Spectroscopic signatures of **spinon Fermi surface** in a rare-earth triangular lattice spin liquid

Gang Chen
Fudan University, Shanghai, China

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Outline

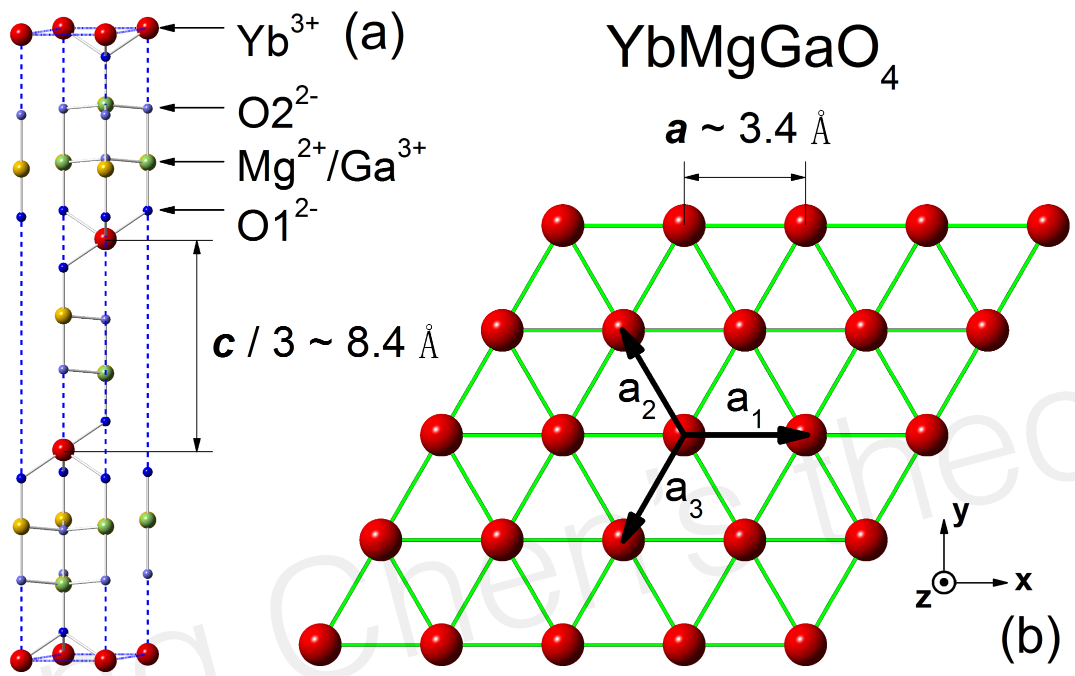
1. Spin quantum number fractionalization in $YbMgGaO_4$?
   Is it a spin liquid with a spinon Fermi surface?

2. Weak field regime: theoretical prediction and measurement

YD Li, XQ Wang, **GC***, PRB 94, 035107 (2016)
YD Li, XQ Wang, **GC***, PRB 94, 201114 (2016)
YD Li, Y Shen, YS Li, J Zhao, **GC***, PRB 97, xxxxxx (2018)
YD Li, YM Lu, **GC***, PRB 96, 054445 (2017)
YD Li, **GC***, PRB 96, 075105 (2017)

YS Li, **GC***, .., QM Zhang*, PRL 115, 167203 (2015)
Y Shen, YD Li, .., **GC***, J Zhao*, Nature, 540, 559 (2016)
Y Shen, YD Li, .., **GC***, J Zhao*, arXiv 1708.06655

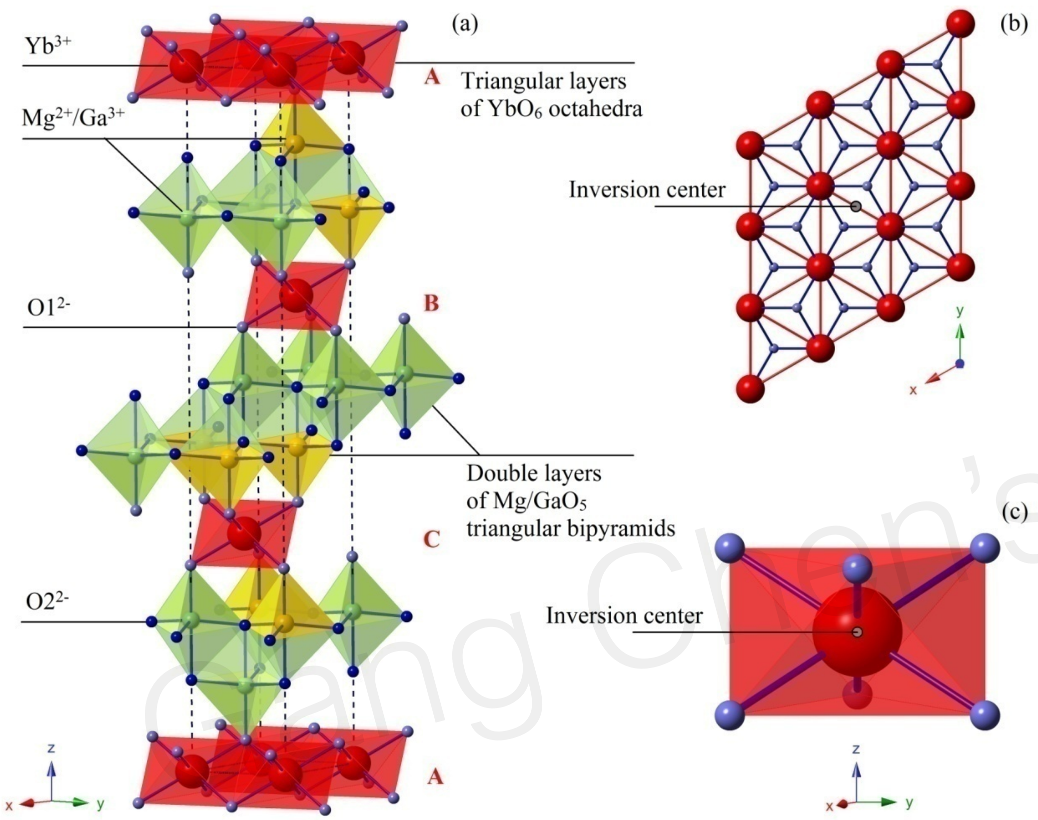
A rare-earth triangular lattice quantum spin liquid: **$YbMgGaO_4$**



Qingming Zhang
(Renmin)

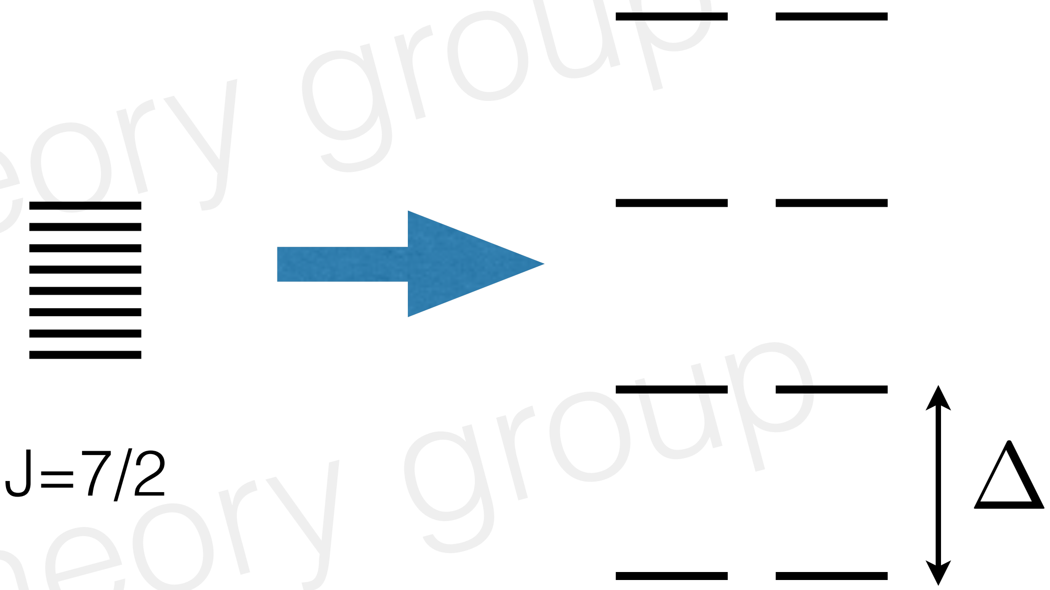
- Hastings-Oshikawa-Lieb-Shultz-Mattis theorem.
- Recent extension to spin-orbit coupled insulators (Watanabe, Po, Vishwanath, Zaletel, PNAS 2015).
- This is likely the **first strong spin-orbit coupled QSL with odd electron filling** and effective spin-1/2.
- It is the first clear observation of $T^{2/3}$ heat capacity. (needs comment.)
- Inelastic neutron scattering is consistent with spinon Fermi surface results.
- I think it is a spinon Fermi surface U(1) QSL.

The microscopics



YS Li, …QM Zhang, Srep 2015

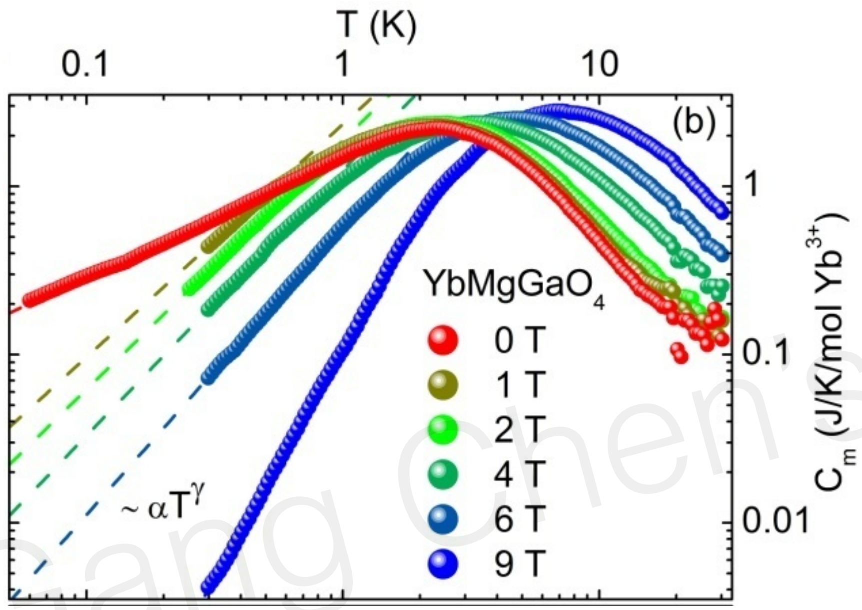
Yb^{3+} ion: $4f^{13}$ has J=7/2 due to SOC.



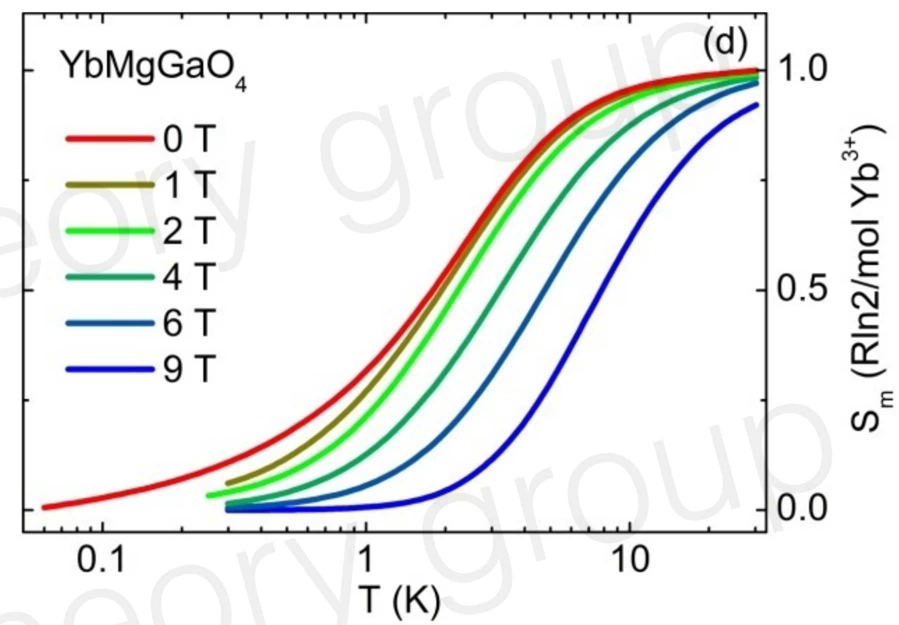
YS Li, **GC**, …, QM Zhang, PRL 2015
YD Li, XQ Wang, **GC**, arXiv1512, PRB 2016

At $T \ll \Delta$, the only active DOF is the ground state doublet that gives rise to an effective spin-1/2.

YbMgGaO$_4$



- observation of $T^{2/3}$ heat capacity



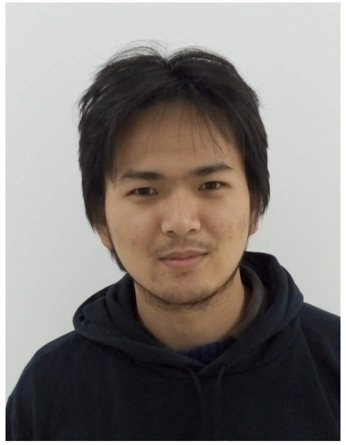
- Entropy: effective spin-1/2 local moments

No breaking of time reversal symmetry at finite temperature.

Our proposal for ground state: spinon Fermi surface U(1) QSL.

Modeling

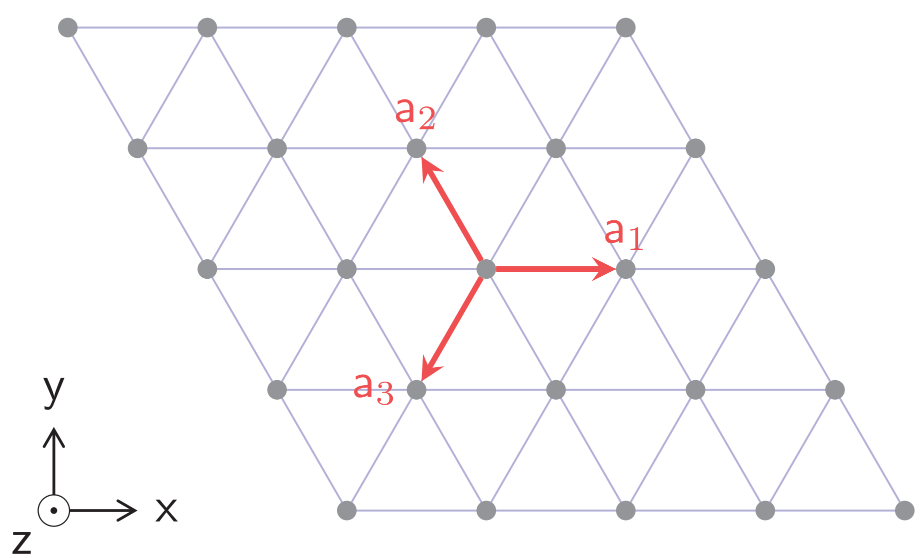
4f electron is very localized, and
dipolar interactions weak.



Yao-Dong Li
(Fudan -> UCSB)

$$\mathcal{H} = \sum_{\langle ij \rangle} \Big[J_{zz} S_i^z S_j^z + J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm}(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) - \frac{i J_{z\pm}}{2}(\gamma_{ij}^* S_i^+ S_j^z - \gamma_{ij} S_i^- S_j^z + \langle i \leftrightarrow j \rangle) \Big], \quad (1)$$

where $S_i^{\pm} = S_i^x \pm i S_i^y$, and the phase factor $\gamma_{ij} = 1, e^{i2\pi/3}, e^{-i2\pi/3}$ for the bond ij along the $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ direction (see Fig. 1), respectively. This generic Hamil-



anisotropic both in spin space and in real space !

YD Li, XQ Wang, GC, arXiv1512, PRB 2016
YD Li, Y Shen, YS Li, J Zhao, GC*, arXiv 1608.06445, PRB

DMRG: Chernyshev, White, 2017
Jize Zhao, XQ Wang, 2017

Polarized neutron scattering

Strong exchange anisotropy in $YbMgGaO_4$ from polarized neutron diffraction

Sándor Tóth,[1,*] Katharina Rolfs,[2] Andrew R. Wildes,[3] and Christian Rüegg[1,4]

[1] *Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland*

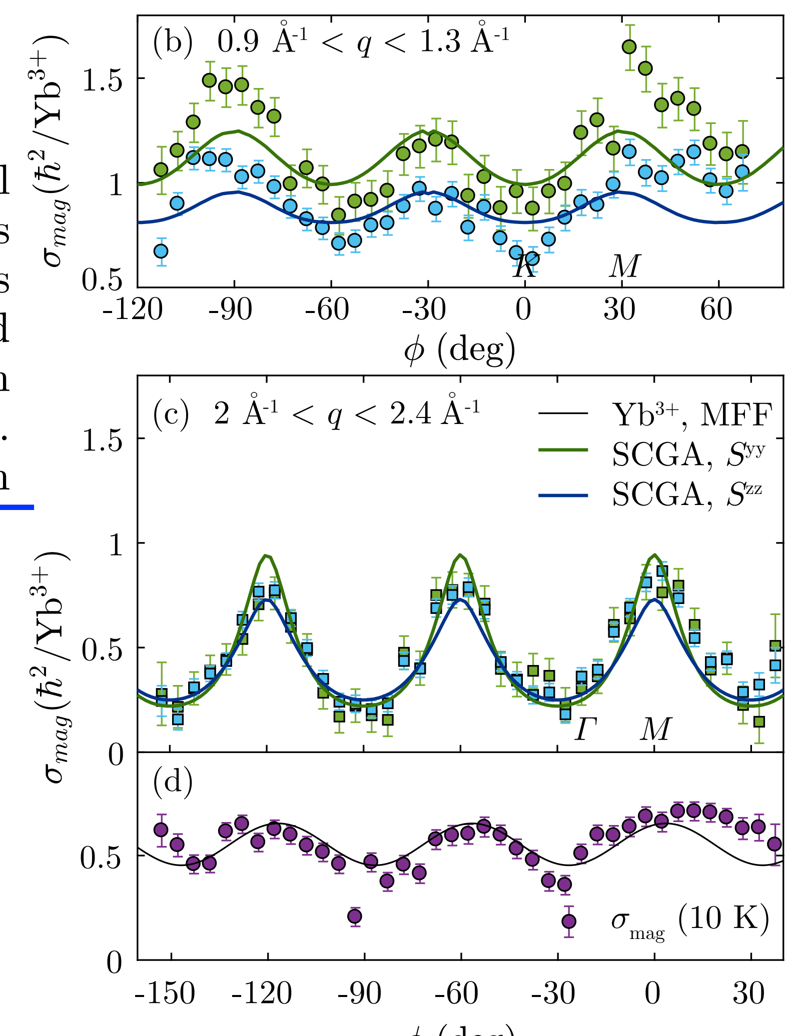
[2] *Laboratory for Scientific Developments and Novel Materials, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland*

[3] *Institut Max von Laue-Paul Langevin, 38042 Grenoble 9, France*

[4] *Department of Quantum Matter Physics, University of Geneva, 1211 Genève, Switzerland*

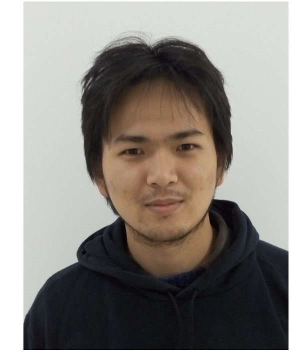
(Dated: May 17, 2017)

We measured the magnetic correlations in the triangular lattice spin-liquid candidate material $YbMgGaO_4$ via polarized neutron diffraction. The extracted in-plane and out-of-plane components of the magnetic structure factor show clear anisotropy. We found that short-range correlations persist at the lowest measured temperature of 52 mK and neutron scattering intensity is centered at the M middle-point of the hexagonal Brillouin-zone edge. Moreover, we found pronounced spin anisotropy, with different correlation lengths for the in-plane and out-of-plane spin components. When comparing to a self-consistent Gaussian appoximation, our data clearly support a model with only first-neighbor coupling and strongly anisotropic exchanges.



arXiv 1705.05699

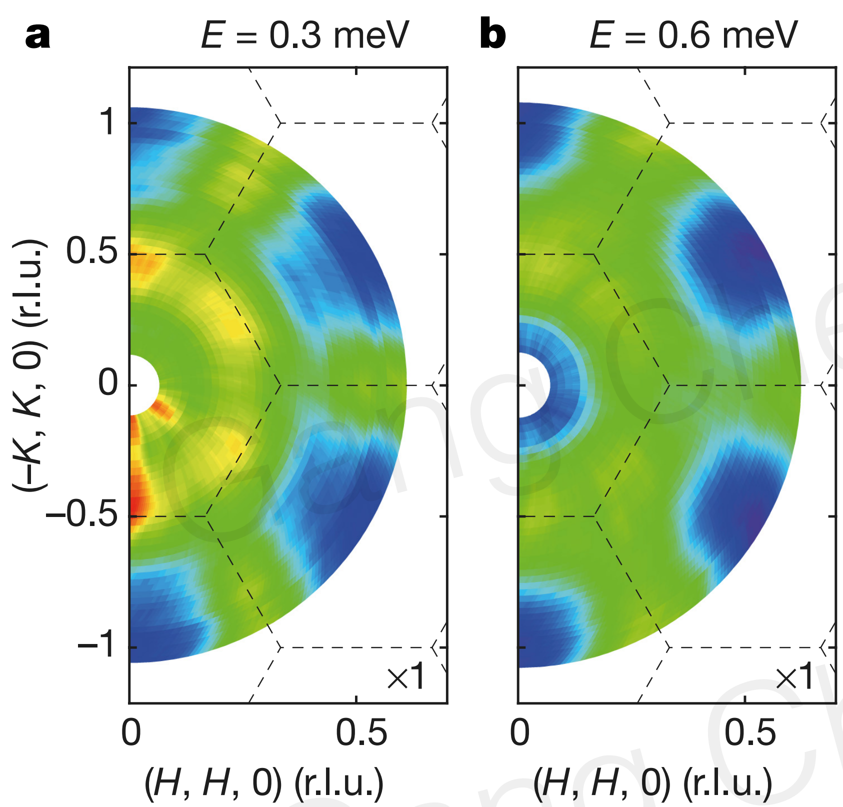
Inelastic neutron scattering

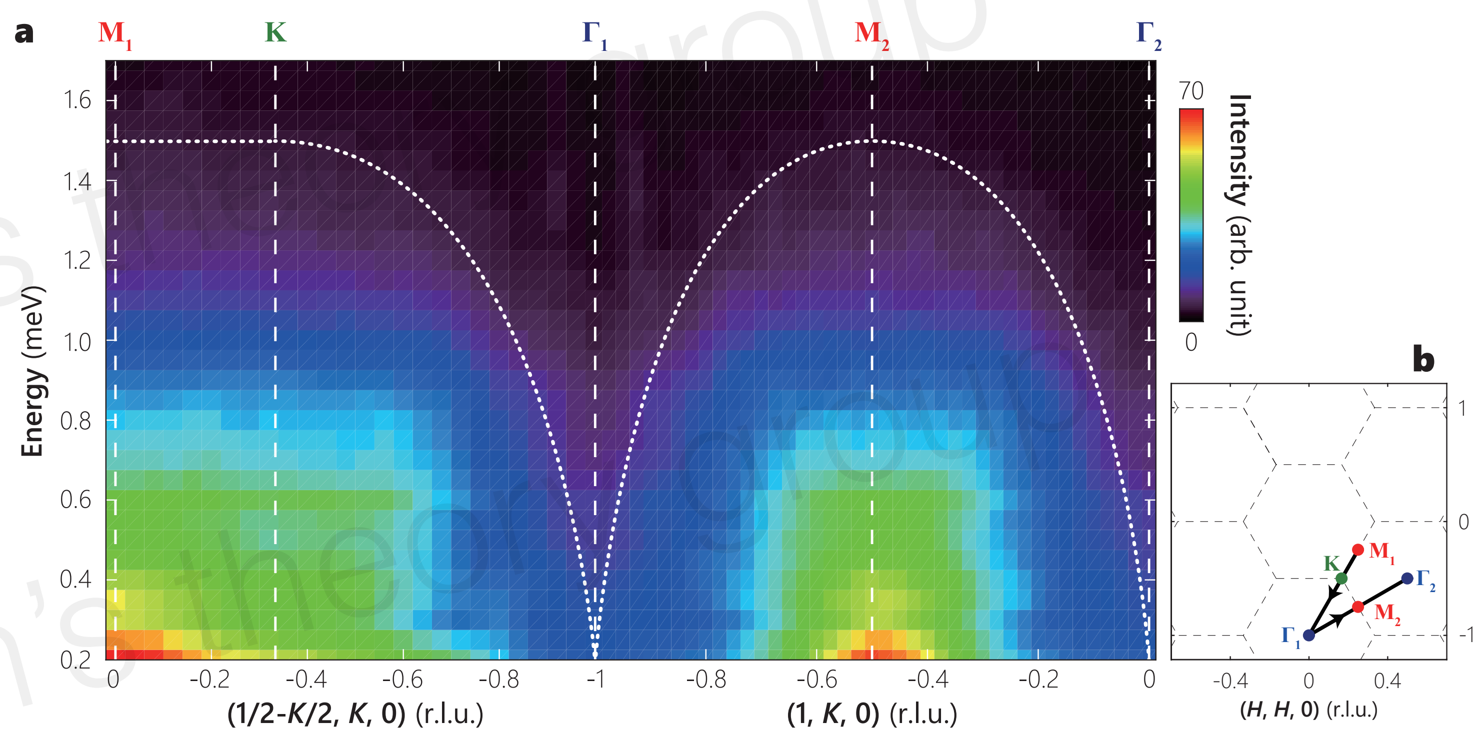


Yao Shen
(Fudan)

Yao-Dong Li
(Fudan->UCSB)

Jun Zhao
(Fudan)

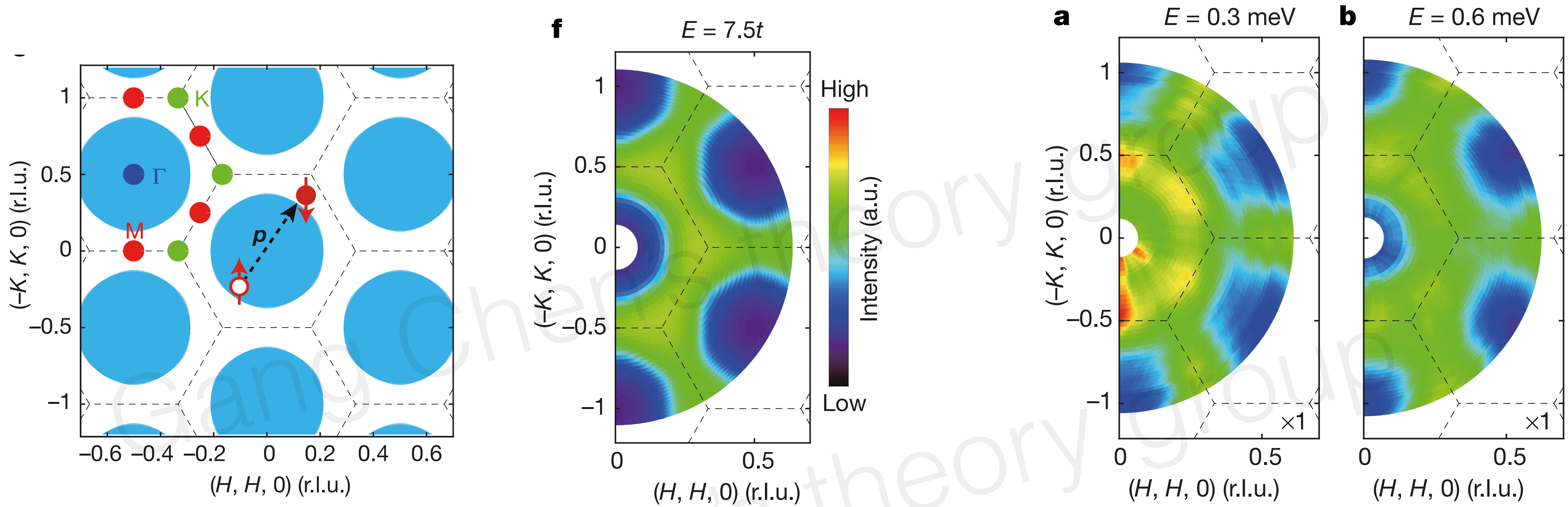




Y Shen, YD Li …GC*, J Zhao* **Nature** 2016

consistent neutron results from Martin Mourigal's group, Nature Physics

Spinon Fermi surface state

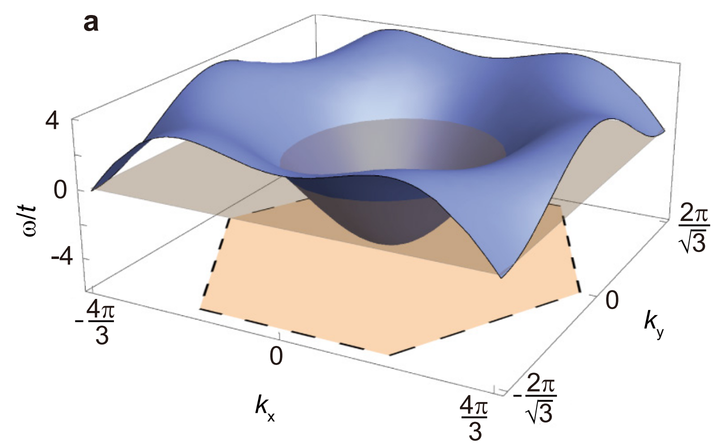


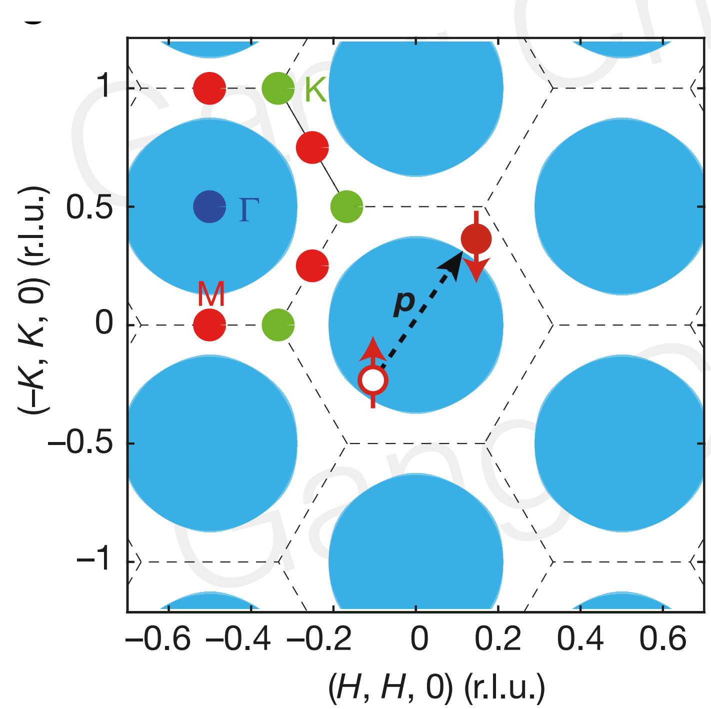
$$S_{\boldsymbol{r}} = \frac{1}{2}\sum_{\alpha,\beta} f^{\dagger}_{\boldsymbol{r}\alpha}\boldsymbol{\sigma}_{\alpha\beta} f_{\boldsymbol{r}\beta}, \qquad H_{\mathrm{MFT}} = -\,t\sum_{\langle ij\rangle}(f^{\dagger}_{i\alpha}f_{j\alpha} + \mathrm{h.c.}) - \mu\sum_{i} f^{\dagger}_{i\alpha}f_{i\alpha}$$

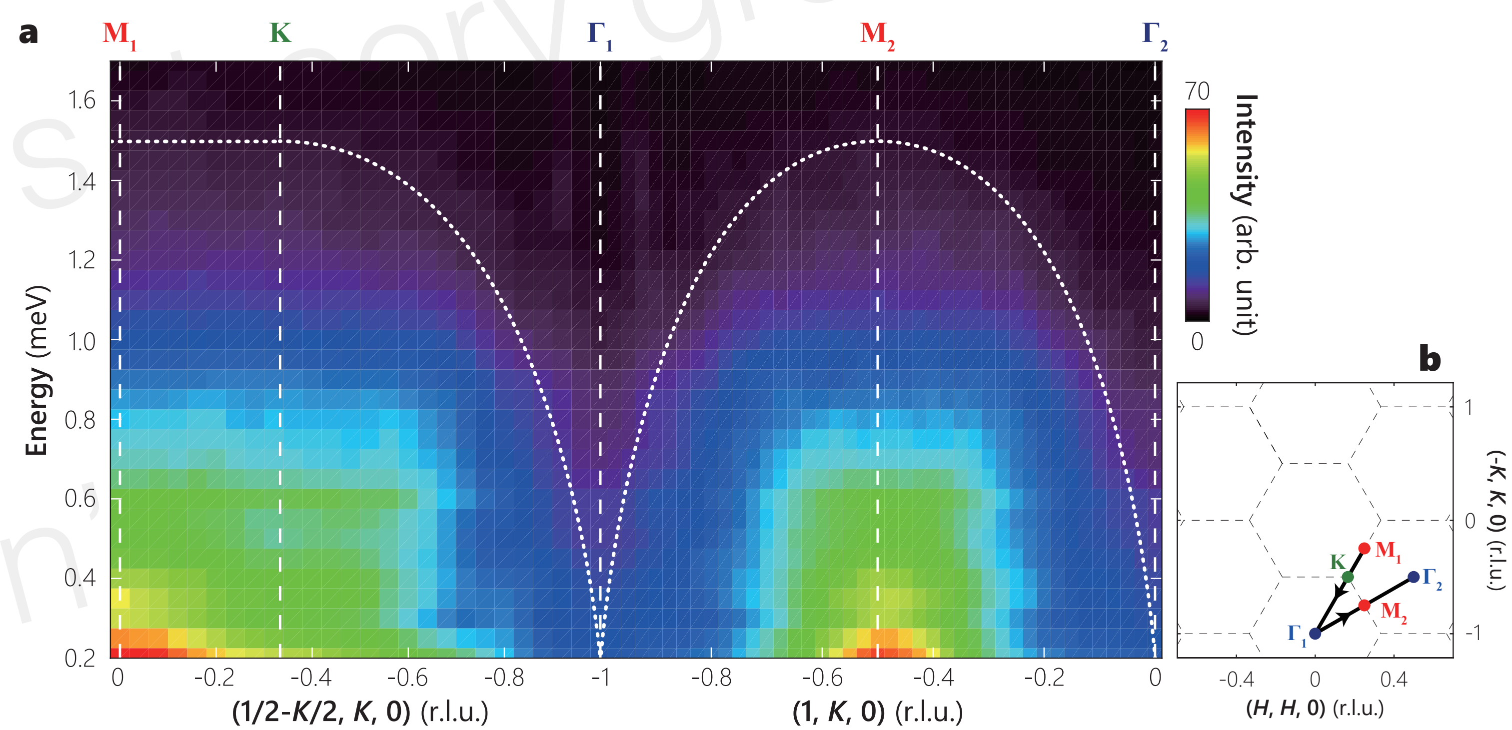
Prediction from the 0 flux uniform spinon hopping

Y Shen, YD Li …GC*, J Zhao* **Nature** 2016

Particle-hole continuum of the spinon Fermi surface

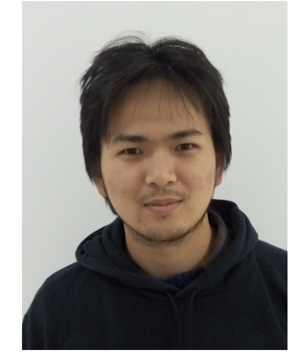






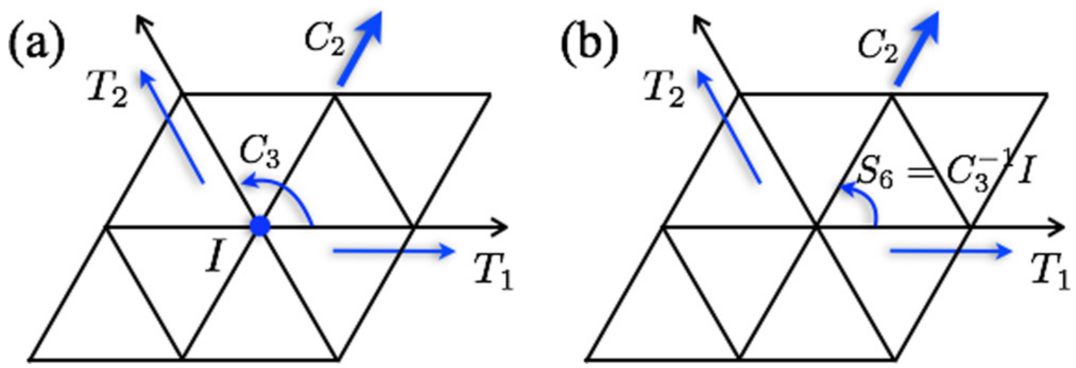
Y Shen, YD Li **…GC*, J Zhao*** **Nature** 2016

More assurance from projective symmetry group analysis



Yao-Dong Li (Fudan->UCSB)

Yuan-Ming Lu (OSU)



$$T_1^{-1} T_2 T_1 T_2^{-1} = T_1^{-1} T_2^{-1} T_1 T_2 = 1,$$

$$C_2^{-1} T_1 C_2 T_2^{-1} = C_2^{-1} T_2 C_2 T_1^{-1} = 1,$$

$$S_6^{-1} T_1 S_6 T_2 = S_6^{-1} T_2 S_6 T_2^{-1} T_1^{-1} = 1,$$

$$(C_2)^2 = (S_6)^6 = (S_6 C_2)^2 = 1.$$

YD Li, XQ Wang, **GC**, arXiv1512, PRB 2016

YD Li, YM Lu, GC, arXiv **1612.03447**, PRB

$$\boldsymbol{S}_{\boldsymbol{r}} = \frac{1}{2} \sum_{\alpha,\beta} f^{\dagger}_{\boldsymbol{r}\alpha} \boldsymbol{\sigma}_{\alpha\beta} f_{\boldsymbol{r}\beta},$$

$$\Psi_{\boldsymbol{r}} = (f_{\boldsymbol{r}\uparrow}, f^{\dagger}_{\boldsymbol{r}\downarrow}, f_{\boldsymbol{r}\downarrow}, -f^{\dagger}_{\boldsymbol{r}\uparrow})^T$$

$$\boldsymbol{S}_{\boldsymbol{r}} = \frac{1}{4} \Psi^{\dagger}_{\boldsymbol{r}} (\boldsymbol{\sigma} \otimes I_{2\times 2}) \Psi_{\boldsymbol{r}},$$

$$\boldsymbol{G}_{\boldsymbol{r}} = \frac{1}{4} \Psi^{\dagger}_{\boldsymbol{r}} (I_{2\times 2} \otimes \boldsymbol{\sigma}) \Psi_{\boldsymbol{r}},$$

$$[S^{\mu}_{\boldsymbol{r}}, G^{\nu}_{\boldsymbol{r}}] = 0.$$

The spin transformation and gauge transformation commute with each other.

XG Wen PRB 2002

Reduction and simplification: classification mean field states

Mean-field model
$$H_{\mathrm{MF}} = -\frac{1}{2}\sum_{(\boldsymbol{r},\boldsymbol{r}')}\left[\Psi_{\boldsymbol{r}}^{\dagger}u_{\boldsymbol{r}\boldsymbol{r}'}\Psi_{\boldsymbol{r}'} + h.c.\right],$$
$$\Psi_{\boldsymbol{r}} = (f_{\boldsymbol{r}\uparrow}, f_{\boldsymbol{r}\downarrow}^{\dagger}, f_{\boldsymbol{r}\downarrow}, -f_{\boldsymbol{r}\uparrow}^{\dagger})^{T}$$

symmetry transformation $\mathcal{O}$
$$u_{\boldsymbol{r}\boldsymbol{r}'} = \mathcal{G}_{\mathcal{O}(\boldsymbol{r})}^{\mathcal{O}\dagger}\mathcal{U}_{\mathcal{O}}^{\dagger}u_{\mathcal{O}(\boldsymbol{r})\mathcal{O}(\boldsymbol{r}')}\mathcal{U}_{\mathcal{O}}\mathcal{G}_{\mathcal{O}(\boldsymbol{r}')}^{\mathcal{O}}.$$

spin rotation

gauge rotation

group relation $\mathcal{O}_1\mathcal{O}_2\mathcal{O}_3\mathcal{O}_4 = 1$

$$\begin{aligned}&\mathcal{U}_{\mathcal{O}_1}\mathcal{G}_{\boldsymbol{r}}^{\mathcal{O}_1}\mathcal{U}_{\mathcal{O}_2}\mathcal{G}_{\mathcal{O}_2\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_2}\mathcal{U}_{\mathcal{O}_3}\mathcal{G}_{\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_3}\mathcal{U}_{\mathcal{O}_4}\mathcal{G}_{\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_4}\\ =&\,\mathcal{U}_{\mathcal{O}_1}\mathcal{U}_{\mathcal{O}_2}\mathcal{U}_{\mathcal{O}_3}\mathcal{U}_{\mathcal{O}_4}\mathcal{G}_{\boldsymbol{r}}^{\mathcal{O}_1}\mathcal{G}_{\mathcal{O}_2\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_2}\mathcal{G}_{\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_3}\mathcal{G}_{\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_4}\\ \in&\,\mathrm{IGG},\end{aligned}$$

$$\mathcal{U}_{\mathcal{O}_1}\mathcal{U}_{\mathcal{O}_2}\mathcal{U}_{\mathcal{O}_3}\mathcal{U}_{\mathcal{O}_4} = \pm I_{4\times4}, \qquad \{\pm I_{4\times4}\}\subset \mathrm{IGG}$$

$$\mathcal{G}_{\boldsymbol{r}}^{\mathcal{O}_1}\mathcal{G}_{\mathcal{O}_2\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_2}\mathcal{G}_{\mathcal{O}_3\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_3}\mathcal{G}_{\mathcal{O}_4(\boldsymbol{r})}^{\mathcal{O}_4}\in\mathrm{IGG}$$

square lattice by J Alicea's group 2014

Projective symmetry group classification

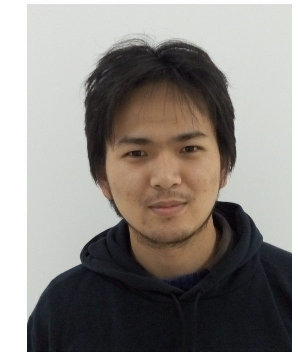
U(1) QSL	$W_{\boldsymbol{r}}^{T_1}$	$W_{\boldsymbol{r}}^{T_2}$	$W_{\boldsymbol{r}}^{C_2}$	$W_{\boldsymbol{r}}^{C_6}$
U1A00	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$
U1A10	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$	$I_{2\times2}$
U1A01	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$
U1A11	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$	$i\sigma^y$
U1B00	$I_{2\times2}$	$(-1)^x I_{2\times2}$	$(-1)^{xy} I_{2\times2}$	$(-1)^{xy-\frac{y(y-1)}{2}} I_{2\times2}$
U1B10	$I_{2\times2}$	$(-1)^x I_{2\times2}$	$i\sigma^y(-1)^{xy}$	$(-1)^{xy-\frac{y(y-1)}{2}} I_{2\times2}$
U1B01	$I_{2\times2}$	$(-1)^x I_{2\times2}$	$(-1)^{xy} I_{2\times2}$	$i\sigma^y(-1)^{xy-\frac{y(y-1)}{2}}$
U1B11	$I_{2\times2}$	$(-1)^x I_{2\times2}$	$i\sigma^y(-1)^{xy}$	$i\sigma^y(-1)^{xy-\frac{y(y-1)}{2}}$

TABLE III. The transformation for the spinons under four U1A PSGs that are labeled by U1A$n_{C_2} n_{S_6}$.

U(1) PSGs	T_1	T_2	C_2	S_6
U1A00	$f_{(x,y),\uparrow} \to f_{(x+1,y),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x+1,y),\downarrow}$	$f_{(x,y),\uparrow} \to f_{(x,y+1),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x,y+1),\downarrow}$	$f_{(x,y),\uparrow} \to e^{i\frac{\pi}{6}} f_{(y,x),\downarrow}$ $f_{(x,y),\downarrow} \to e^{i\frac{5\pi}{6}} f_{(y,x),\uparrow}$	$f_{(x,y),\uparrow} \to e^{-i\frac{\pi}{3}} f_{(x-y,x),\uparrow}$ $f_{(x,y),\downarrow} \to e^{+i\frac{\pi}{3}} f_{(x-y,x),\downarrow}$
U1A10	$f_{(x,y),\uparrow} \to f_{(x+1,y),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x+1,y),\downarrow}$	$f_{(x,y),\uparrow} \to f_{(x,y+1),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x,y+1),\downarrow}$	$f_{(x,y),\uparrow} \to e^{i\frac{\pi}{6}} f^{\dagger}_{(y,x),\uparrow}$ $f_{(x,y),\downarrow} \to e^{-i\frac{\pi}{6}} f^{\dagger}_{(y,x),\downarrow}$	$f_{(x,y),\uparrow} \to e^{-i\frac{\pi}{3}} f_{(x-y,x),\uparrow}$ $f_{(x,y),\downarrow} \to e^{+i\frac{\pi}{3}} f_{(x-y,x),\downarrow}$
U1A01	$f_{(x,y),\uparrow} \to f_{(x+1,y),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x+1,y),\downarrow}$	$f_{(x,y),\uparrow} \to f_{(x,y+1),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x,y+1),\downarrow}$	$f_{(x,y),\uparrow} \to e^{i\frac{\pi}{6}} f_{(y,x),\downarrow}$ $f_{(x,y),\downarrow} \to e^{i\frac{5\pi}{6}} f_{(y,x),\uparrow}$	$f_{(x,y),\uparrow} \to -e^{-i\frac{\pi}{3}} f^{\dagger}_{(x-y,x),\downarrow}$ $f_{(x,y),\downarrow} \to e^{+i\frac{\pi}{3}} f^{\dagger}_{(x-y,x),\uparrow}$
U1A11	$f_{(x,y),\uparrow} \to f_{(x+1,y),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x+1,y),\downarrow}$	$f_{(x,y),\uparrow} \to f_{(x,y+1),\uparrow}$ $f_{(x,y),\downarrow} \to f_{(x,y+1),\downarrow}$	$f_{(x,y),\uparrow} \to e^{i\frac{\pi}{6}} f^{\downarrow\dagger}_{(y,x),\uparrow}$ $f_{(x,y),\downarrow} \to e^{-i\frac{\pi}{6}} f^{\downarrow\dagger}_{(y,x),\downarrow}$	$f_{(x,y),\uparrow} \to -e^{-i\frac{\pi}{3}} f^{\dagger}_{(x-y,x),\downarrow}$ $f_{(x,y),\downarrow} \to e^{+i\frac{\pi}{3}} f^{\dagger}_{(x-y,x),\uparrow}$

Gang Chen's theory group

Spectroscopic constraints

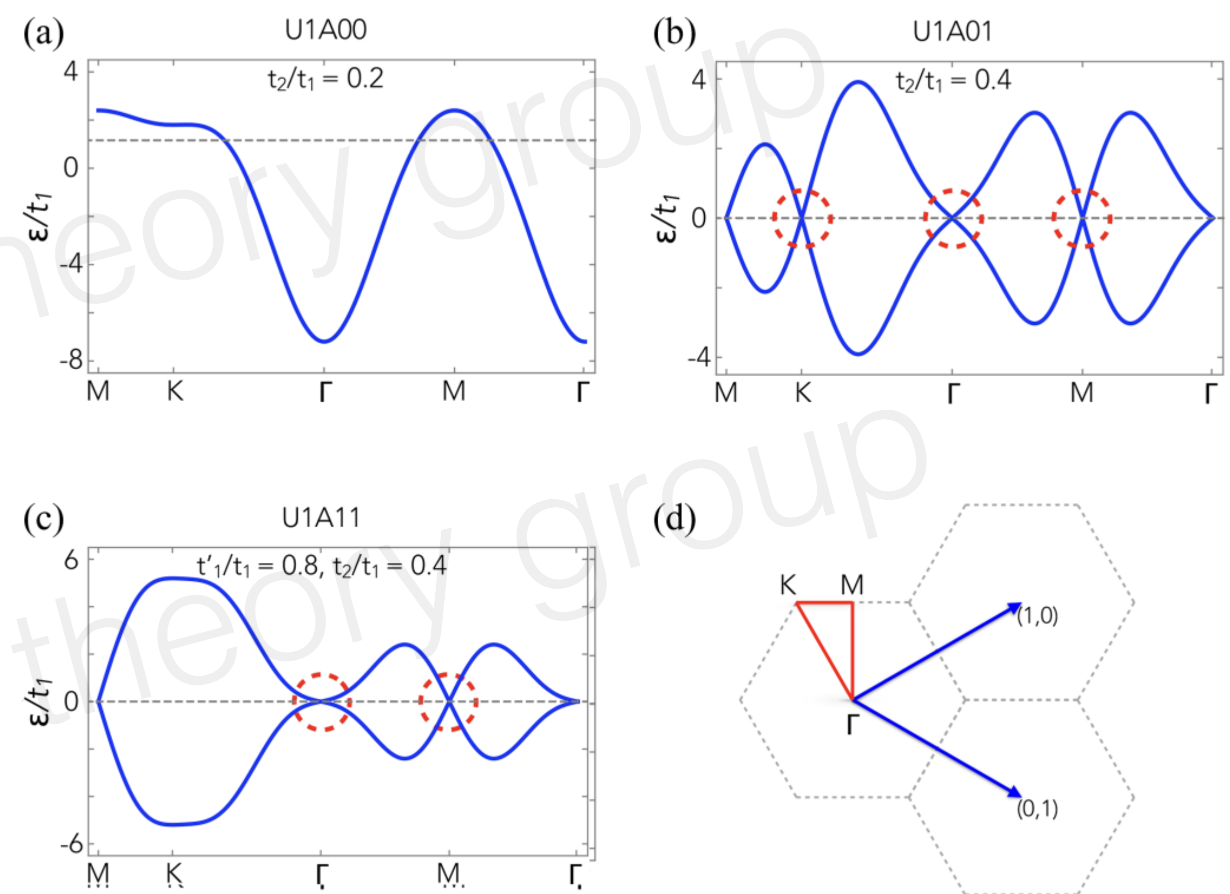


Yao-Dong Li

We use PSG to predict the corresponding spectrum.

$$H_{\rm MF} = -\sum_{(\boldsymbol{r}\boldsymbol{r}')}\sum_{\alpha\beta}\big[\,t_{\boldsymbol{r}\boldsymbol{r}',\alpha\beta} f^{\dagger}_{\boldsymbol{r}\alpha} f_{\boldsymbol{r}'\beta} + h.c.\,\big],$$

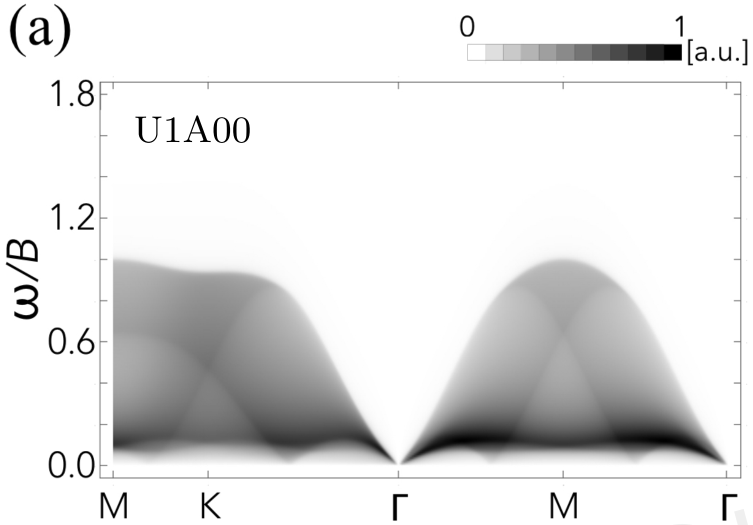
U(1) QSL	$W_{\boldsymbol{r}}^{T_1}$	$W_{\boldsymbol{r}}^{T_2}$	$W_{\boldsymbol{r}}^{C_2}$	$W_{\boldsymbol{r}}^{C_6}$
U1A00	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$
U1A10	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$	$I_{2\times2}$
U1A01	$I_{2\times2}$	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$
U1A11	$I_{2\times2}$	$I_{2\times2}$	$i\sigma^y$	$i\sigma^y$



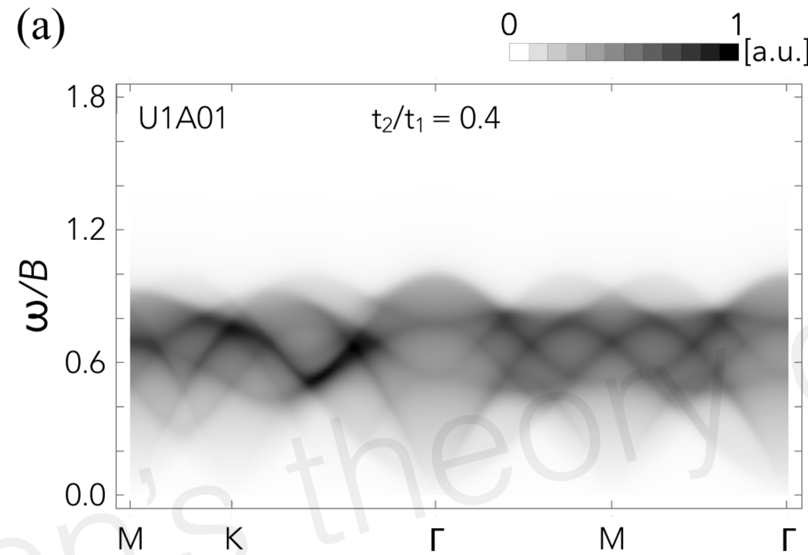
The U1A00 state is the spinon Fermi surface state that we proposed in Shen, et al, Nature.

VMC study has been done bty Balents' group

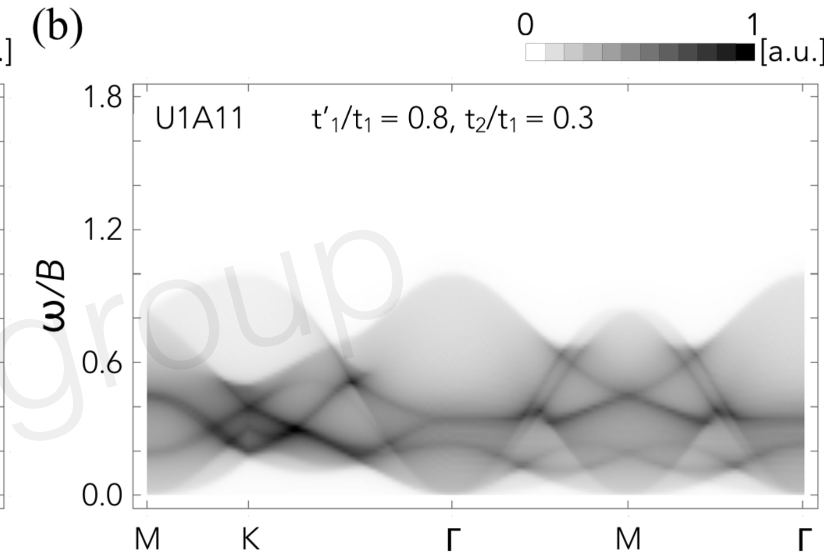
Dynamic spin structure factor



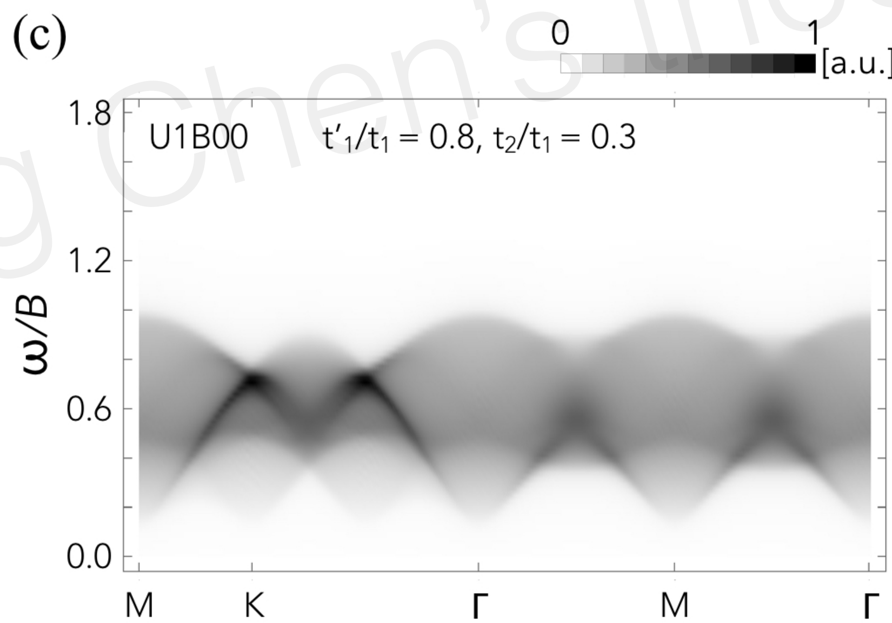
U1A00



U1A01



U1A11

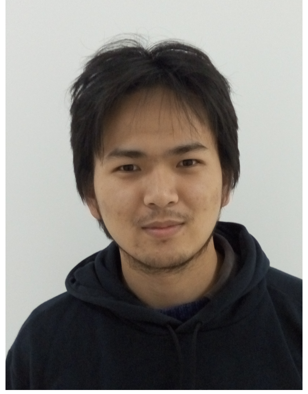


U1B state

2. Weak field regime: theoretical prediction and measurement

YD Li, **GC***,	PRB 96, 075105 (2017)
Y Shen, YD Li, .., **GC***, J Zhao*,	arXiv 1708.06655

Explore the weak field regime



Yao-Dong Li
(Fudan -> UCSB)

Continuing the recent proposal of the spinon Fermi surface U(1) spin liquid state for $YbMgGaO_4$ in Yao-Dong Li, *et al*, arXiv:1612.03447 and Yao Shen, *et al*, Nature 2016, we explore the experimental consequences of the external magnetic fields on this exotic state. Specifically, we focus on the *weak field regime* where the spin liquid state is preserved and the fractionalized spinon excitations remain to be a good description of the magnetic excitations. From the spin-1/2 nature of the spinon excitation, we predict the unique features of spinon continuum when the magnetic field is applied to the system. Due to the small energy scale of the rare-earth magnets, our proposal for the spectral weight shifts in the magnetic fields can be immediately tested by inelastic neutron scattering experiments. Several other experimental aspects about the spinon Fermi surface and spinon excitations are discussed and proposed. Our work provides a new way to examine the fractionalized spinon excitation and the candidate spin liquid states in the rare-earth magnets like $YbMgGaO_4$.

Reasonable, Feasible, and Predictable.

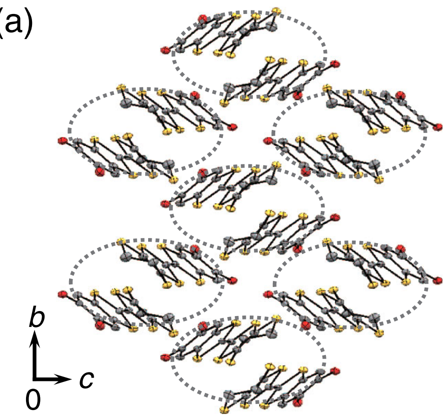
YD Li, **GC**, arXiv: **1703.01876**
PhysRevB, 96, 075105

ESR response in a field by Oleg Starykh's group, 2017

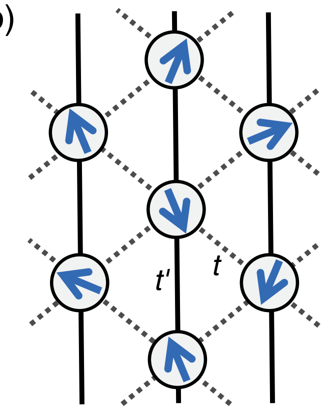
Organic spin liquids?

Kanoda

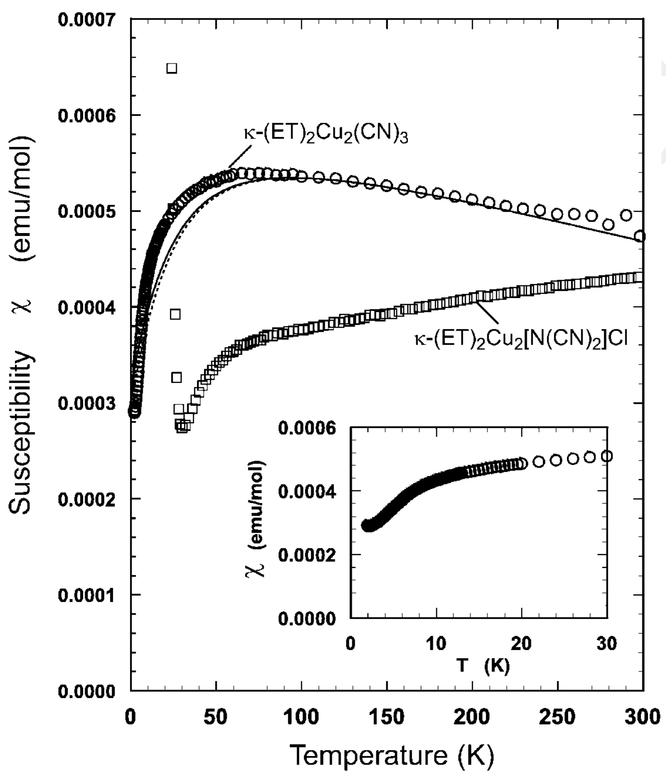
(a)

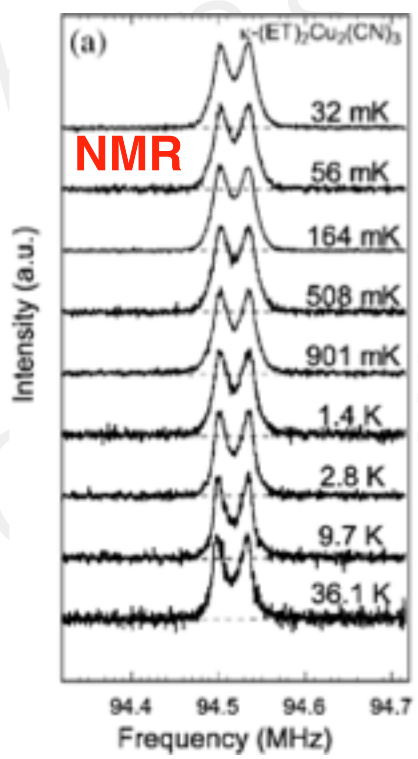


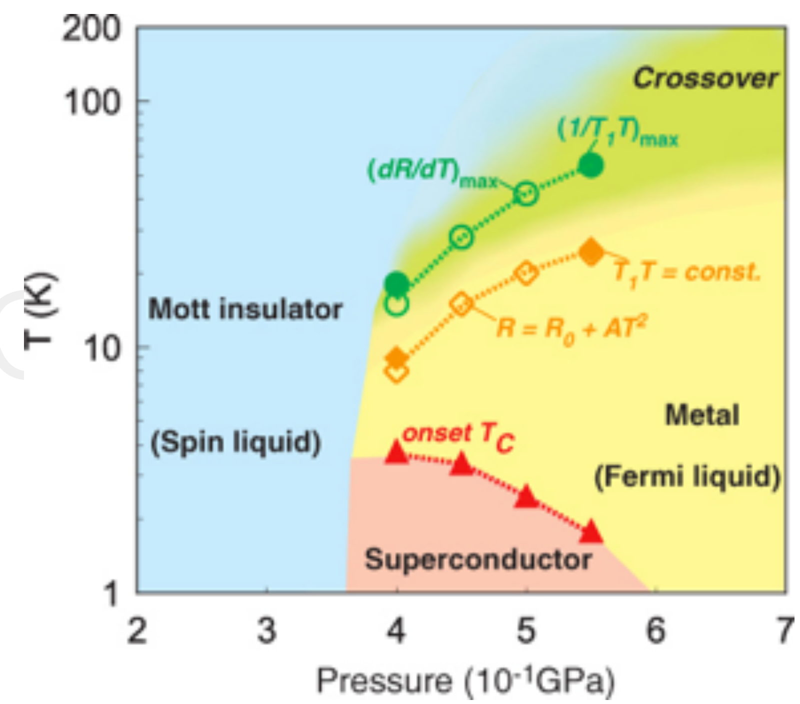
(b)



kappa-(BEDT-TTF)2Cu2(CN)3,
EtMe3Sb[Pd(dmit)2]2,
kappa–H3(Cat-EDT-TTF)2 **a new one!**



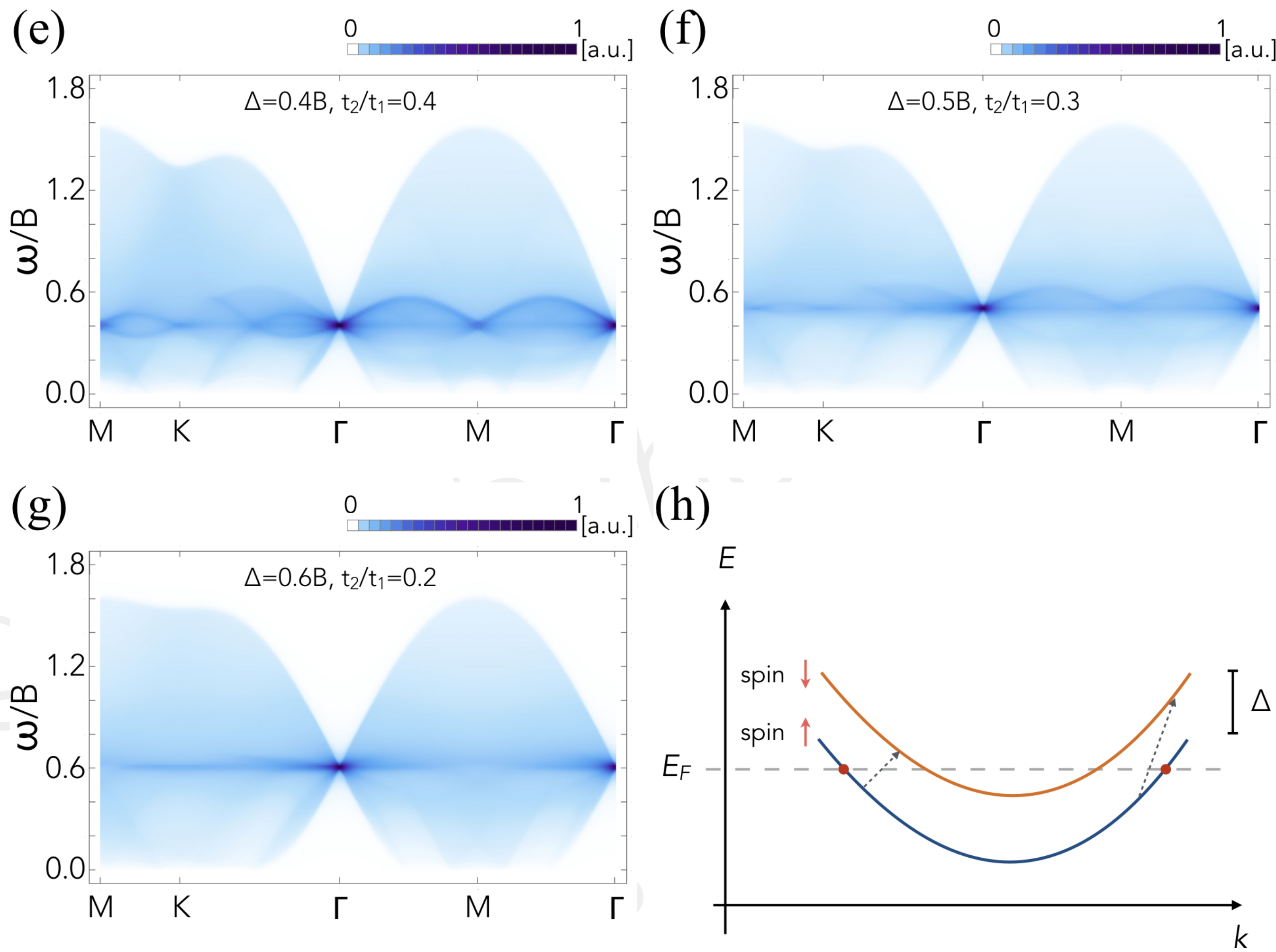




* No magnetic order down to 32mK
* Constant spin susceptibility at zero temperature

Other experiments: transport,
heat capacity, optical absorption, etc,
Unfortunately, **no neutron scattering** so far.

Prediction for dynamic spin structure factor



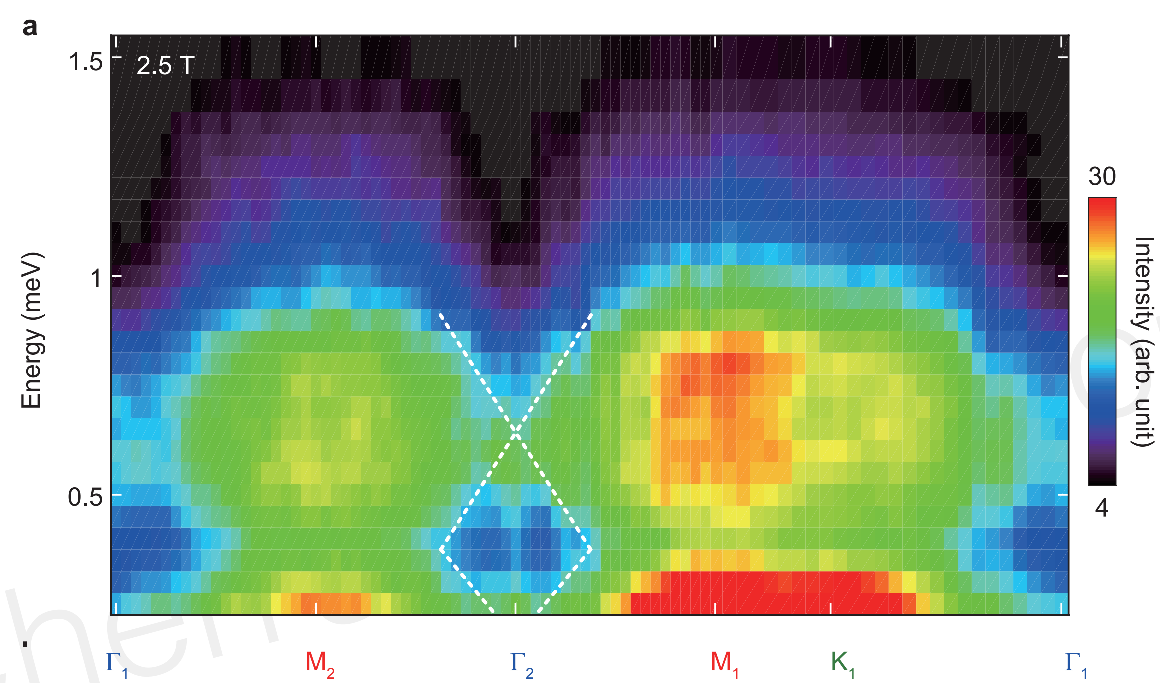
We predict:

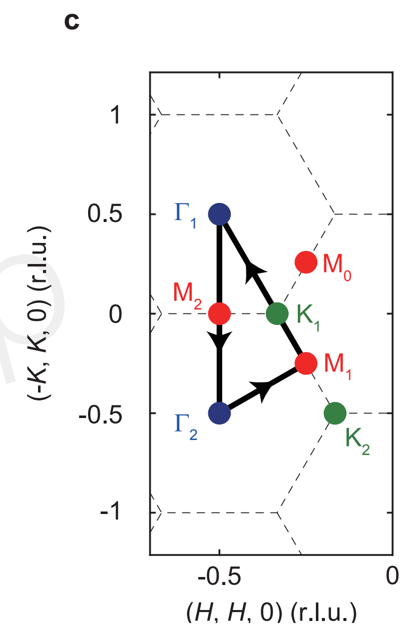
1. The system remains gapless and spinon continuum persists
2. spectral weight shifts
3. the spectral crossing at Gamma point
4. the presence of lower and upper excitation edges

Very different from magnon in the field !!

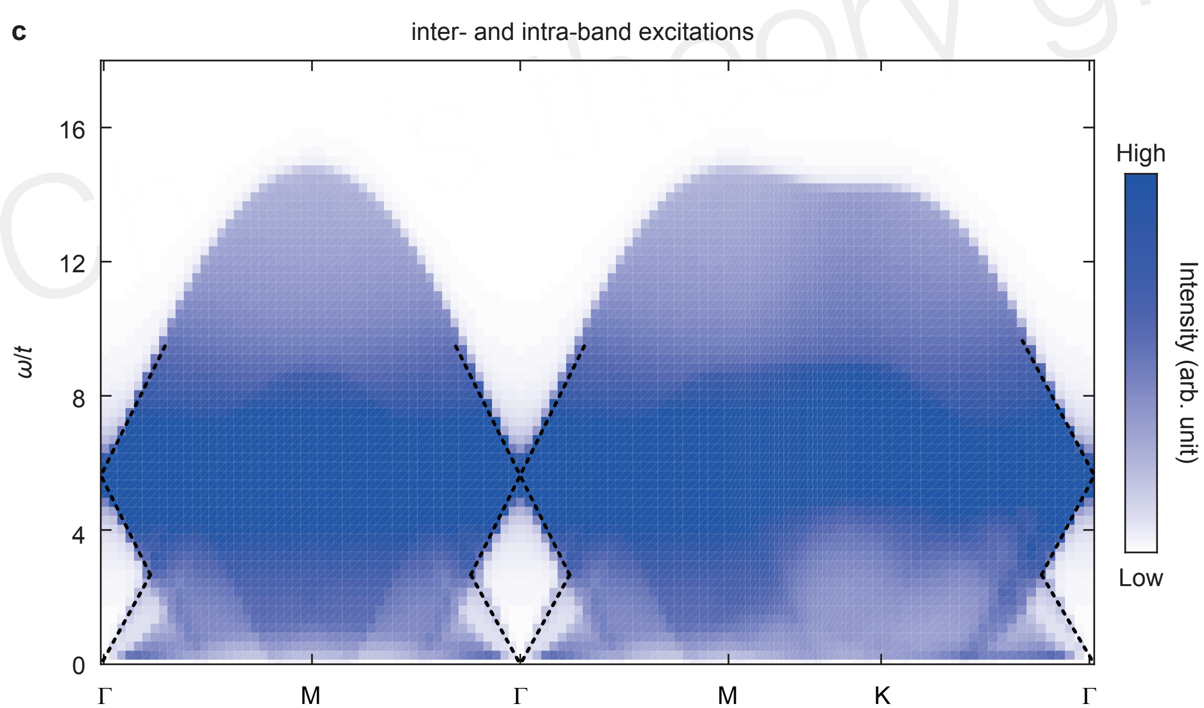
Excitation continuum in weakly magnetized YbMgGaO4

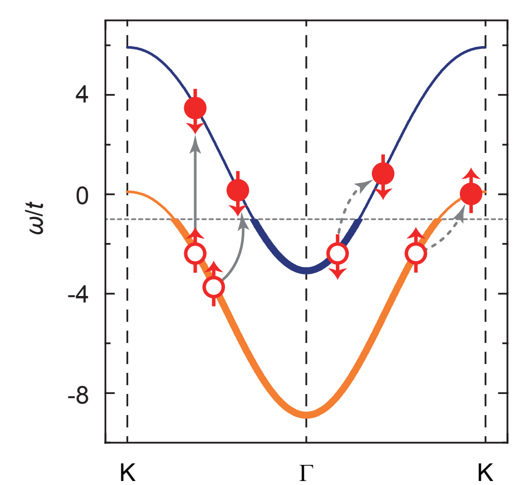
Experiment:
Y Shen, YD Li, …, GC*, J Zhao*
arXiv: 1708.06655





Theoretical results for
the experimental parameter





YD Li, **GC***, PRB 96, 075105 (2017)

Finally, lots of isostructural materials

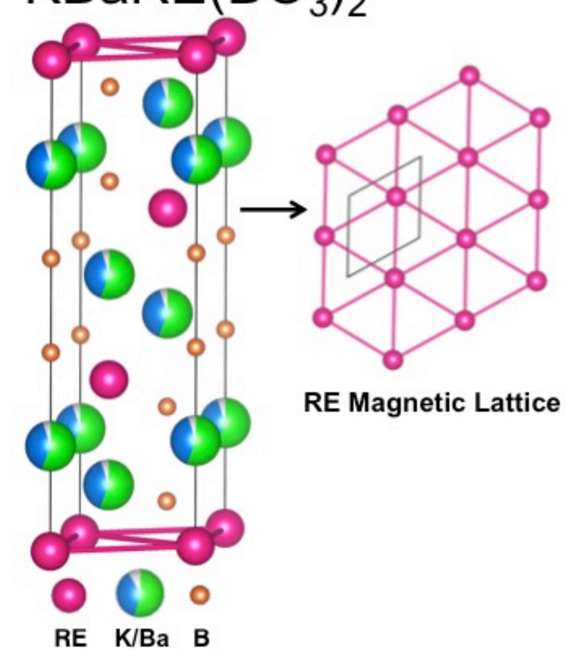
Compound	Magnetic ion	Space group	Local moment	Θ_{CW} (K)	Magnetic transition	Frustration para. f	Refs.
$YbMgGaO_4$	$Yb^{3+}(4f^{13})$	$R\bar{3}m$	Kramers doublet	-4	PM down to 60 mK	$f > 66$	[4]
$CeCd_3P_3$	$Ce^{3+}(4f^{1})$	$P6_3/mmc$	Kramers doublet	-60	PM down to 0.48 K	$f > 200$	[5]
$CeZn_3P_3$	$Ce^{3+}(4f^{1})$	$P6_3/mmc$	Kramers doublet	-6.6	AFM order at 0.8 K	$f = 8.2$	[7]
$CeZn_3As_3$	$Ce^{3+}(4f^{1})$	$P6_3/mmc$	Kramers doublet	-62	Unknown	Unknown	[8]
$PrZn_3As_3$	$Pr^{3+}(4f^{2})$	$P6_3/mmc$	Non-Kramers doublet	-18	Unknown	Unknown	[8]
$NdZn_3As_3$	$Nd^{3+}(4f^{3})$	$P6_3/mmc$	Kramers doublet	-11	Unknown	Unknown	[8]

YD Li, XQ Wang, GC*, PRB 94, 035107 (2016)

Magnetism in the $KBaRE(BO_3)_2$ (RE=Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) series: materials with a triangular rare earth lattice

M. B. Sanders, F. A. Cevallos, R. J. Cava
Department of Chemistry, Princeton University, Princeton, New Jersey 08544

$KBaRE(BO_3)_2$



Summary

1. We propose $YbMgGaO_4$ to be a spin-orbit-coupled spin liquid.

2. The signature of spin fractionalization has been discovered and interpreted as spinons.

3. Predictions have been made for the weakly magnetized regime. It can be immediately tested by inelastic neutron. It has been **confirmed** in Jun Zhao's recent experiment.