

How to characterise spin liquids ?

IBS-PCS, Daejeon

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Collaborators



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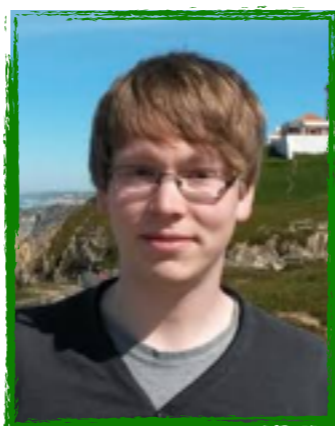
*Mathieu
Taillefumier*



*Owen
Benton*



*Roderich
Moessner*



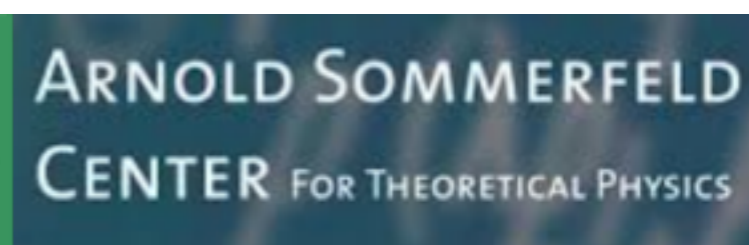
*Jonas
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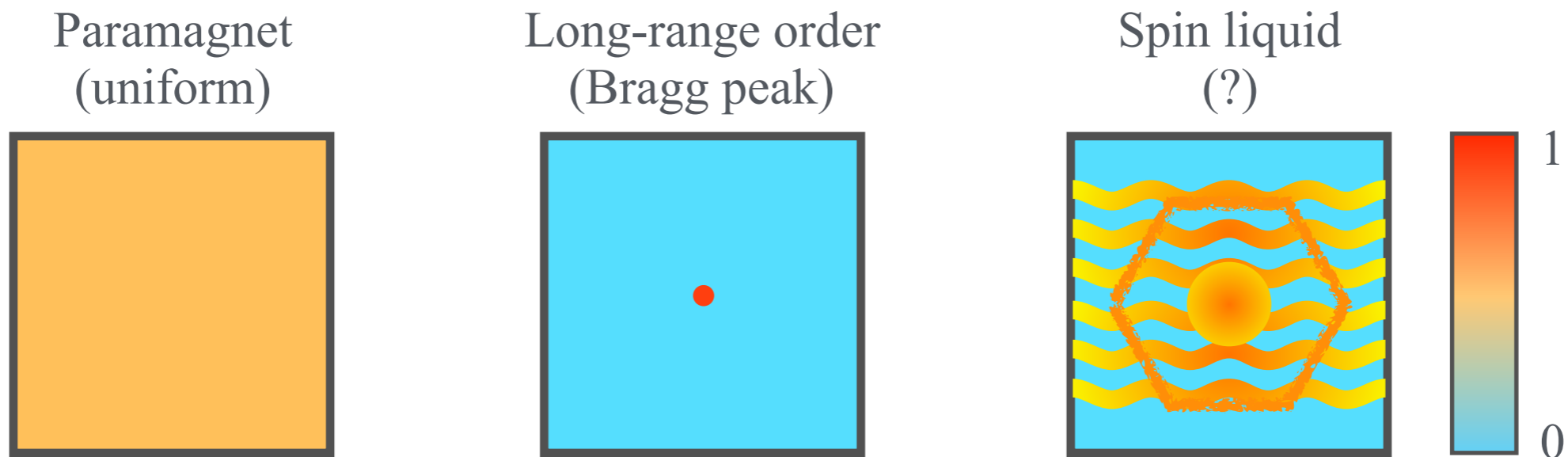


*Lode
Pollet*



Spin liquids & Neutron scattering

Neutron scattering = Fourier transform of spin-spin correlations
= *extensive* amount of data



Motivation

Long-range order implies Bragg peaks, but what about spin liquids ?

There is no unique signature of a spin liquid.

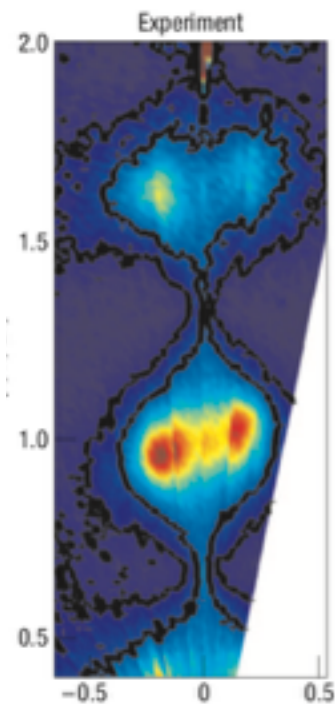
=> **Zoology of ~~spin liquids~~ in neutron scattering**

strongly correlated, disordered, phases

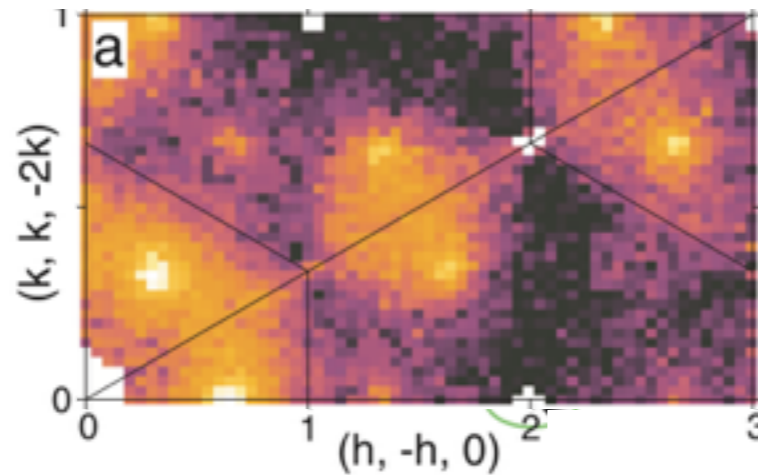
Spin ice & pinch points

Harris *et al* PRL 1997

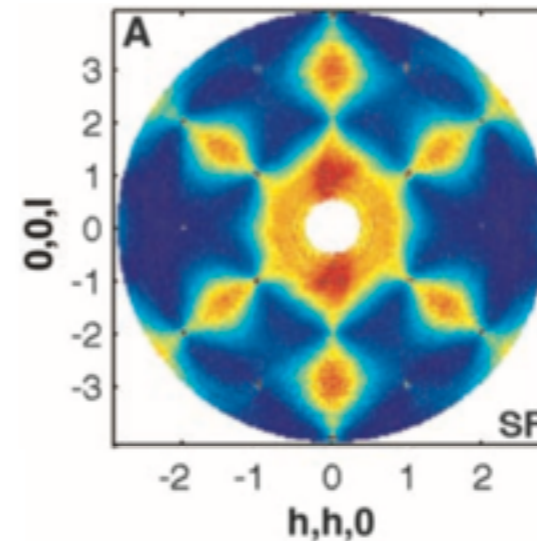
Dy₂Ti₂O₇, Ho₂Ti₂O₇, Dy₂Ge₂O₇...



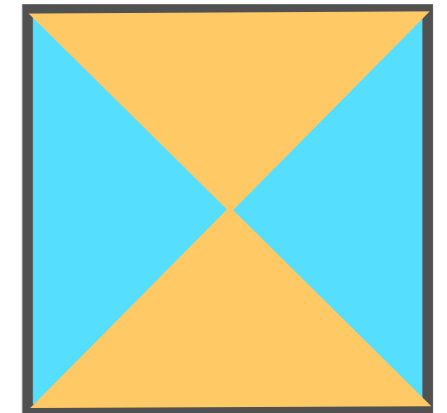
Fennell *et al*
Nat. Phys. 2007



Kadowaki *et al*
JPSJ 2009



Fennell *et al*
Science 2009



Schematic
pinch points

Theory of pinch points: Youngblood & Axe PRB (1981), Isakov *et al* PRL (2004), Henley PRB (2005) ...

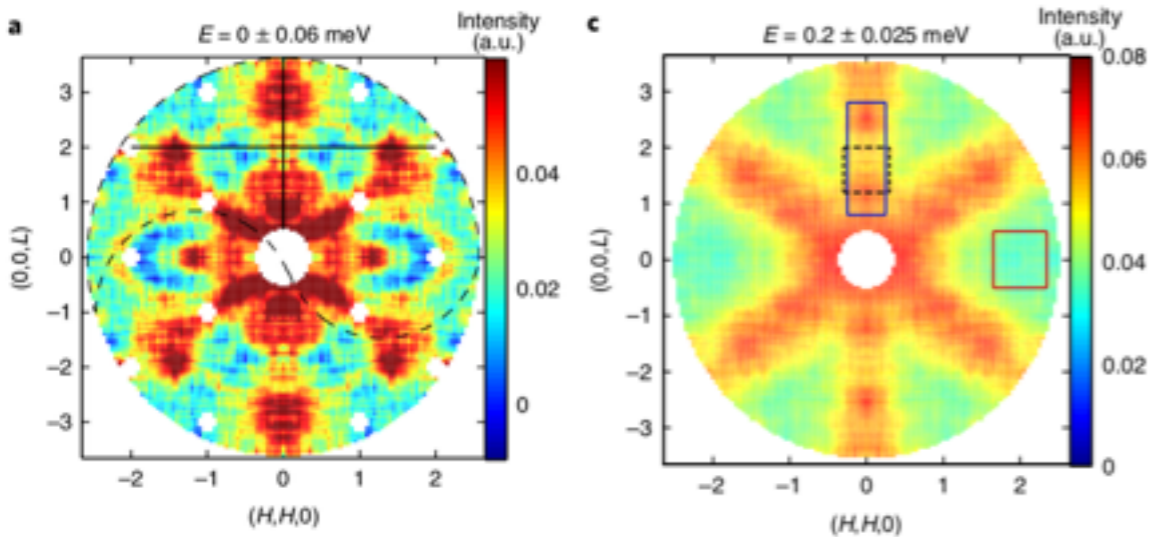
$$F_{\text{tot}}(\{\mathbf{P}(\mathbf{r})\})/T \propto \int d^3\mathbf{r} \frac{1}{2} \kappa |\mathbf{P}(\mathbf{r})|^2 \xrightarrow{\text{Fourier transform}} \sum_{\mathbf{k}} \frac{1}{2} \kappa |\mathbf{P}(\mathbf{k})|^2 \xrightarrow{\text{equipartition}} \langle P_{\mu}(-\mathbf{k}) P_{\nu}(\mathbf{k}) \rangle = (1/\kappa) \delta_{\mu\nu}$$

Equations of the magnetic field: Coulomb phase

$$\begin{aligned} \nabla \cdot \mathbf{P}(\mathbf{r}) &= 0 \\ \mathbf{k} \cdot \mathbf{P}(\mathbf{k}) &= 0 \end{aligned}$$

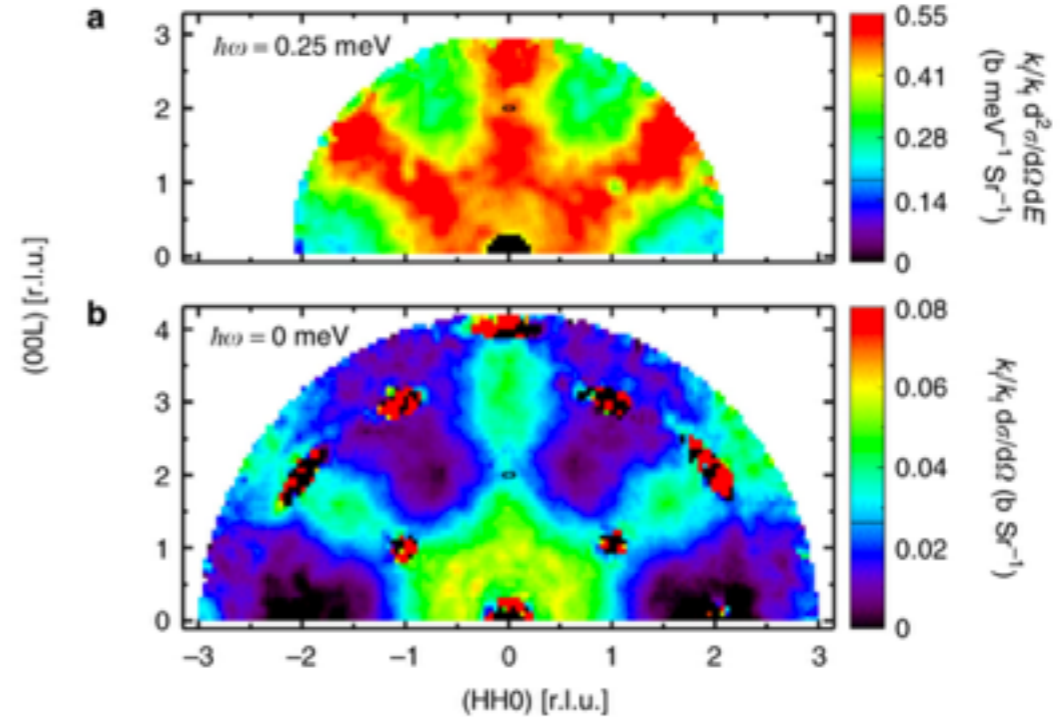
$$\langle P_{\mu}(0) P_{\nu}(\mathbf{r}) \rangle \cong \frac{4\pi}{\kappa} \left[\delta(\mathbf{r}) + \frac{1}{r^3} (\delta_{\mu\nu} - 3\hat{r}_{\mu}\hat{r}_{\nu}) \right] \xleftarrow{\text{inverse Fourier transform}} \langle P_{\mu}(-\mathbf{k}) P_{\nu}(\mathbf{k}) \rangle = \frac{1}{\kappa} \left(\delta_{\mu\nu} - \frac{k_{\mu}k_{\nu}}{|\mathbf{k}|^2} \right)$$

Pinch points in rare-earth pyrochlores



$\text{Pr}_2\text{Hf}_2\text{O}_7$ — a QSI ?

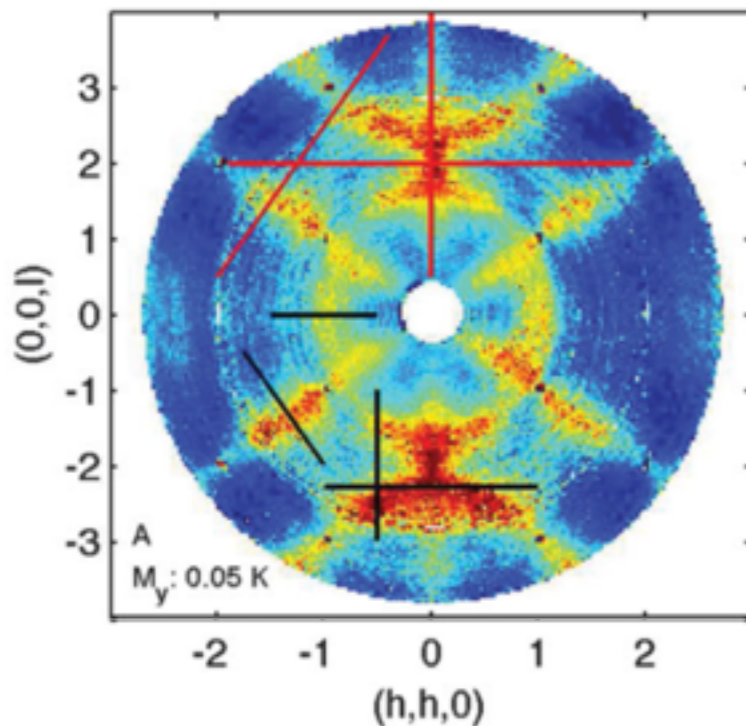
Sibille *et al* Nat. Phys. 2018



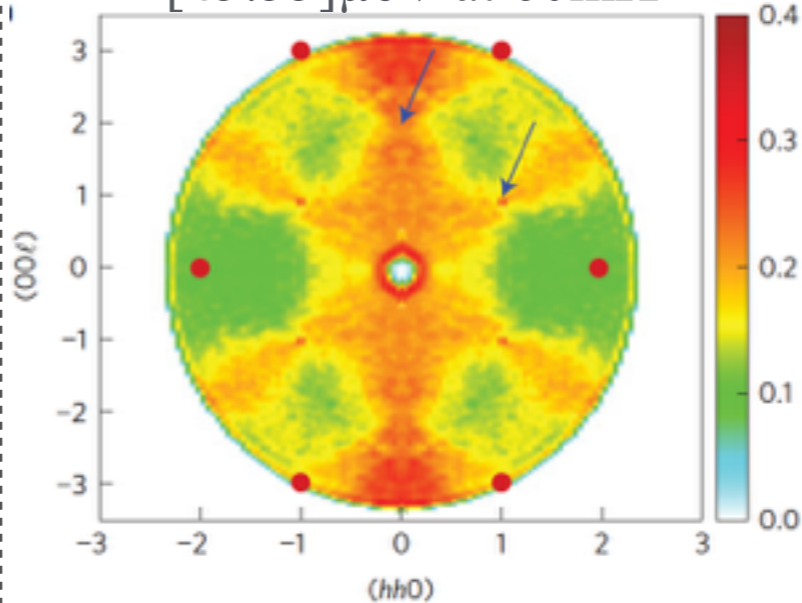
$\text{Pr}_2\text{Zr}_2\text{O}_7$

Kimura *et al* Nat. Comm. 2013

$\text{Tb}_2\text{Ti}_2\text{O}_7$ Fennell *et al* PRL 2012



$\text{Nd}_2\text{Zr}_2\text{O}_7$ averaged over
[45:55] μeV at 60mK



Petit *et al* Nat. Phys. 2016

Benton, PRB 2016

Magnetic fragmentation

Brooks-Bartlett *et al*

PRX 2014

$\text{Nd}_2\text{Hf}_2\text{O}_7$

Anand *et al* PRB 2017

$\text{Ho}_2\text{Ir}_2\text{O}_7$

Lefrançois *et al*

Nat. Comm. 2017

Structure factors

Total: $\frac{1}{N} \left| \sum_n \mathbf{S}_n e^{i\mathbf{q}\cdot\mathbf{r}_n} \right|^2$

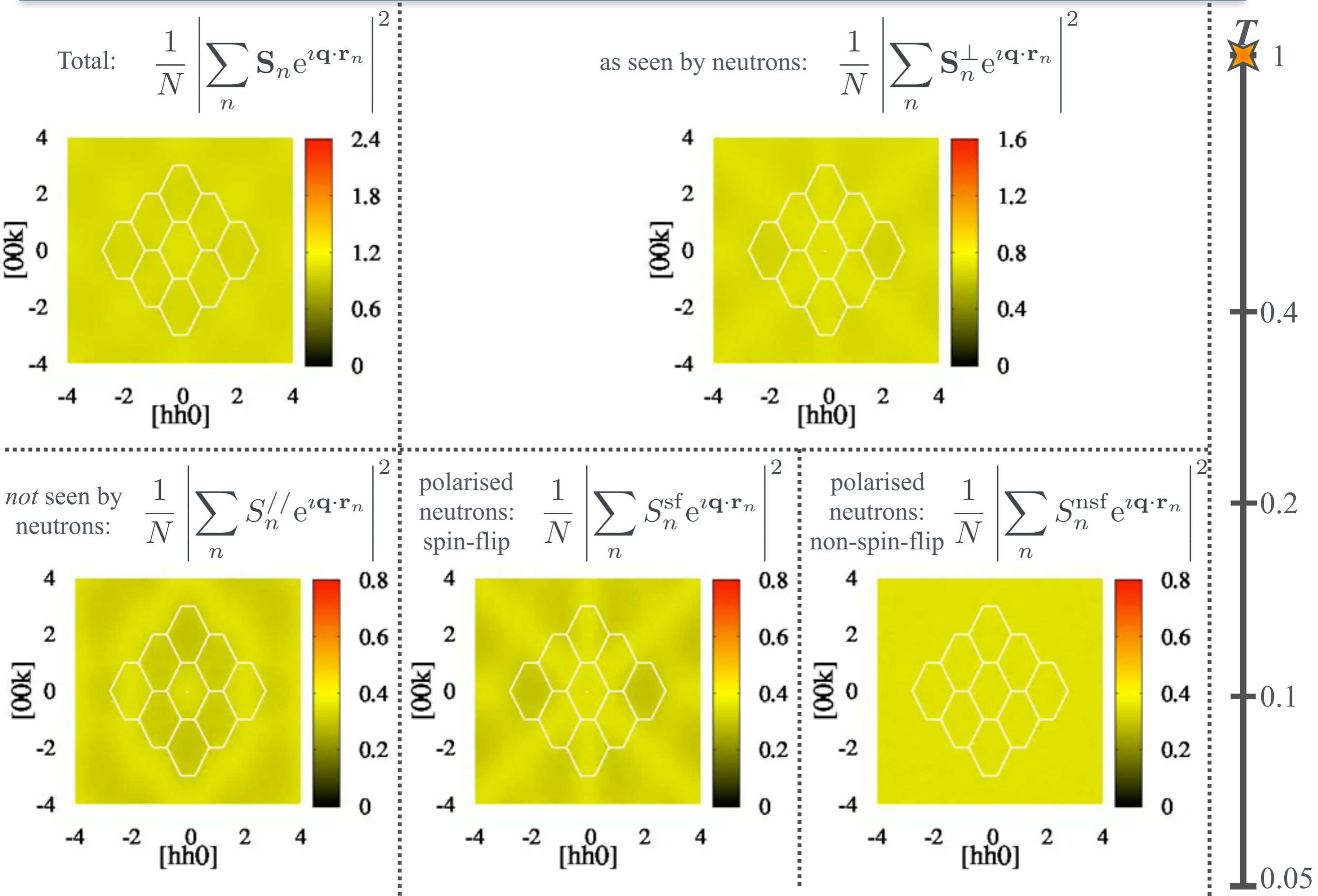
as seen by neutrons: $\frac{1}{N} \left| \sum_n \mathbf{S}_n^\perp e^{i\mathbf{q}\cdot\mathbf{r}_n} \right|^2$
 $(\mathbf{S}_n \perp \mathbf{q})$

not seen by neutrons: $\frac{1}{N} \left| \sum_n S_n^{//} e^{i\mathbf{q}\cdot\mathbf{r}_n} \right|^2$
 $(\mathbf{S}_n // \mathbf{q})$

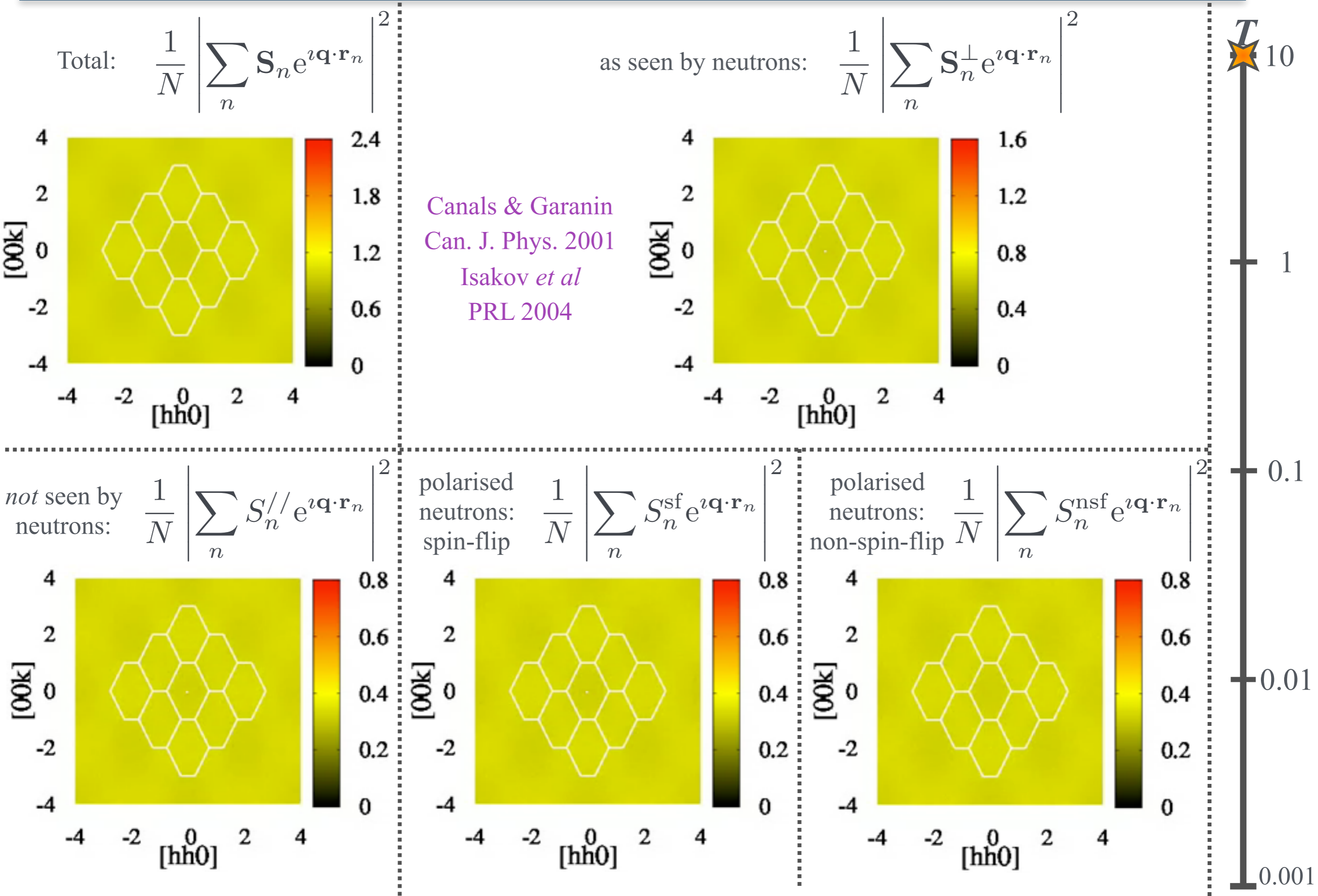
polarised neutrons: spin-flip $\frac{1}{N} \left| \sum_n S_n^{\text{sf}} e^{i\mathbf{q}\cdot\mathbf{r}_n} \right|^2$

polarised neutrons: non-spin-flip $\frac{1}{N} \left| \sum_n S_n^{\text{nssf}} e^{i\mathbf{q}\cdot\mathbf{r}_n} \right|^2$

Structure factors: spin ice



Structure factors: Heisenberg antiferromagnet

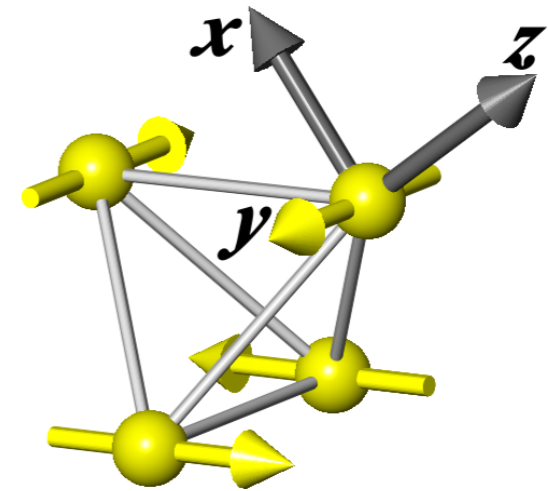


U(1) gauge fields

Heisenberg antiferro (HAF): $\sum_{i \in \text{tet}} \mathbf{S}_i = 0 \Rightarrow U(1) \times U(1) \times U(1)$

spin ice (SI): $\sum_{i \in \text{tet}} S_i^{z_\ell} = 0 \Rightarrow U(1)$

Can we extend it to other gauge fields ?





*Han
Yan*



*Nic
Shannon*



*Owen
Benton*

Rank-2 $U(1)$ gauge field

Heisenberg AF as a tensor gauge field

$(S_0^x S_0^y S_0^z S_1^x S_1^y S_1^z S_2^x S_2^y S_2^z S_3^x S_3^y S_3^z)$

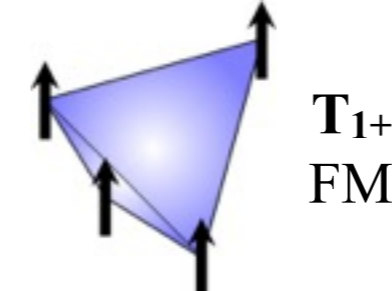
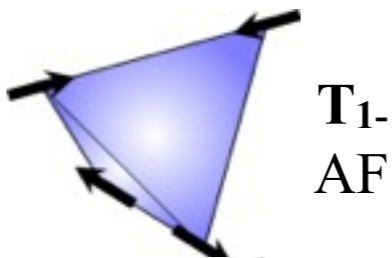
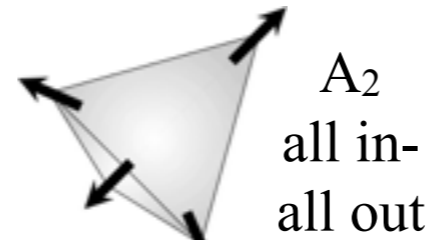
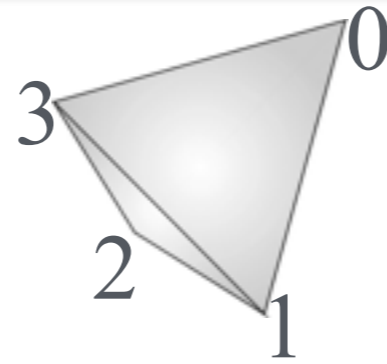
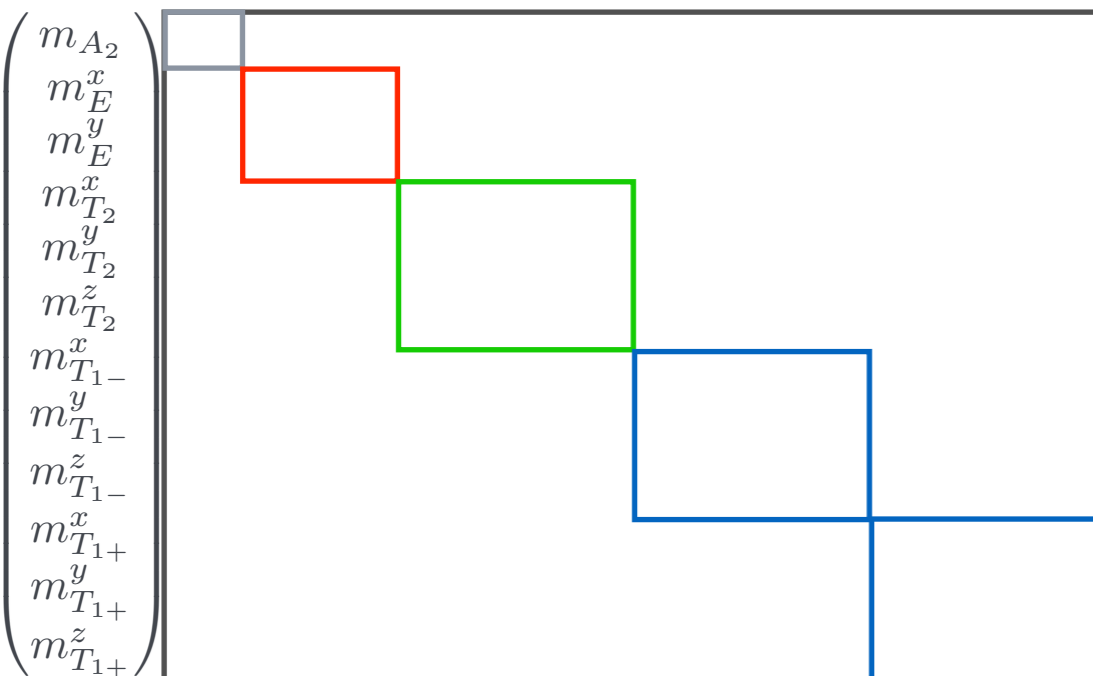
12 × 12 Interaction matrix

Generic nearest-neighbour Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} \vec{S}_i \bar{\mathcal{J}}_{ij} \vec{S}_j \quad \text{with} \quad \bar{\mathcal{J}} = \begin{pmatrix} J_2 & J_4 & J_4 \\ -J_4 & J_1 & J_3 \\ -J_4 & J_3 & J_1 \end{pmatrix}$$

diagonalisation

$(m_{A_2} m_E^x m_E^y m_{T_2}^x m_{T_2}^y m_{T_2}^z m_{T_{1-}}^x m_{T_{1-}}^y m_{T_{1-}}^z m_{T_{1+}}^x m_{T_{1+}}^y m_{T_{1+}}^z)$



Quadratic Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} \vec{S}_i \bar{\mathcal{J}}_{ij} \vec{S}_j = \sum_i a_i \mathbf{m}_i^2$$

For the Heisenberg AF:

fields fluctuating in the ground state

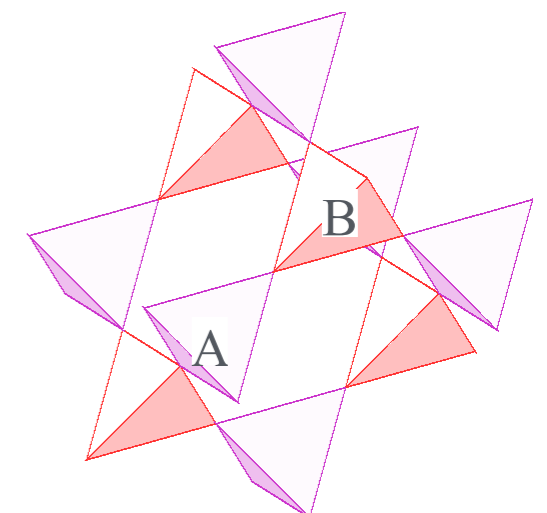
$m_{A_2} \mathbf{m}_E, \mathbf{m}_{T_2}, \mathbf{m}_{T_{1-}}$

defined on A tetrahedra

fields vanishing in the ground state

$\mathbf{m}_{T_{1+}} = 0$

constraint applied on B tetrahedra



Heisenberg AF as a tensor gauge field

$$\mathbf{E}^{\text{HAF}} = \begin{bmatrix} \frac{2}{\sqrt{3}}m_{\text{E}}^1 - \sqrt{\frac{2}{3}}m_{\text{A}_2} & m_{\text{T}_{1,-}}^z + m_{\text{T}_2}^z & m_{\text{T}_{1,-}}^y - m_{\text{T}_2}^y \\ m_{\text{T}_{1,-}}^z - m_{\text{T}_2}^z & -\frac{1}{\sqrt{3}}m_{\text{E}}^1 - m_{\text{E}}^2 - \sqrt{\frac{2}{3}}m_{\text{A}_2} & m_{\text{T}_{1,-}}^x + m_{\text{T}_2}^x \\ m_{\text{T}_{1,-}}^y + m_{\text{T}_2}^y & m_{\text{T}_{1,-}}^x - m_{\text{T}_2}^x & -\frac{1}{\sqrt{3}}m_{\text{E}}^1 + m_{\text{E}}^2 - \sqrt{\frac{2}{3}}m_{\text{A}_2} \end{bmatrix}$$

The low-energy fluctuations of the HAF can be described by a **rank-2 tensor field** (generalised electric field) satisfying the constraint of **zero vector charge**:

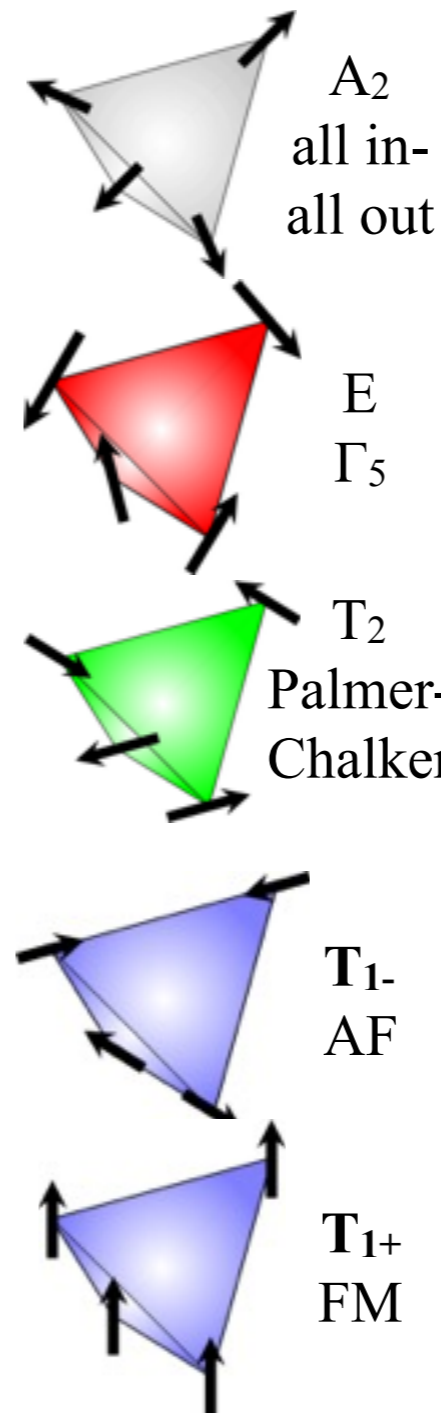
$$\partial_i E_{ij}^{\text{HAF}} = \rho_j = 0$$

$$\mathbf{E}^{\text{HAF}} = \mathbf{E}_{\text{sym.}}^{\text{HAF}} + \mathbf{E}_{\text{antisym.}}^{\text{HAF}} + \mathbf{E}_{\text{trace}}^{\text{HAF}}$$

$$\mathbf{E}_{\text{trace}}^{\text{HAF}} = \begin{bmatrix} -\sqrt{\frac{2}{3}}m_{\text{A}_2} & 0 & 0 \\ 0 & -\sqrt{\frac{2}{3}}m_{\text{A}_2} & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}}m_{\text{A}_2} \end{bmatrix}$$

$$\mathbf{E}_{\text{antisym.}}^{\text{HAF}} = \begin{bmatrix} 0 & m_{\text{T}_2}^z & -m_{\text{T}_2}^y \\ -m_{\text{T}_2}^z & 0 & m_{\text{T}_2}^x \\ m_{\text{T}_2}^y & -m_{\text{T}_2}^x & 0 \end{bmatrix}$$

$$\mathbf{E}_{\text{sym.}}^{\text{HAF}} = \begin{bmatrix} \frac{2}{\sqrt{3}}m_{\text{E}}^1 & m_{\text{T}_{1,-}}^z & m_{\text{T}_{1,-}}^y \\ m_{\text{T}_{1,-}}^z & -\frac{1}{\sqrt{3}}m_{\text{E}}^1 - m_{\text{E}}^2 & m_{\text{T}_{1,-}}^x \\ m_{\text{T}_{1,-}}^y & m_{\text{T}_{1,-}}^x & -\frac{1}{\sqrt{3}}m_{\text{E}}^1 + m_{\text{E}}^2 \end{bmatrix}$$



For the Heisenberg AF:

fields fluctuating in the ground state

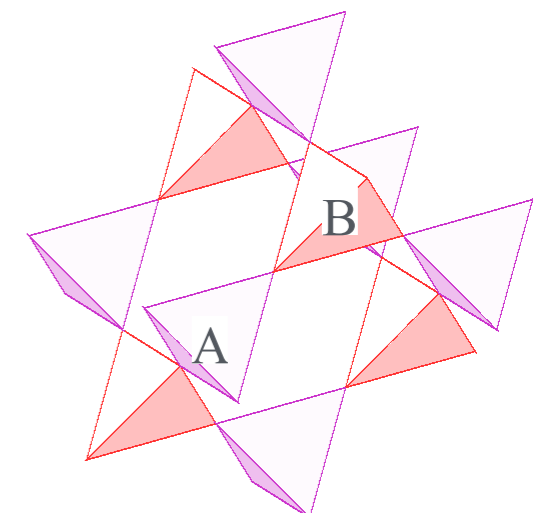
$$m_{\text{A}_2} \mathbf{m}_{\text{E}}, \mathbf{m}_{\text{T}_2}, \mathbf{m}_{\text{T}_{1,-}}$$

defined on A tetrahedra

fields vanishing in the ground state

$$\mathbf{m}_{\text{T}_{1,+}} = 0$$

constraint applied on B tetrahedra



Higher-rank tensor gauge fields

PHYSICAL REVIEW B 74, 224433 (2006)

Gapless bosonic excitation without symmetry breaking: An algebraic spin liquid with soft gravitons

Cenke Xu

Stable Gapless Bose Liquid Phases without Any Symmetry

Alex Rasmussen,¹ Yi-Zhuang You,¹ and Cenke Xu¹

¹Department of physics, University of California, Santa Barbara, CA 93106, USA
(Dated: February 1, 2016)

PHYSICAL REVIEW B 96, 035119 (2017)

Generalized electromagnetism of subdimensional particles: A spin liquid story

Michael Pretko

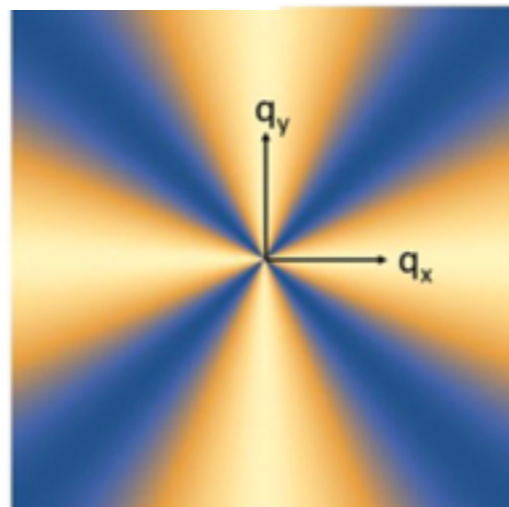
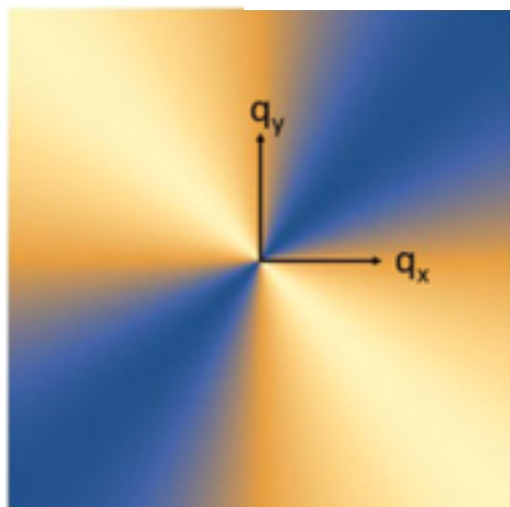
PHYSICAL REVIEW B 95, 115139 (2017)



Subdimensional particle structure of higher rank $U(1)$ spin liquids

Michael Pretko

$$\langle E^{ij}(q) E^{k\ell}(-q) \rangle$$



PHYSICAL REVIEW B 98, 165140 (2018)

Pinch point singularities of tensor spin liquids

Abhinav Prem,^{1,*} Sagar Vijay,² Yang-Zhi Chou,¹ Michael Pretko,¹ and Rahul M. Nandkishore¹

characteristic 4-fold pinch points \Rightarrow symmetric rank-2 $U(1)$ tensor gauge field

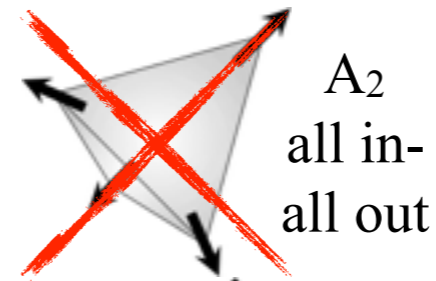
Symmetric U(1) tensor gauge field

$$\mathbf{E}^{\text{HAF}} = \mathbf{E}_{\text{sym.}}^{\text{HAF}} + \mathbf{E}_{\text{antisym.}}^{\text{HAF}} + \mathbf{E}_{\text{trace}}^{\text{HAF}}$$

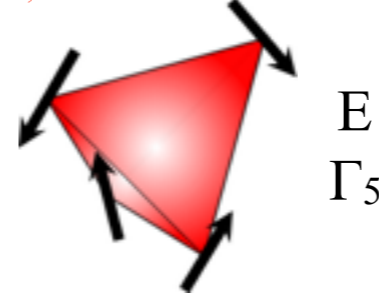
~~$$\mathbf{E}_{\text{trace}}^{\text{HAF}} = \begin{bmatrix} -\sqrt{\frac{2}{3}}m_{A_2} & 0 & 0 \\ 0 & -\sqrt{\frac{2}{3}}m_{A_2} & 0 \\ 0 & 0 & -\sqrt{\frac{2}{3}}m_{A_2} \end{bmatrix}$$~~

~~$$\mathbf{E}_{\text{antisym.}}^{\text{HAF}} = \begin{bmatrix} 0 & m_{T_2}^z & -m_{T_2}^y \\ -m_{T_2}^z & 0 & m_{T_2}^x \\ m_{T_2}^y & -m_{T_2}^x & 0 \end{bmatrix}$$~~

$$\mathbf{E}_{\text{sym.}}^{\text{HAF}} = \begin{bmatrix} \frac{2}{\sqrt{3}}m_E^1 & m_{T_{1-}}^z & m_{T_{1-}}^y \\ m_{T_{1-}}^z & -\frac{1}{\sqrt{3}}m_E^1 - m_E^2 & m_{T_{1-}}^x \\ m_{T_{1-}}^y & m_{T_{1-}}^x & -\frac{1}{\sqrt{3}}m_E^1 + m_E^2 \end{bmatrix}$$



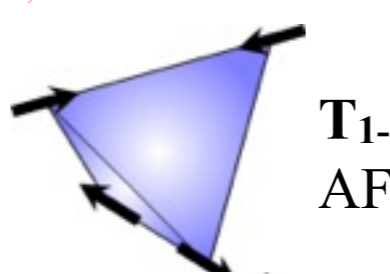
A_2
all in-
all out



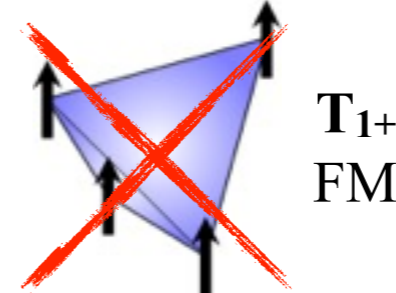
E
 Γ_5



T_2
Palmer-
Chalker



T_{1-}
AF



T_{1+}
FM

Breathing anisotropy

fields fluctuating in the ground state

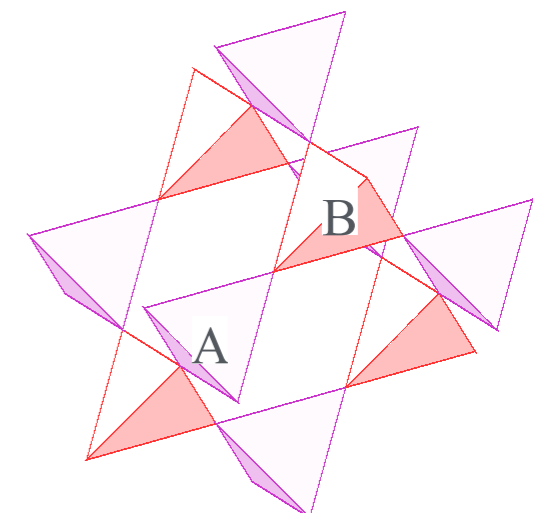
~~m_{A_2}~~ m_E , ~~m_{T_2}~~ , $m_{T_{1-}}$

defined on A tetrahedra

fields vanishing in the ground state

$$m_{T_{1+}} = 0$$

constraint applied on B tetrahedra



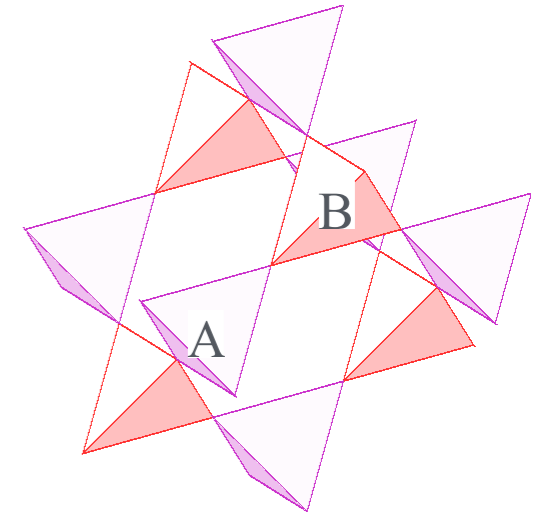
Rank-2 U(1) tensor gauge field

Breathing pyrochlore

$$\mathcal{H} = \sum_{\langle ij \rangle \in A} \left[J_A \mathbf{S}_i \cdot \mathbf{S}_j + D_A \hat{\mathbf{d}}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \right] + \sum_{\langle ij \rangle \in B} \left[J_B \mathbf{S}_i \cdot \mathbf{S}_j + D_B \hat{\mathbf{d}}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \right]$$

Heisenberg antiferromagnet
with Dzyaloshinskii–Moriya
on A tetrahedra

$$J_A = J_B > 0 \\ D_A < 0, D_B = 0$$



The generalised electric field is
a symmetric, traceless,
rank-2 tensor field.

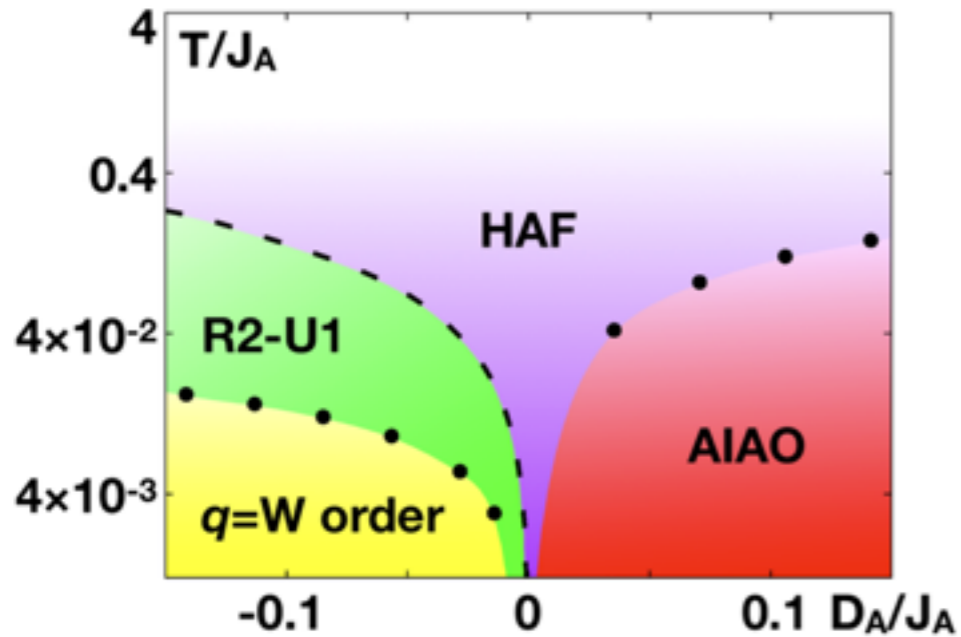
$$\mathbf{E} = \begin{bmatrix} \frac{2}{\sqrt{3}} m_E^1 & m_{T_{1-}}^z & m_{T_{1-}}^y \\ m_{T_{1-}}^z & -\frac{1}{\sqrt{3}} m_E^1 - m_E^2 & m_{T_{1-}}^x \\ m_{T_{1-}}^y & m_{T_{1-}}^x & -\frac{1}{\sqrt{3}} m_E^1 + m_E^2 \end{bmatrix}$$

with zero
vector charge

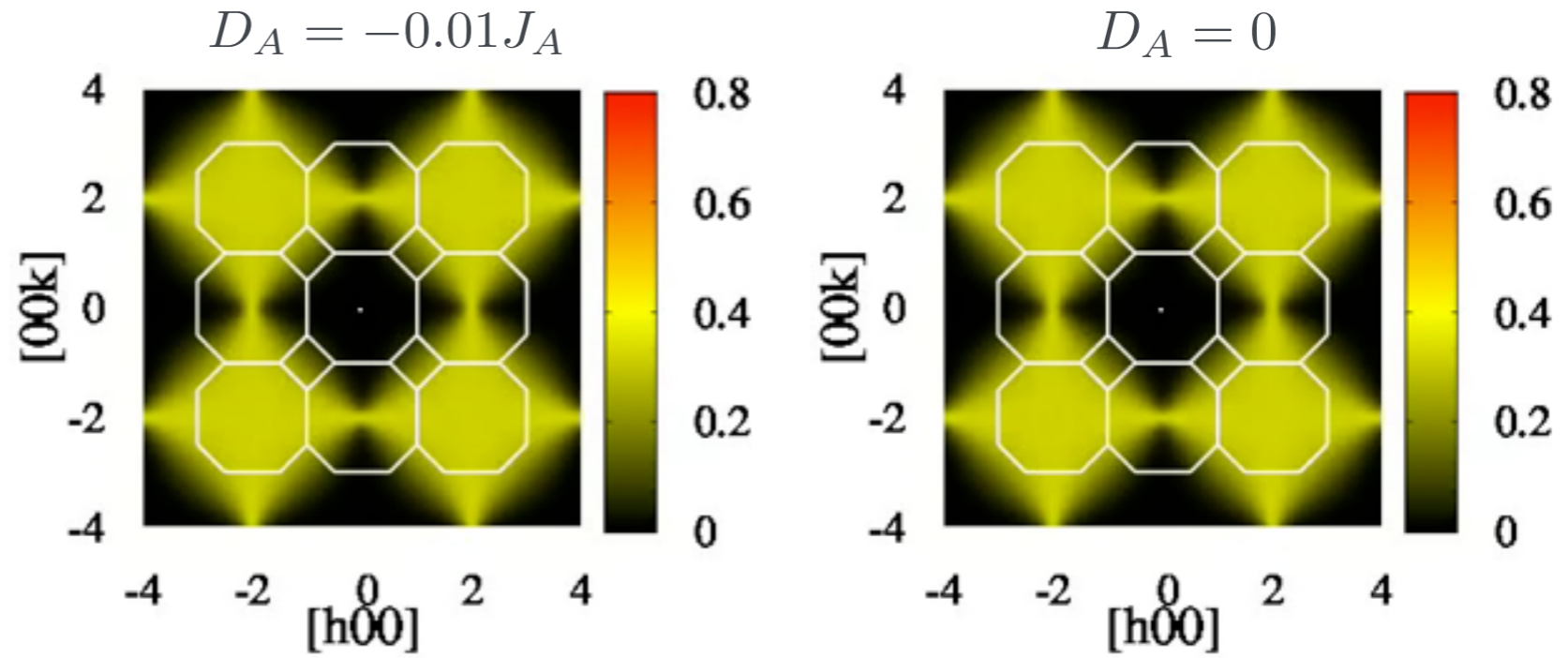
$$\partial_i E_{ij} = 0$$

4-fold pinch points in neutron scattering ?

Phase diagram



Spin-flip channel as seen in neutron scattering



Breathing Pyrochlore $Ba_3Yb_2Zn_5O_{11}$

Kimura et al PRB 2014

single-tetrahedron parametrisation

Rau et al PRL 2016

$$\begin{aligned} J_1 &= +0.587 \text{ meV} \\ J_2 &= +0.573 \text{ meV} \\ J_3 &= -0.011 \text{ meV} \\ J_4 &= -0.117 \text{ meV} \end{aligned}$$

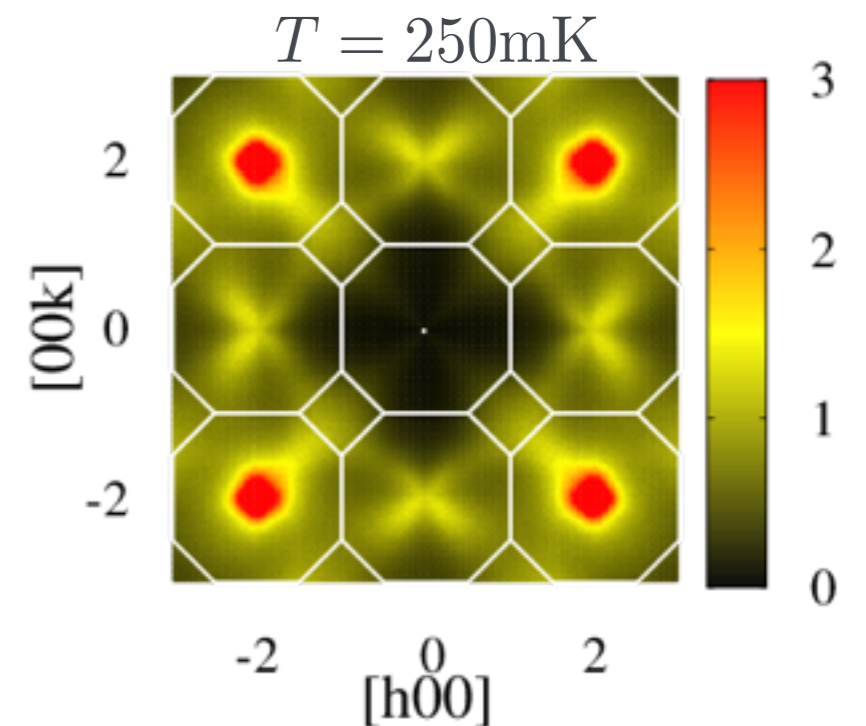
Haku et al PRB 2016

$$\begin{aligned} J_1 &= -0.570 \pm 0.033 \text{ meV}, \\ J_2 &= -0.558 \pm 0.028 \text{ meV}, \\ J_3 &= 0.000 \pm 0.023 \text{ meV}, \\ J_4 &= 0.113 \pm 0.014 \text{ meV}. \end{aligned}$$

(!) opposite sign convention

We chose:

$$\begin{aligned} J_A &= J_1 = J_2 = +0.57 \text{ meV} \\ J_3 &= 0 \text{ meV} \\ D_A &= \sqrt{2} J_4 = -0.16 \text{ meV} \\ J_B &= J_A/20, \quad D_B = D_A/20 \end{aligned}$$





*Masafumi
Udagawa*



*Tomonari
Mizoguchi*



*Roderich
Moessner*

Half moon patterns

Ghost modes in the kagome antiferromagnet

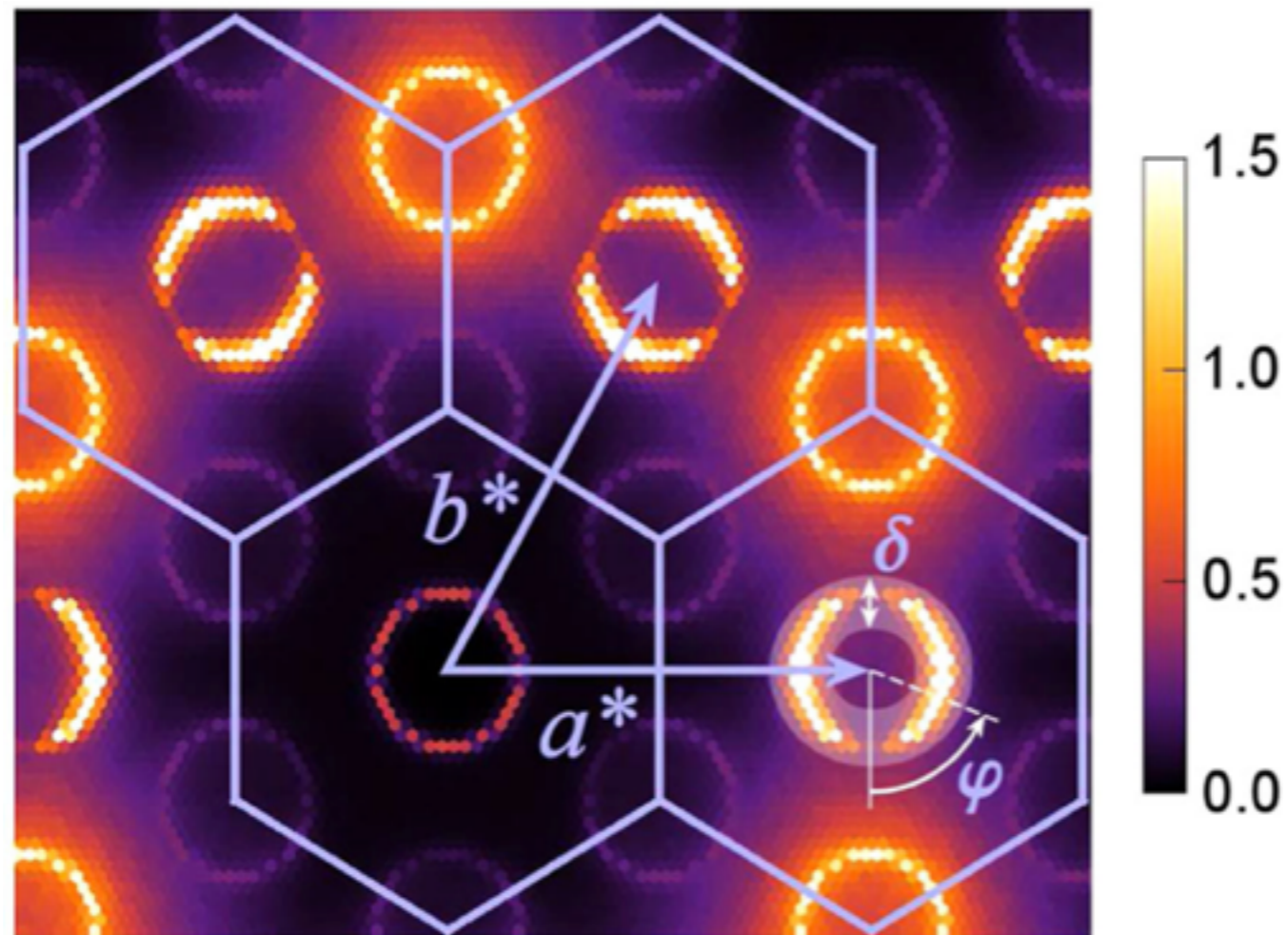
Intensity map at finite energy ω

The spectral weight fades out in certain directions

=

“ghost” modes

Robert et al PRL 2008



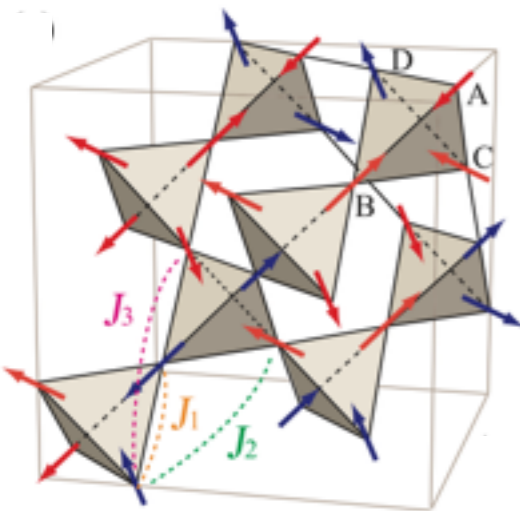
Half moons in Ising models

in terms of spins

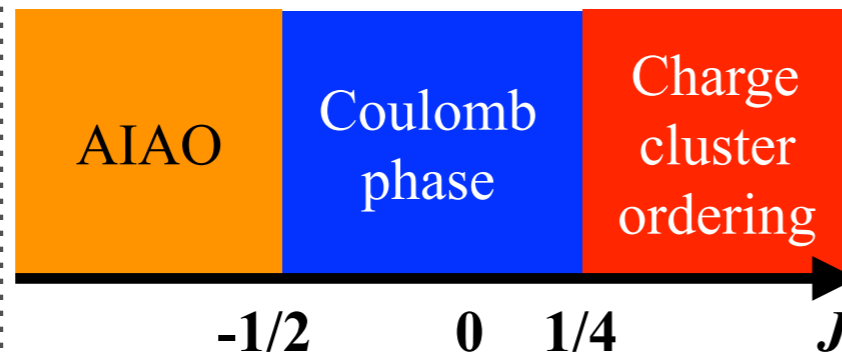
$J = \tilde{J}_2 = \tilde{J}_3$ in terms of topological charges

$$\mathcal{H} = \tilde{J}_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_2 \sum_{\text{2nd.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_3 \sum_{\text{3rd.}} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow \mathcal{H} = \left(\frac{1}{2} - J\right) \sum_p Q_p^2 - J \sum_{\langle p,q \rangle} Q_p Q_q.$$

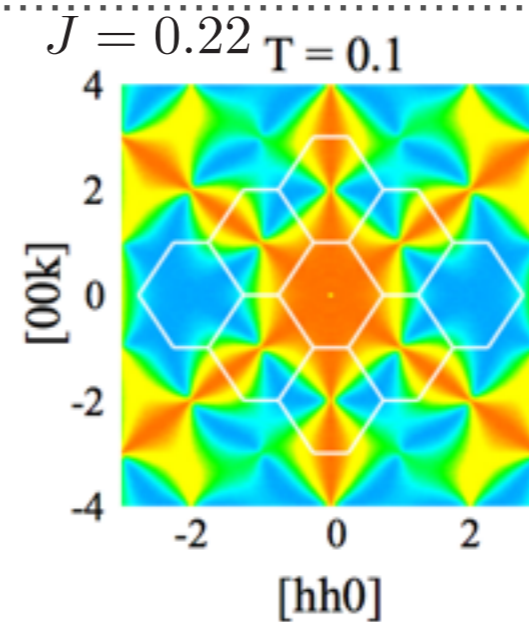
Models



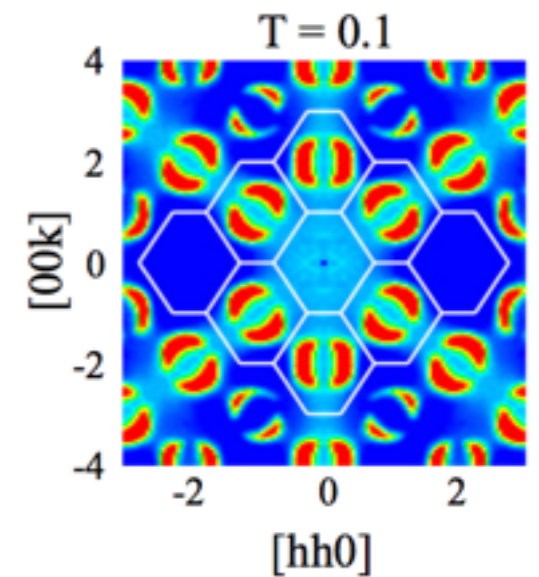
Phase Diagram



Pinch Points

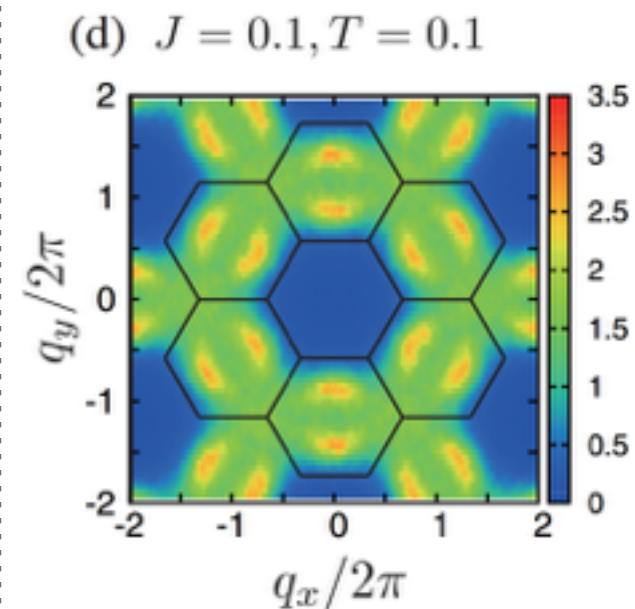
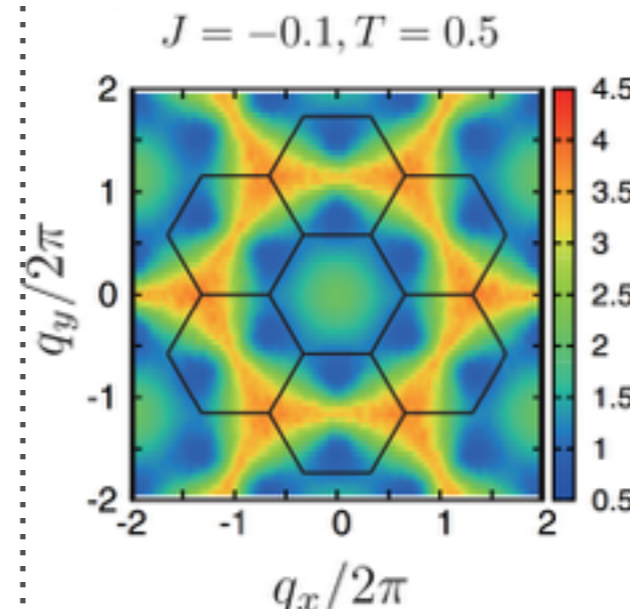
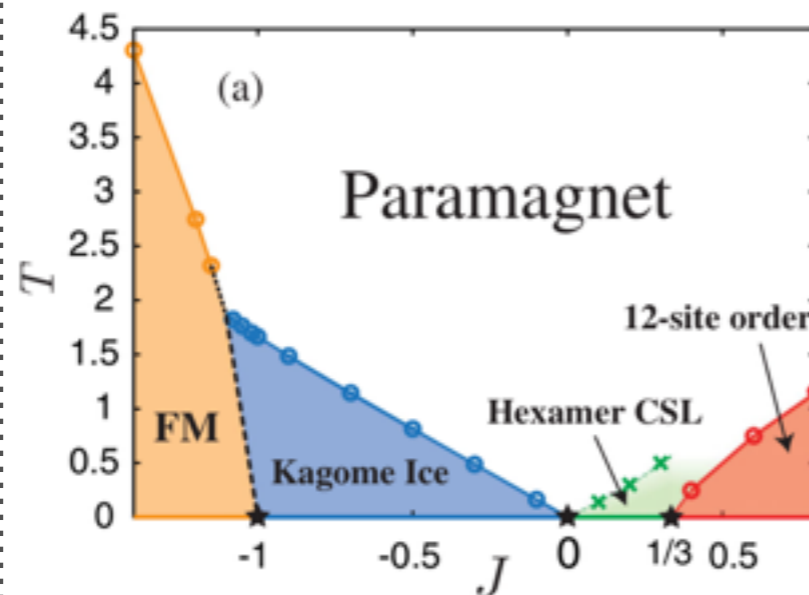
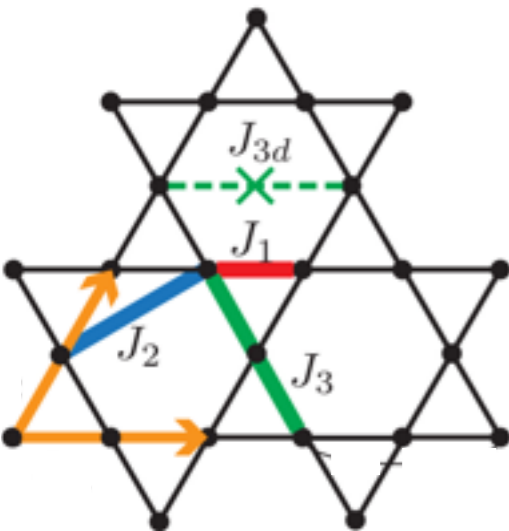


Half moons



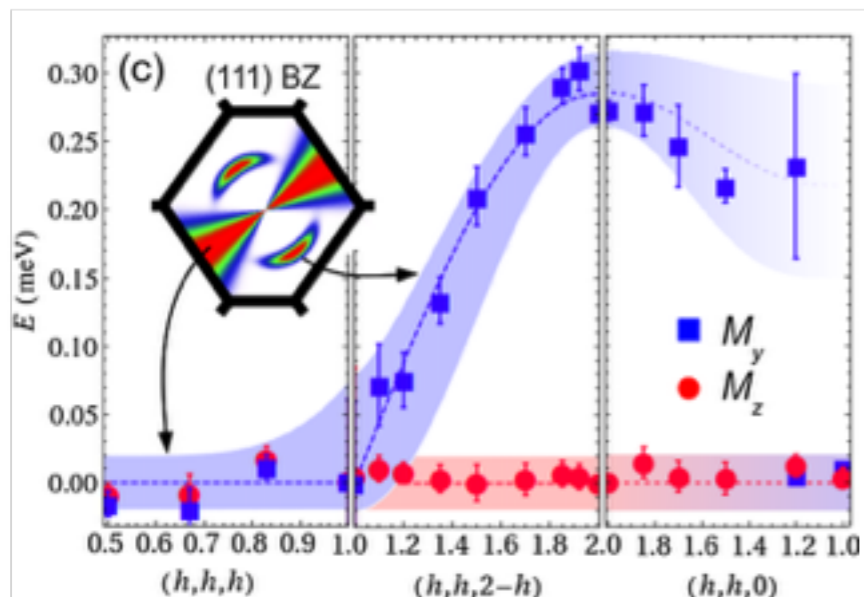
Udagawa, Jaubert, Castelnovo, Moessner PRB 2016

// Rau & Gingras Nature Comm. 2016



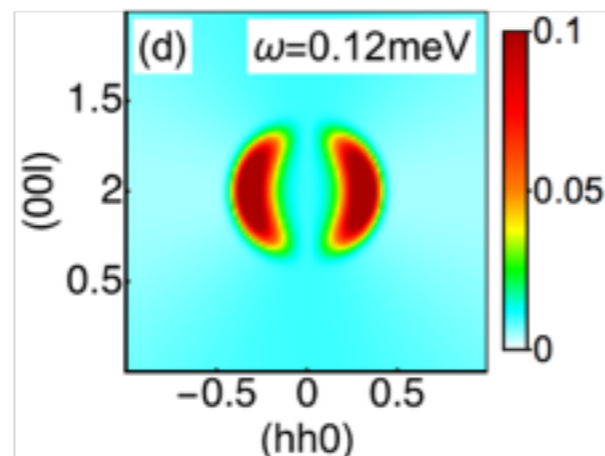
Mizoguchi, Jaubert, Udagawa PRB 2016

Half moons in materials



Schematic map of polarised neutron scattering of $\text{Tb}_2\text{Ti}_2\text{O}_7$

Guitteny et al PRL 2013

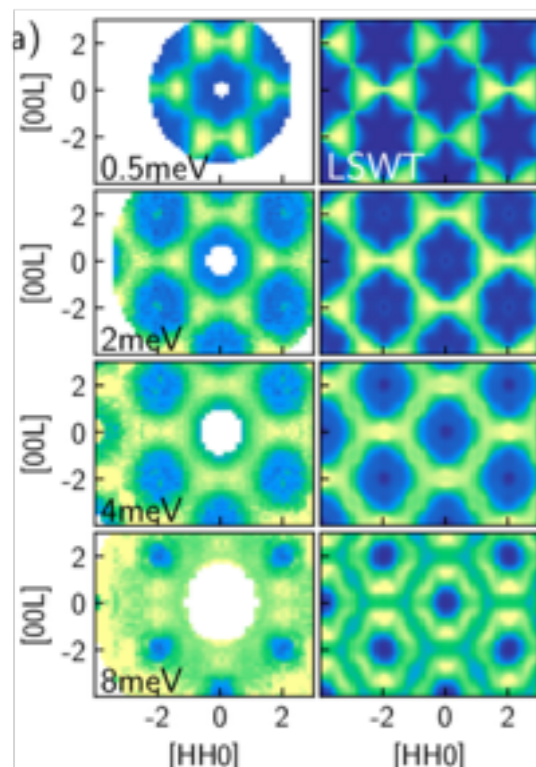


Predictions for the dynamic structure factor (at finite energy ω)

Han, Pohle, Shannon PRB 2018

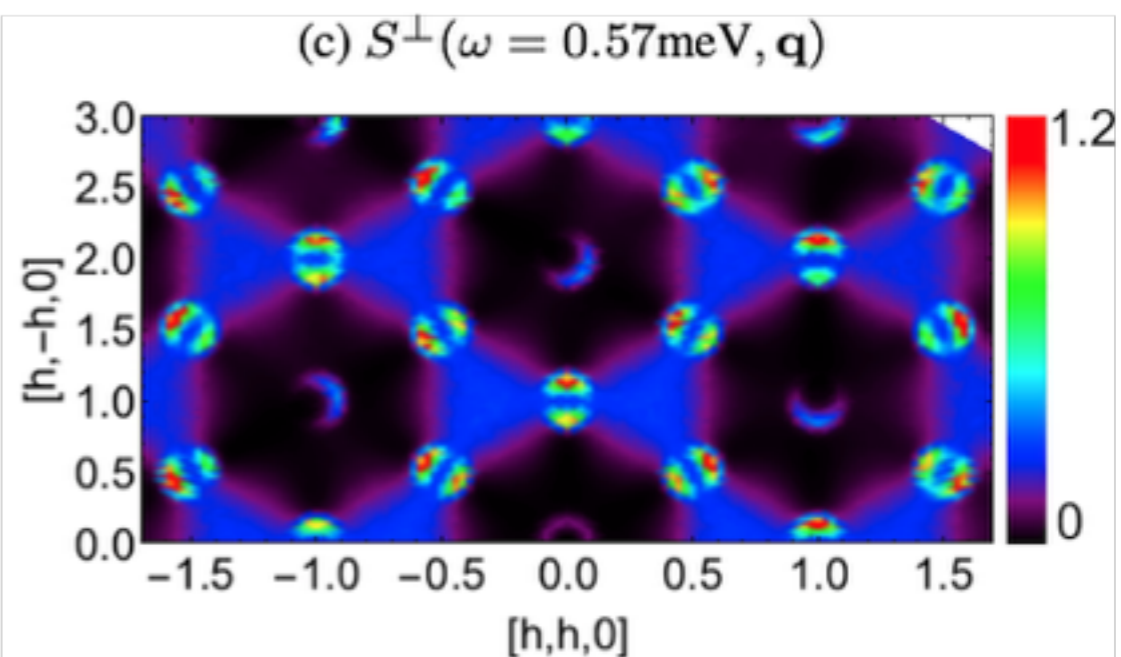
for parameters of $\text{Nd}_2\text{Zr}_2\text{O}_7$

Benton PRB 2016



Inelastic neutron scattering experiments on $\text{NaCaNi}_2\text{F}_7$ (left) and linear spin wave theory (right)

Zhang et al PRL 2019



Molecular dynamics simulation of transverse spin excitations (at finite energy ω)

Pohle, Han, Shannon arXiv 2017

for parameters of $\text{Ca}_{10}\text{Cr}_7\text{O}_{28}$

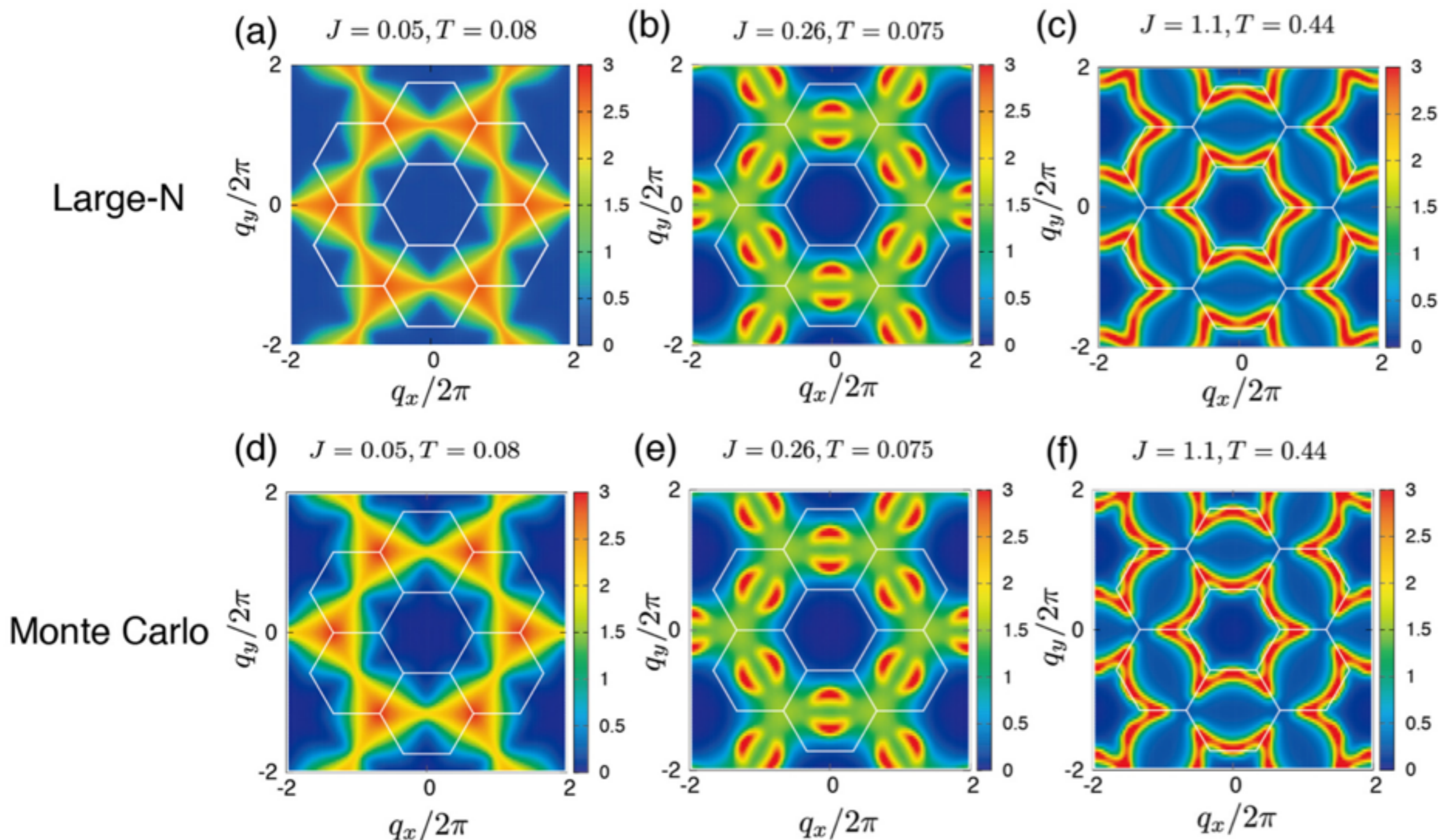
Balz et al Nature Phys. 2016

Half moons in Heisenberg models

in terms of spins

 $J = \tilde{J}_2 = \tilde{J}_3$ in terms of a coarse-grained field

$$\mathcal{H} = \tilde{J}_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_2 \sum_{\text{2nd.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_3 \sum_{\text{3rd.}} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow H = \left(\frac{1}{2} - J\right) \sum_n |\mathbf{M}_n|^2 - J \sum_{\langle n,m \rangle} \mathbf{M}_n \cdot \mathbf{M}_m,$$



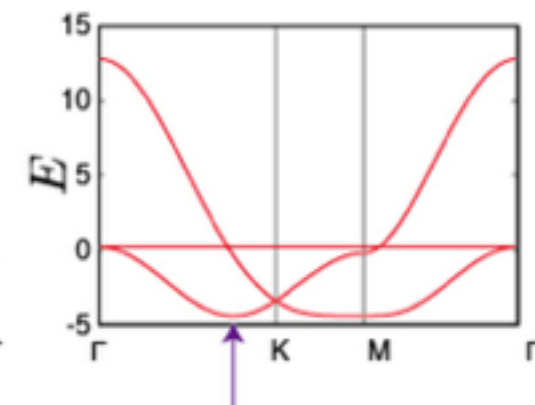
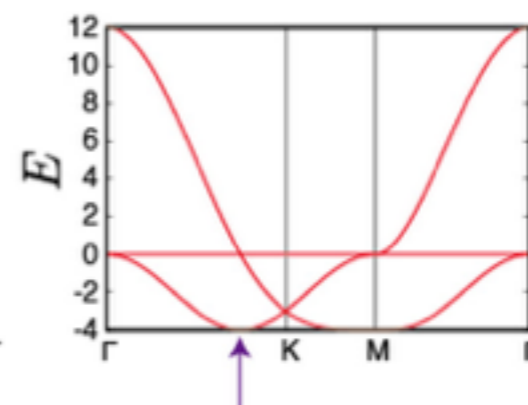
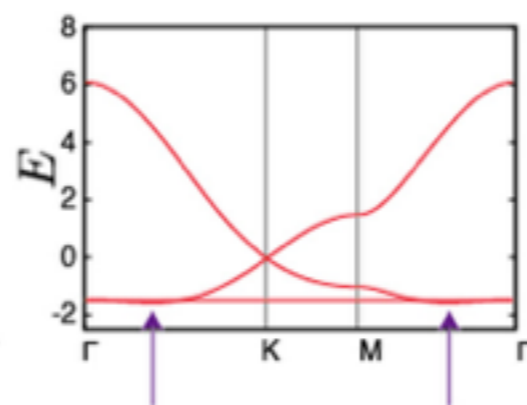
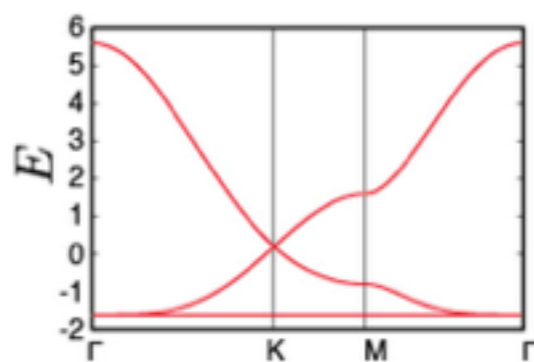
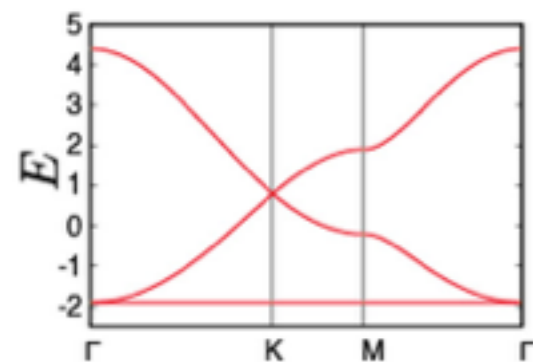
Half moons in Heisenberg models

in terms of spins

$$J = \tilde{J}_2 = \tilde{J}_3$$

in terms of a coarse-grained field

$$\mathcal{H} = \tilde{J}_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_2 \sum_{\text{2nd.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_3 \sum_{\text{3rd.}} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow H = \left(\frac{1}{2} - J\right) \sum_n |\mathbf{M}_n|^2 - J \sum_{\langle n,m \rangle} \mathbf{M}_n \cdot \mathbf{M}_m$$

 $J = 0.05$ $J = 1/5$ $J = 0.26$ $J = 1$ $J = 1.1$ 

Origin of the Half moons

in terms of spins

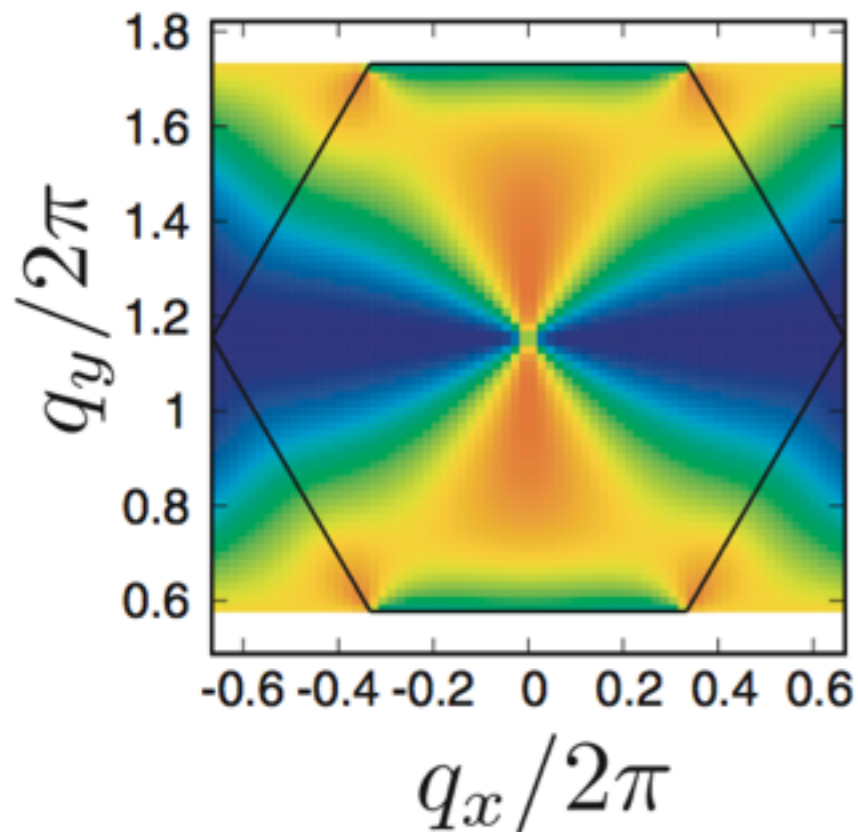
$$J = \tilde{J}_2 = \tilde{J}_3$$

in terms of a coarse-grained field

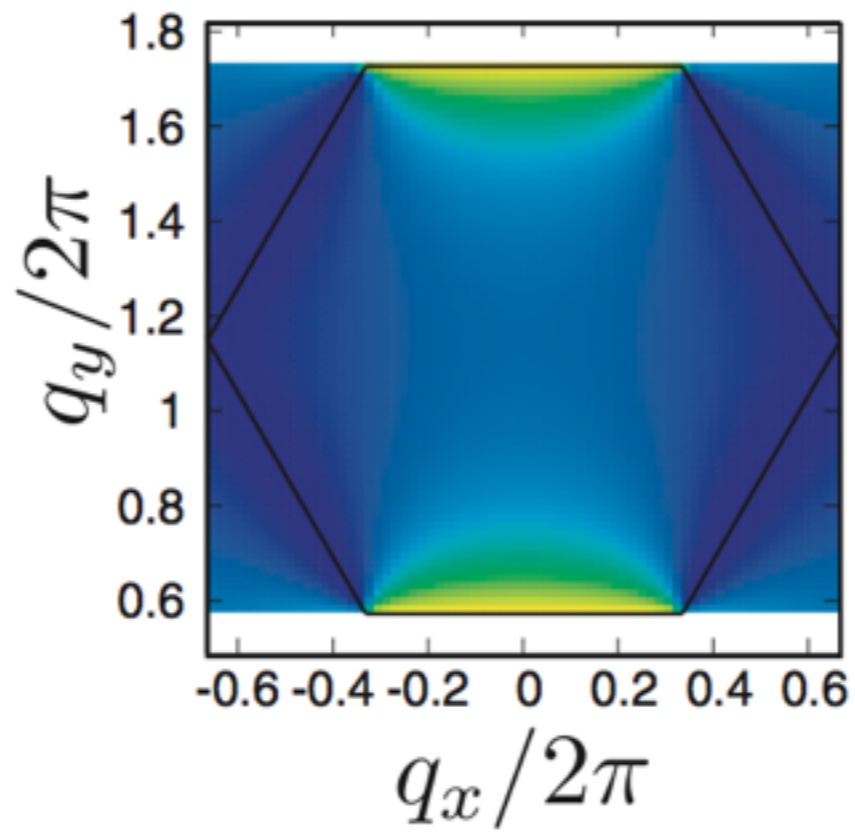
$$\mathcal{H} = \tilde{J}_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_2 \sum_{\text{2nd.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_3 \sum_{\text{3rd.}} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow H = \left(\frac{1}{2} - J\right) \sum_n |\mathbf{M}_n|^2 - J \sum_{\langle n,m \rangle} \mathbf{M}_n \cdot \mathbf{M}_m,$$

Weight of the eigenvectors in a 2nd Brillouin zone

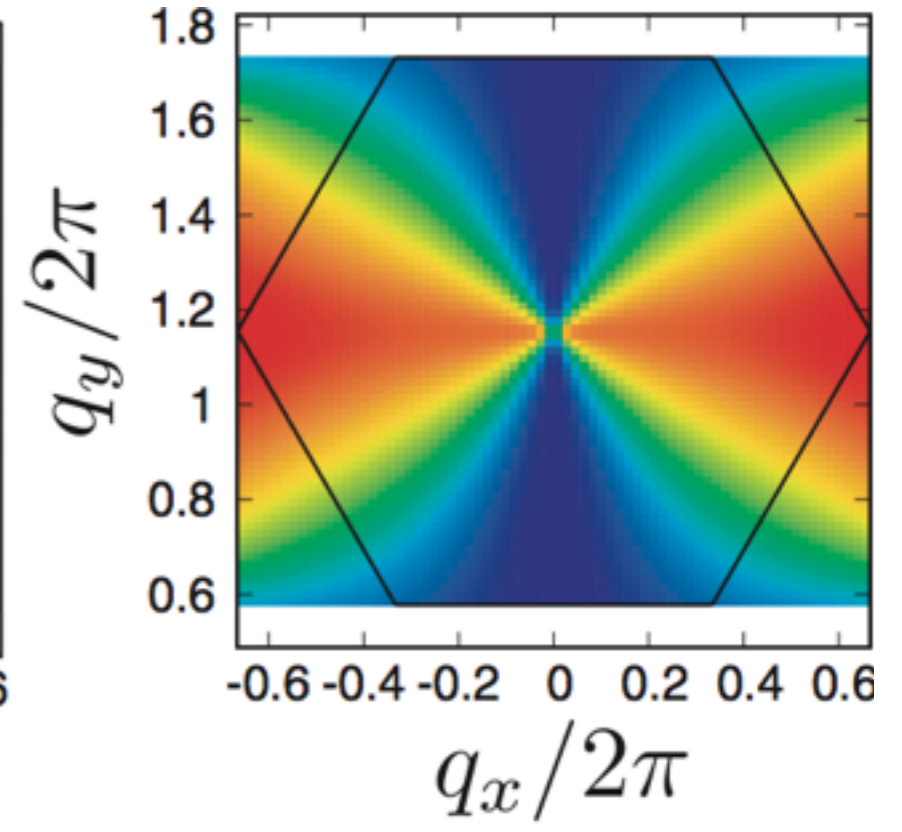
Lower dispersive band



Higher dispersive band



Flat band



Origin of the Half moons

in terms of spins

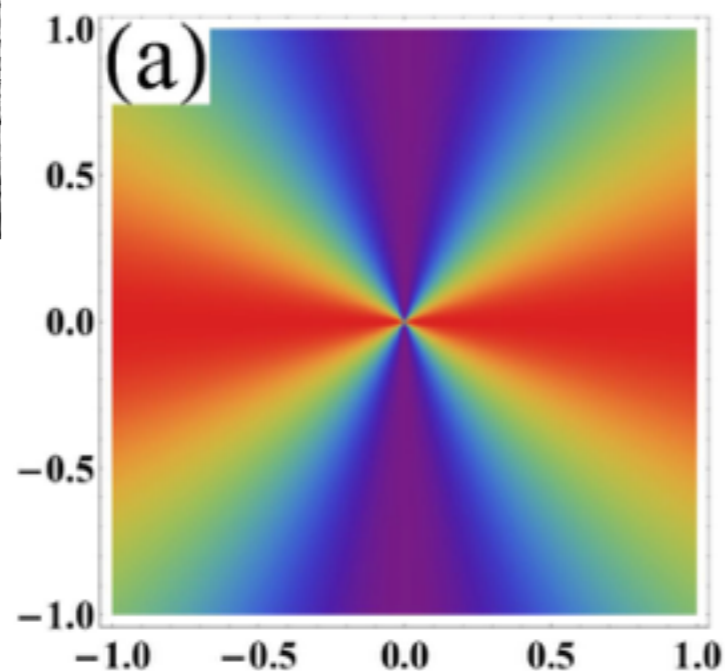
$$J = \tilde{J}_2 = \tilde{J}_3$$

in terms of a coarse-grained field

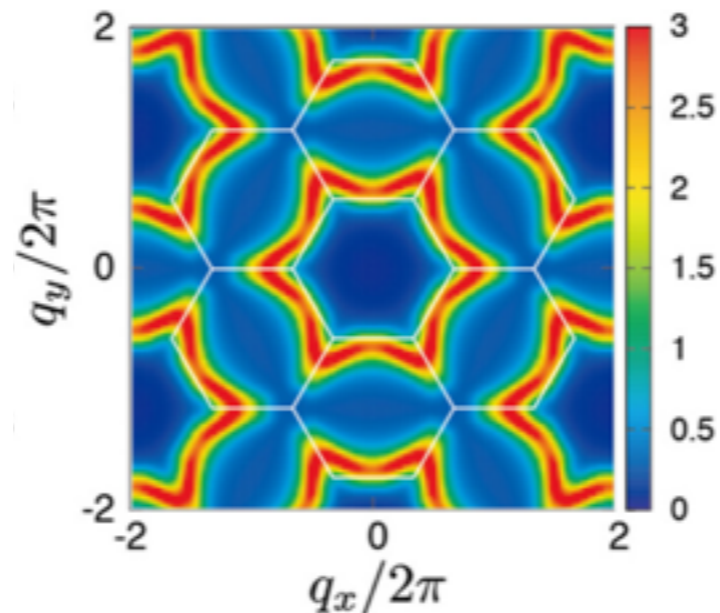
$$\mathcal{H} = \tilde{J}_1 \sum_{\text{n.n.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_2 \sum_{\text{2nd.}} \mathbf{S}_i \cdot \mathbf{S}_j + \tilde{J}_3 \sum_{\text{3rd.}} \mathbf{S}_i \cdot \mathbf{S}_j \longrightarrow H = \left(\frac{1}{2} - J\right) \sum_n |\mathbf{M}_n|^2 - J \sum_{\langle n,m \rangle} \mathbf{M}_n \cdot \mathbf{M}_m,$$

Field theory by
Han, Pohle, Shannon
PRB 2018

pinch point

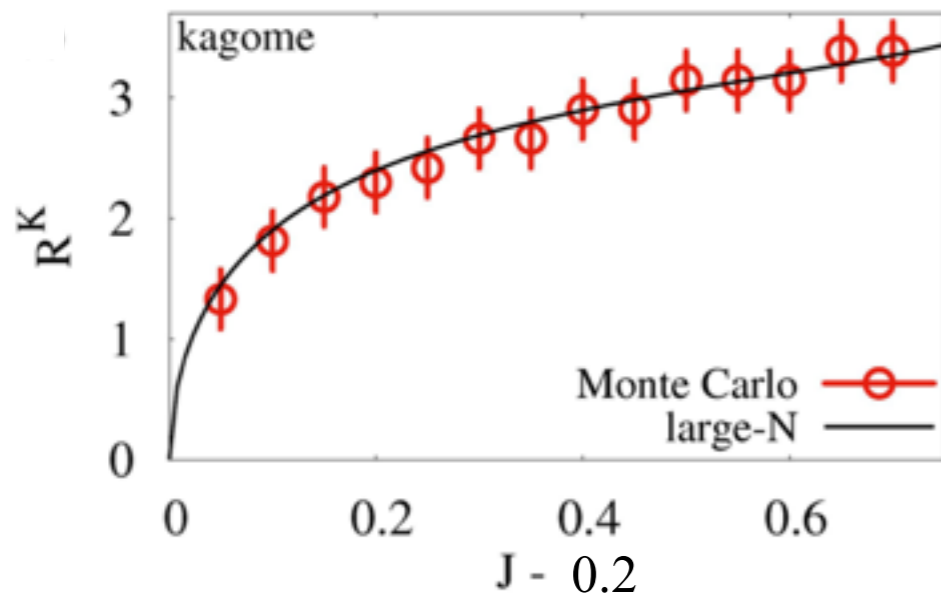


Origin of the Star patterns

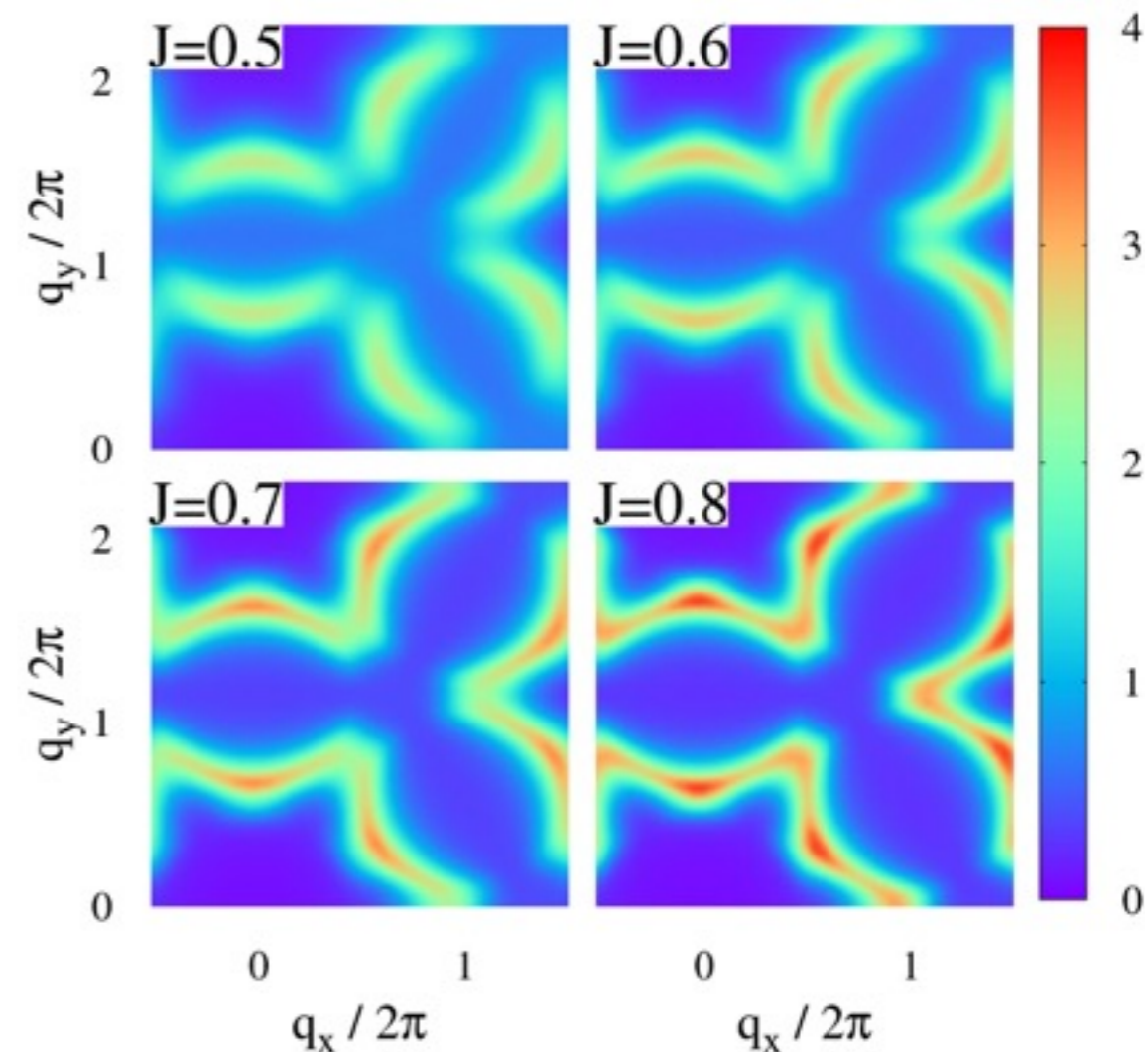


The radius of the half moons increase with J .

$$R^K = \frac{4}{\sqrt{3}} \arccos \sqrt{\frac{1}{8} \left[\left(\frac{1+J}{2J} \right)^2 - 1 \right]},$$



The half moons merge into stars.



Conclusion

Manipulate the gauge fields from a higher manifold
Rank-2 U(1) tensor spin liquids in breathing geometry with 4-fold pinch points

Half moons are dispersive pinch points,
and common neutron-scattering features near a Coulomb phase.
The star patterns are half moons reaching the limit of the Brillouin zone.

Machine Learning can build an entire phase diagram
without being taught the nature of the phases beforehand.
It can characterise the local spin constraints of spin liquids,
and measure crossovers (i.e. not only phase transitions).

- ◆ Yan, Benton, Jaubert, Shannon, arXiv:1902.10934
- ◆ Udagawa, Jaubert, Castelnovo, Moessner, PRB 2016
- ◆ Mizoguchi, Jaubert, Udagawa, PRL 2017
- ◆ Mizoguchi, Jaubert, Moessner, Udagawa, PRB 2018
- ◆ Taillefumier, Benton, Han, Jaubert, Shannon, PRX 2017
- ◆ Benton, Jaubert, Singh, Oitmaa, Shannon, PRL 2018
- ◆ Greitemann et al, PRB 2019 (in press)

Fundings

