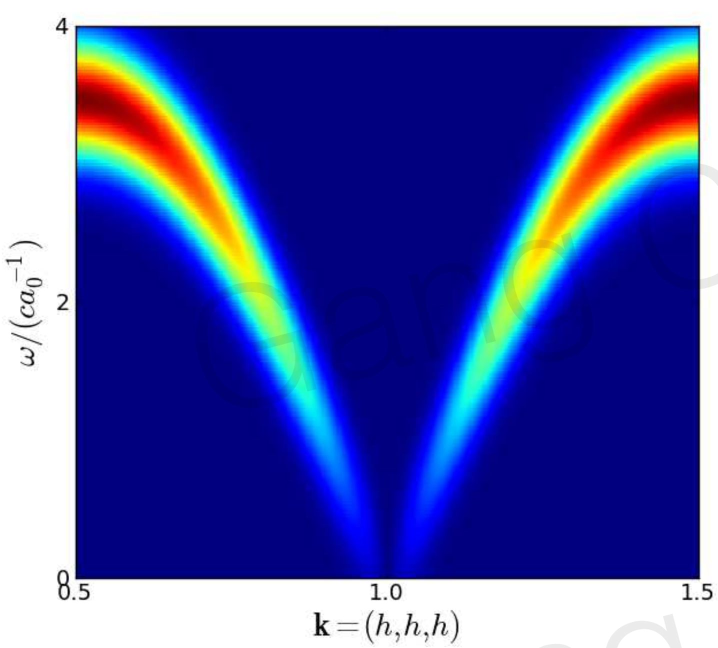


When the charge bosons are condensed, the $U(1)_{ch}$ gauge field is gapped from the Higgs' mechanism. The charge fractionalization is then destroyed. The charge rotor is also condensed from which the $U(1)_{sp}$ gauge field picks up a mass. The spinon and charge rotor are then combined back into a full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

- (Inelastic) X-ray scattering measures $U(1)_{ch}$ gauge field correlation

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

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



O. Benton *et al*, 2012

$I(\omega) \sim \omega$

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

Pinch points in equal-time charge structure factor

Pyrochlore Mott insulators 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

M. M. Abd-Elmeguid,[1] B. Ni,[1] D. I. Khomskii,[1,*] R. Pocha,[2] D. Johrendt,[2] X. Wang,[3] and K. Syassen[3]
[1]*II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany*
[2]*Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstrasse 5-13 (Haus D), 81377 München, Germany*
[3]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany*
(Received 30 April 2004; published 16 September 2004)

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

VOLUME 85, NUMBER 5 PHYSICAL REVIEW LETTERS 31 JULY 2000

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

C. Urano,[1] M. Nohara,[1] S. Kondo,[1] F. Sakai,[2] H. Takagi,[1,3] T. Shiraki,[4] and T. Okubo[4]
[1]*Department of Advanced Materials Science and Department of Superconductivity, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[2]*Institute for Solid State Physics, University of Tokyo, Kashiwanoha, Kashiwa-shi, Chiba 277-8581, Japan*
[3]*CREST, Japan Science and Technology Corporation, Japan*
[4]*Department of Chemical System Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
(Received 27 January 2000)

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

and many others

Summary

- We propose an interesting exotic state 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.