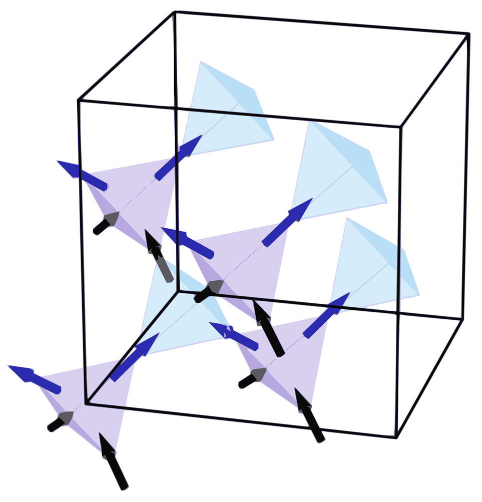
Fragmentation in spin ices: quantum and thermodynamic aspects

Flavien Museur[1,2], Elsa Lhotel[1], Peter Holdsworth[2]

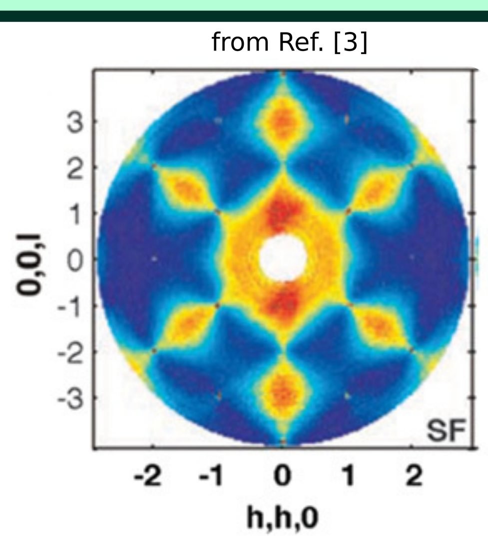
1: Institut Néel, CNRS and Université Grenoble Alpes 2: Laboratoire de Physique, ENS de Lyon

Fragmentation in the Dumbbell model of spin ice

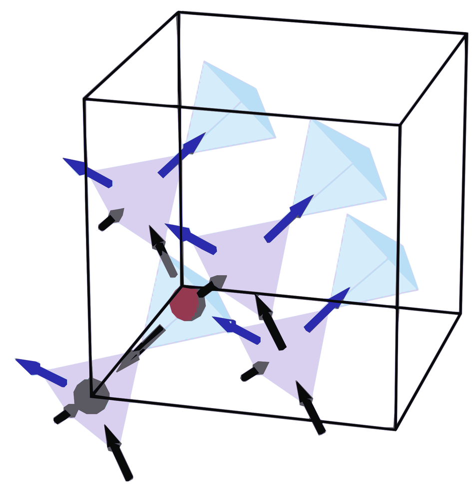


- 2 in / 2 out: **ice rule**
- Extensive residual entropy (Pauling):

$\Longrightarrow$ Lead to pinch-point pattern in neutron scattering (dipolar correlations)



- Flipping a spin breaks the ice rule
- Deconfined excitations: **monopoles**



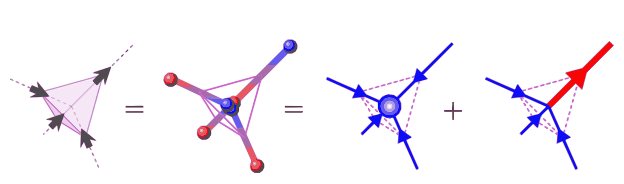
$$\mathcal{H}_{\mathrm{DSI}} = -J\sum_{<i,j>}\mathbf{S}_i\cdot\mathbf{S}_j + Dr_{nn}^3\sum_{i>j}\frac{(\mathbf{S}_i\cdot\mathbf{S}_j)\cdot(\mathbf{r}_{ij}\cdot\mathbf{r}_{ij})-3(\mathbf{S}_i\cdot\mathbf{r}_{ij})(\mathbf{S}_j\cdot\mathbf{r}_{ij})}{|\mathbf{r}_{ij}^5|}$$

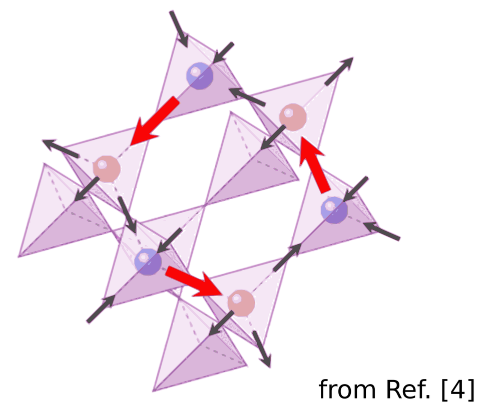
$$\Downarrow$$

$$\mathcal{H}_{\mathrm{Dumbbell}} = -\mu\sum_{\mathbf{r}}Q_{\mathbf{r}}^2 + \frac{1}{2}\sum_{\mathbf{p}\neq\mathbf{q}}\frac{\mu_0 Q_{\mathbf{p}}Q_{\mathbf{q}}}{4\pi|\mathbf{p}-\mathbf{q}|}$$

$$\mathcal{H}_{\mathrm{Dumbbell}} + \Delta\sum_{\mathbf{r}}\eta_{\mathbf{r}}Q_{\mathbf{r}}$$

Consider a crystal of monopoles:





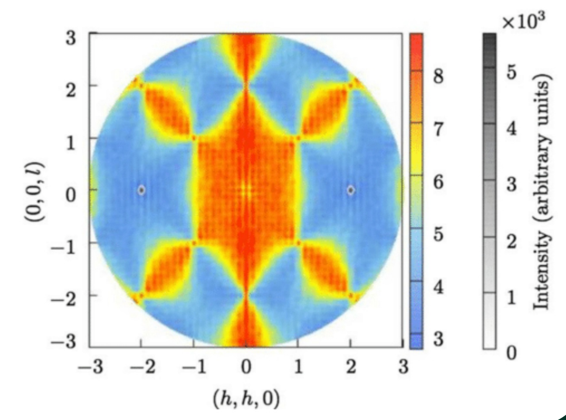
$$\mathbf{M} = \nabla\Psi + \nabla\times\mathbf{A}$$

$$[M_{\mathbf{r}\mu}]\,\frac{a}{m} = (-1,-1,-1,1) = \left(-\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{1}{2}\right) + \left(-\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{1}{2},\tfrac{3}{2}\right)$$

Coexistence of order and disorder:

- Bragg peaks
- Diffuse background

$\Rightarrow$ fragmented entropy

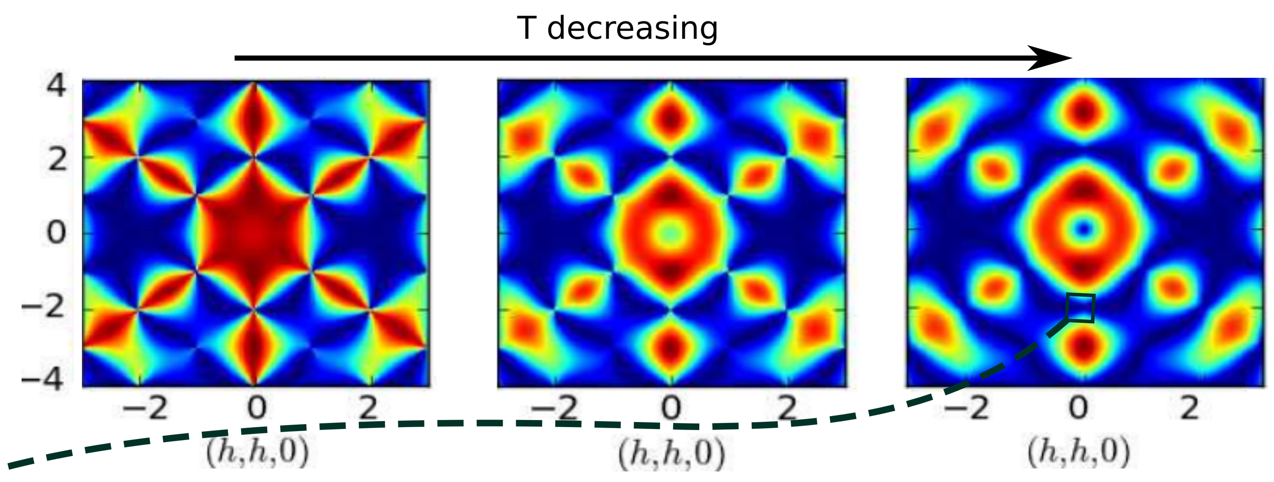


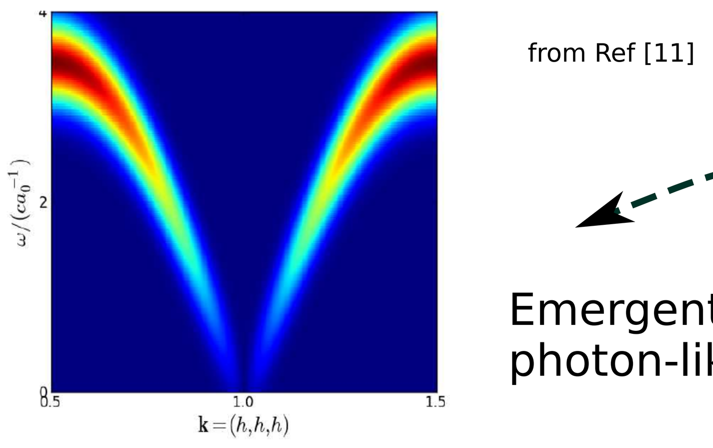
Quantum fluctuations

XXZ hamiltonian:

$$\mathcal{H}_{\mathrm{Quantum}} = -\mu\sum_{\mathbf{r}}Q_{\mathbf{r}}^2 + \Delta\sum_{\mathbf{r}}\eta_{\mathbf{r}}Q_{\mathbf{r}} - J_{\pm}\sum_{<i,j>}\left(S_i^+S_j^- + S_i^-S_j^+\right)$$

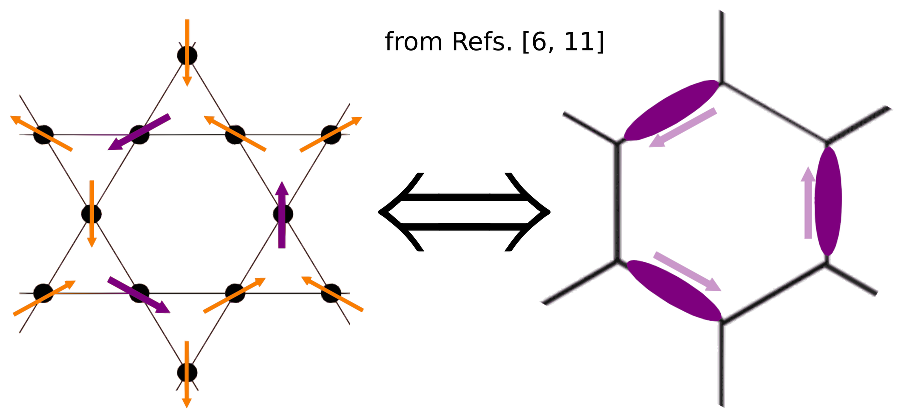
At low T, maps to a compact U(1) lattice gauge theory





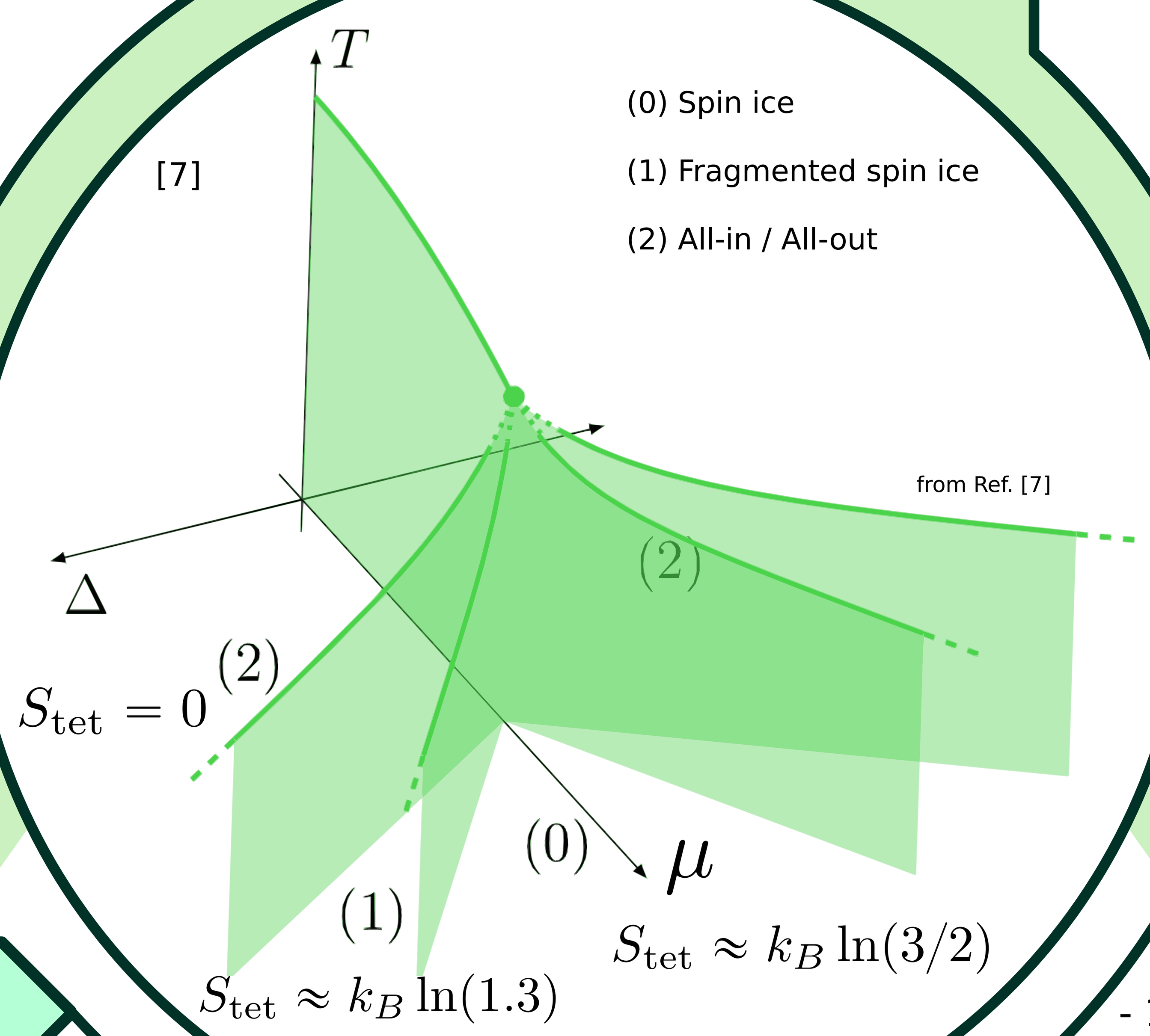
Emergent QEM with a photon-like excitation

The transverse part maps to a hardcore bosons / dimer model on the dual lattice:

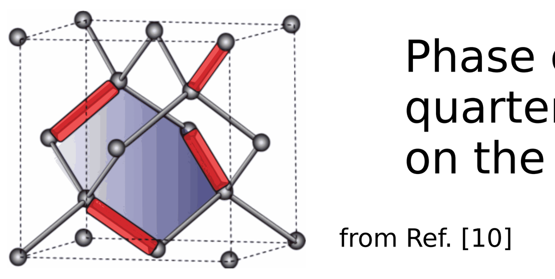


Effective perturbative hamiltonian:

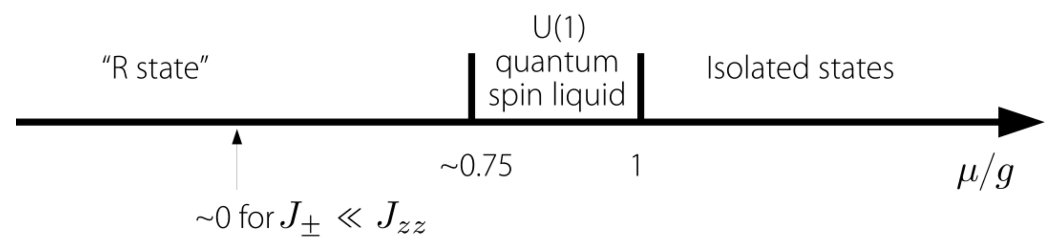
$$\mathrm{H}_{eff} = \mu\sum_{\hexagon}|\triangleright\rangle\langle\triangleright| + |\triangleleft\rangle\langle\triangleleft| - g\sum_{\hexagon}|\triangleright\rangle\langle\triangleleft| + |\triangleleft\rangle\langle\triangleright|$$



Low temperature phases

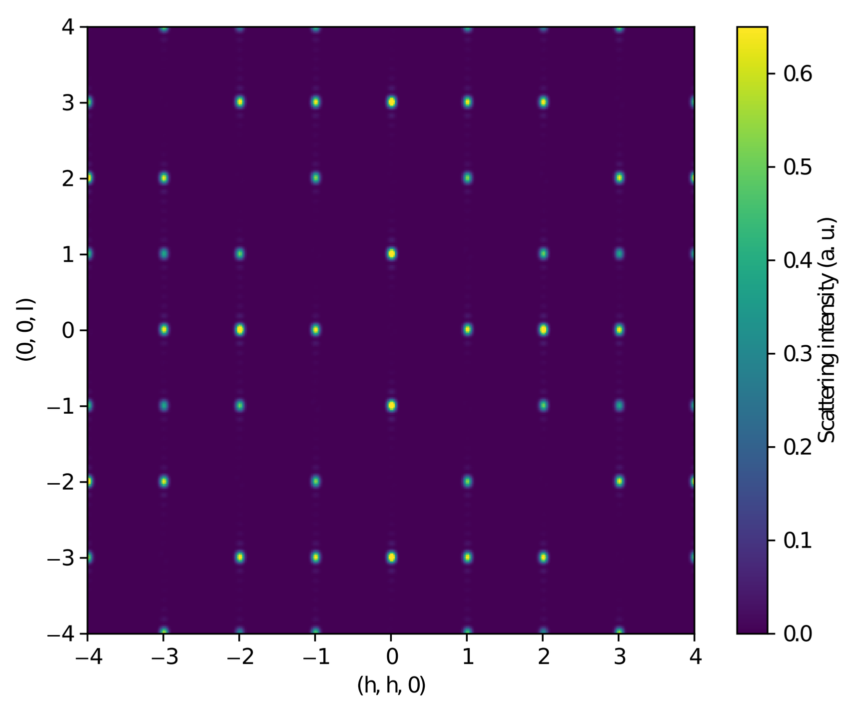


Phase diagram for the quarter-filled dimer model on the diamond lattice:



No interference between the fragments' neutron signals

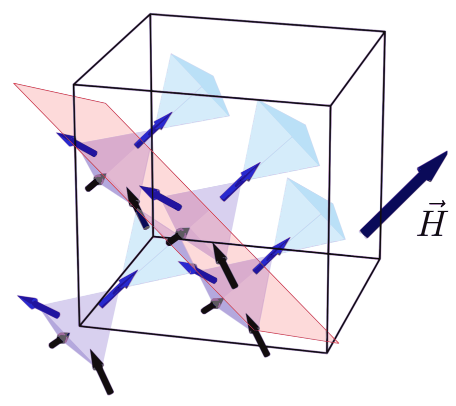
$$\Rightarrow\quad I_{\mathrm{Total}} = I_{\mathrm{Long}} + I_{\mathrm{trans}}$$



Fragmentation order parameters

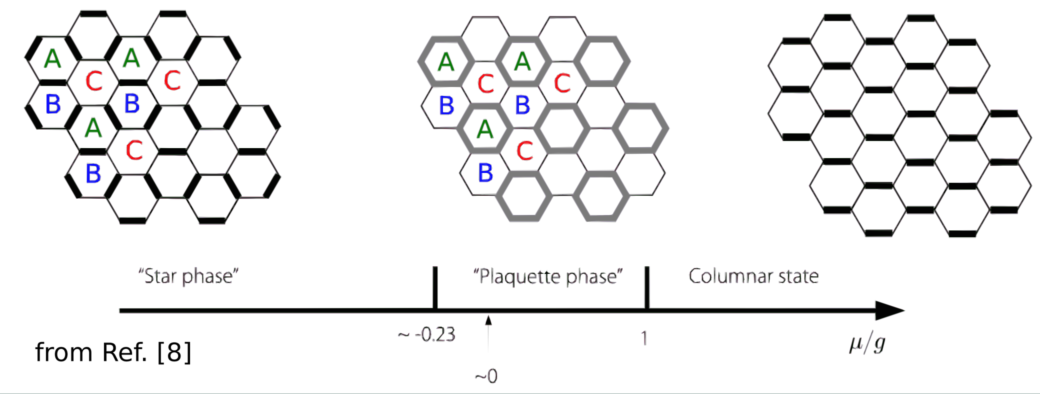
Spin ice in a [111] field

- 1 spin per tetrahedra is pinned, the other 3 obey the kagome ice rules
- Complete decomposition uses three fragments:



$$\mathbf{M} = \nabla\Psi + \nabla\times\mathbf{A} + \mathbf{h}$$

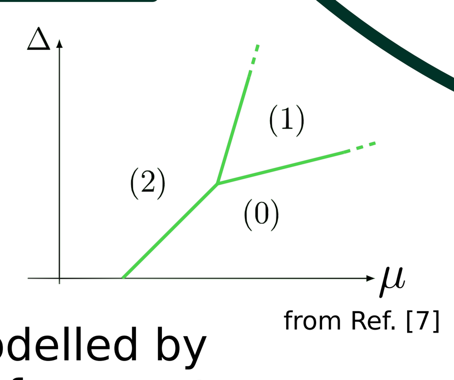
$$[M_{\mathbf{r}\mu}]\,\frac{a}{m} = (-1,-1,1,1) = [0] + \left(-\frac{2}{3},-\frac{2}{3},\frac{4}{3},0\right) + \left(-\frac{1}{3},-\frac{1}{3},-\frac{1}{3},1\right)$$



from Ref. [8]

Thermodynamics

At low T the spin ice phase should prevail close to the critical point because it has the largest entropy



Fragmented phase entropy can be modelled by considering the spectral intensities of fragments in the Pauling approximation

$$S \approx k_B\ln(3/2) \approx k_B A^2\ln(3/2) = k_B\left(1-\tfrac{1}{4}(\rho_1^2+4\rho_2^2)\right)\ln(3/2)$$

$\Longrightarrow$ Should resolve the multicritical region

Experiments:

- $Ho_2Ir_2O_7$ neutron diffraction under pressure
- $Dy_2Ir_2O_7$ specific heat under pressure
- $Ho_2Ru_2O_7$ magnetic and neutron measurements

References

[1] M. J. Harris, S. T. Bramwell, D. F. McMorrow et al., Physical Review Letters 79, 2554 (1997)
[2] C. Castelnovo, R. Moessner, and S. L. Sondhi, Nature 451, 42 (2008)
[3] T. Fennell, P. P. Deen, A. R. Wildes et al., Science (2009)
[4] M. E. Brooks-Bartlett, S. T. Banks, L. D. C. Jaubert, A. Harman-Clarke, and P. C. W. Holdsworth, Physical Review X 4, (2014).
[5] E. Lhotel, L. D. C. Jaubert, and P. C. W. Holdsworth, Journal of Low Temperature Physics (2020)
[6] R. Moessner and S. L. Sondhi, Phys. Rev. B 68, 064411 (2003)
[7] V. Raban, C. T. Suen, L. Berthier, and P. C. W. Holdsworth, Phys. Rev. B 99, 224425 (2019)
[8] T. M. Schlittler, R. Mosseri, and T. Barthel, Physical Review B 96, (2017)
[9] E. Lefrançois, V. Cathelin, E. Lhotel et al., Nature Communications 8, (2017)
[10] O. Sikora, N. Shannon, F. Pollmann, K. Penc, and P. Fulde, Physical Review B 84, (2011)
[11] O. Benton, O. Sikora, and N. Shannon, Phys. Rev. B 86, 075154 (2012)

institut NÉEL cnrs UGA Université Grenoble Alpes ENS DE LYON

flavien.museur@neel.cnrs.fr December 2021