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Phase transitions and spin dynamics of the quasi-1D Ising-like antiferromagnet $BaCo_2V_2O_8$ in a longitudinal magnetic field

Béatrice GRENIER

Univ. Grenoble Alpes & CEA-IRIG-MEM

Grenoble, France

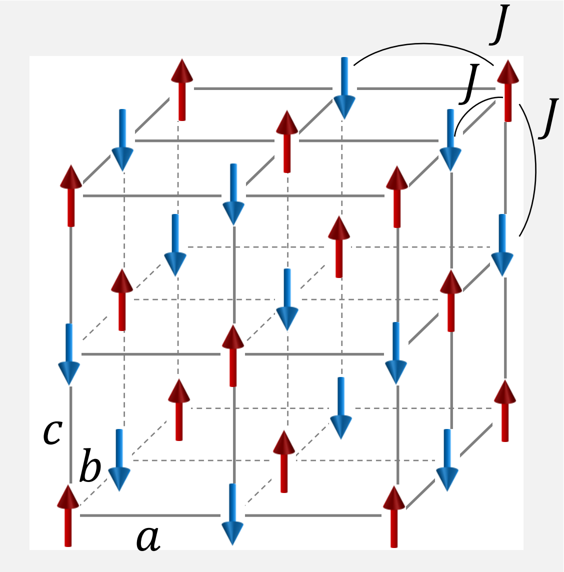
Introduction on XXZ 1D spin ½ antiferromagnets

Introduction: Classical 3D vs quantum 1D spin ½ antiferromagnets

$$\mathcal{H} = J \sum_i \vec{S}_i . \vec{S}_{i+1}$$

Conventional Heisenberg 3D antiferromagnet

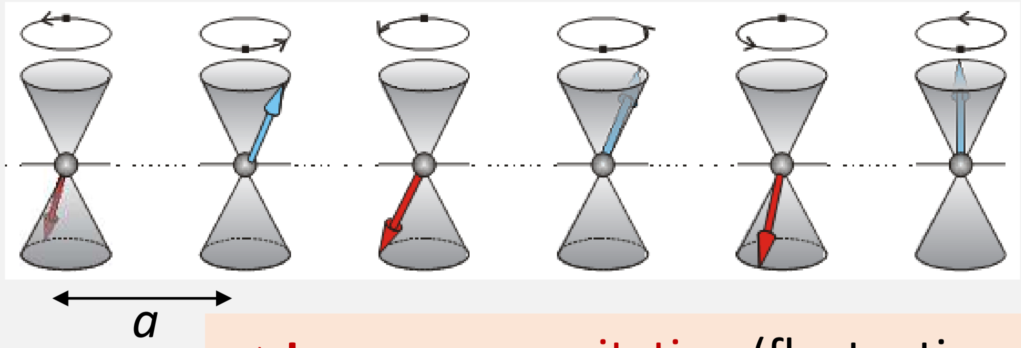
isotropic spins — $J > 0$



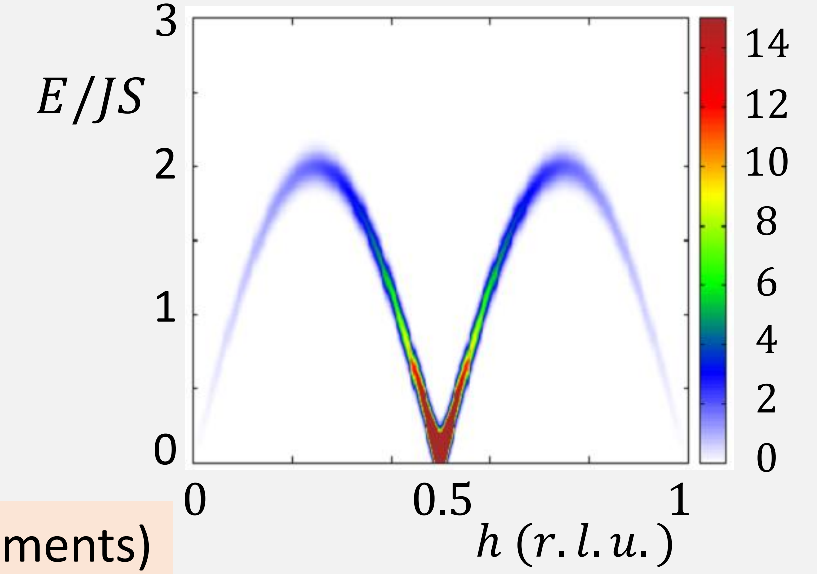
• **Ground state: AF (Néel) ordering** below $T_N \sim J$

Example: cubic AF → same J along the 3 directions of space → $\vec{k} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$

• **Excitations: spin waves / magnons**
(precession of the spin around its equilibrium position)



$$E(k) = 2JS|\sin(ka)|$$

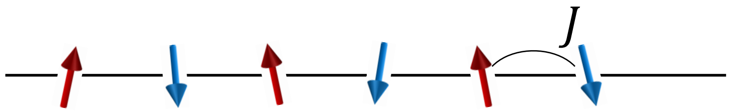


→ **transverse** excitation (fluctuations ⊥ ordered magnetic moments)

Introduction: *Classical 3D vs* ***quantum 1D spin ½ antiferromagnets***

$$\mathcal{H} = J \sum_i \vec{S}_i.\vec{S}_{i+1}$$

Quantum Heisenberg 1D antiferromagnet



J along a single direction of space

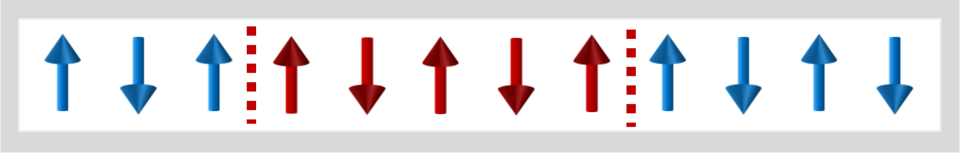
Quantum fluctuations ⇒ **exotic static and dynamical properties**

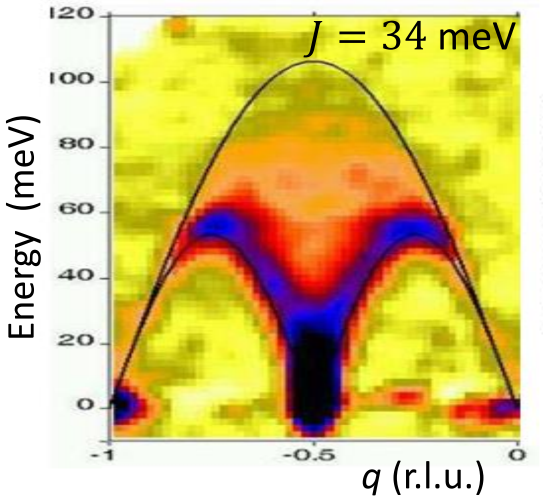
- **Ground state: Tomonaga-Luttinger Liquid (TLL)**

  No magnetic LRO down to $T = 0$

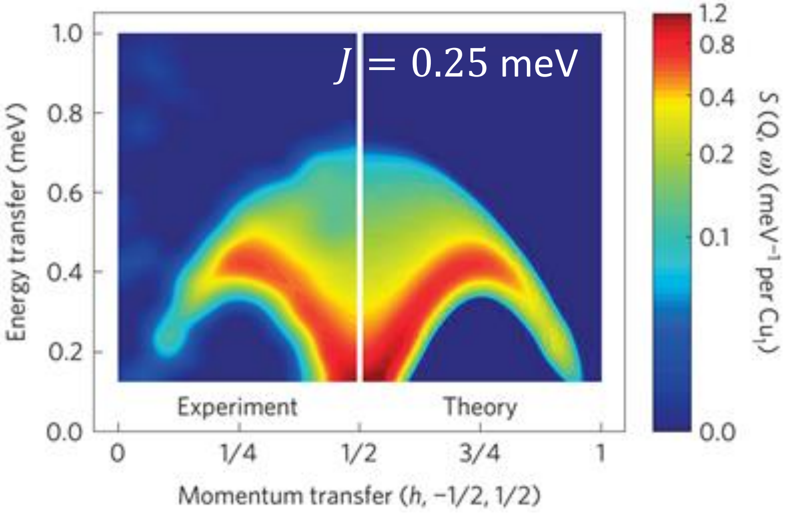
- **Excitations: Ungapped 2-spinons continuum**

  (= "domain walls")





$KCuF_3$
Nagler *et al.*, PRB (1991)



$CuSO_4 \bullet 5D_2O$
Mourigal *et al.*, Nat. Phys. (2013)

Bethe, Z. Phys. (1931); Haldane, PRL (1983)

Introduction: XXZ *antiferromagnetic spin 1/2 chains*

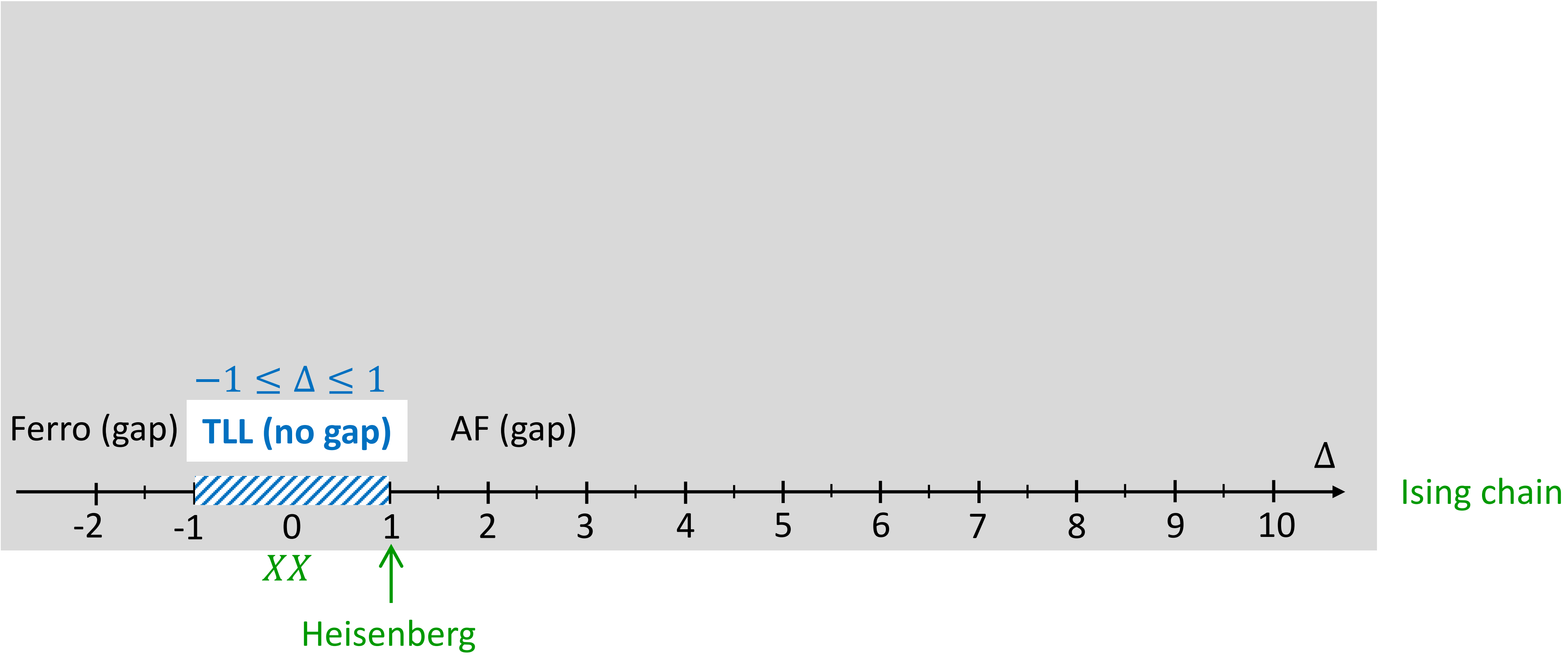
$$\mathcal{H}_{XXZ} = J \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta\, S_i^z S_{i+1}^z \right)$$

anisotropy parameter

$\Delta = 1$: Heisenberg

$0 < \Delta < 1$: XX-like ($\Delta = 0$: pure XX)

$\Delta > 1$: Ising-like ($\Delta \to +\infty$: pure Ising)



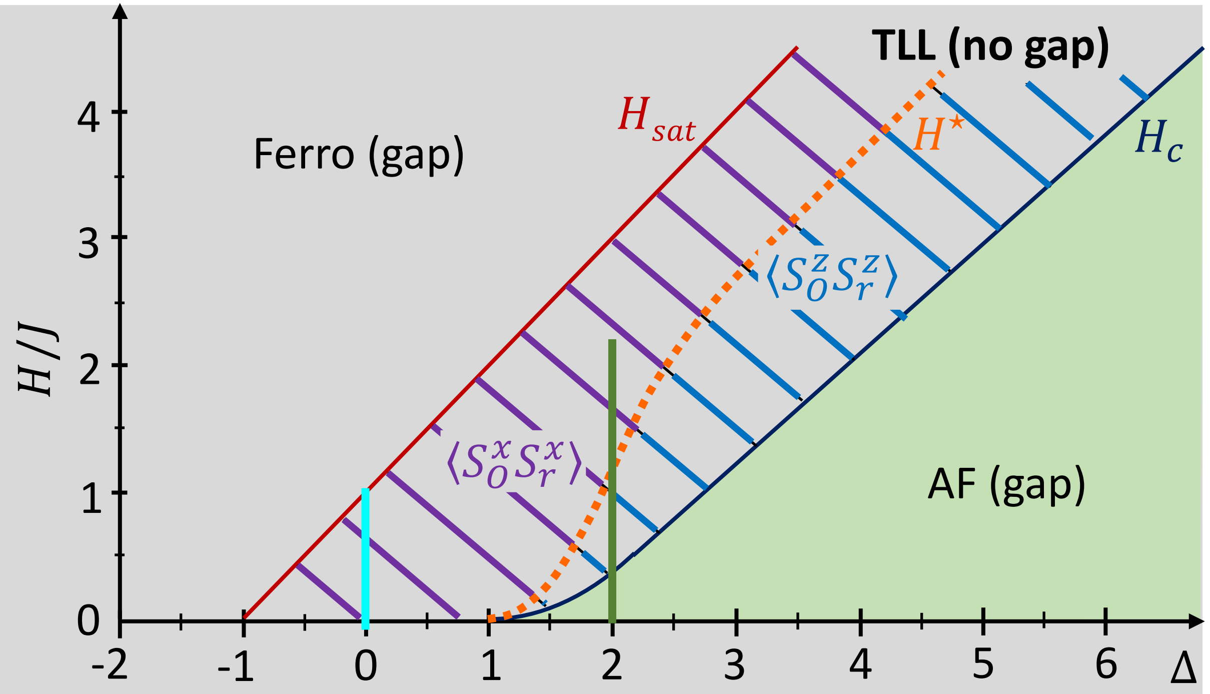
Introduction: *XXZ antiferromagnetic spin 1/2 chains*

$$\mathcal{H}_{XXZ} = J \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta\, S_i^z S_{i+1}^z \right)$$

XXZ AF $S = 1/2$ chain
in a magnetic field $H \parallel z$

$$\mathcal{H} = \mathcal{H}_{XXZ} - H \sum_i S_i^z$$

S. Wessel and S. Haas,
PRB (2000)



$\langle S_0^x S_r^x \rangle$:
Commensurate
Transverse AF correlations

$\langle S_0^z S_r^z \rangle$:
Incommensurate
longitudinal AF correlations
incommensurability increases with increasing the field

$\langle S_0^z S_r^z \rangle$:
Commensurate
Longitudinal AF correlations

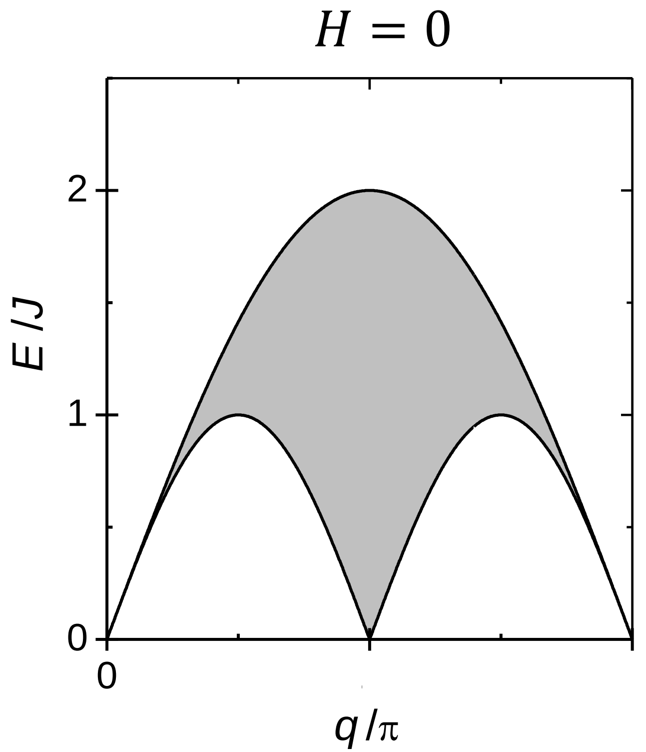
Experimental realizations:

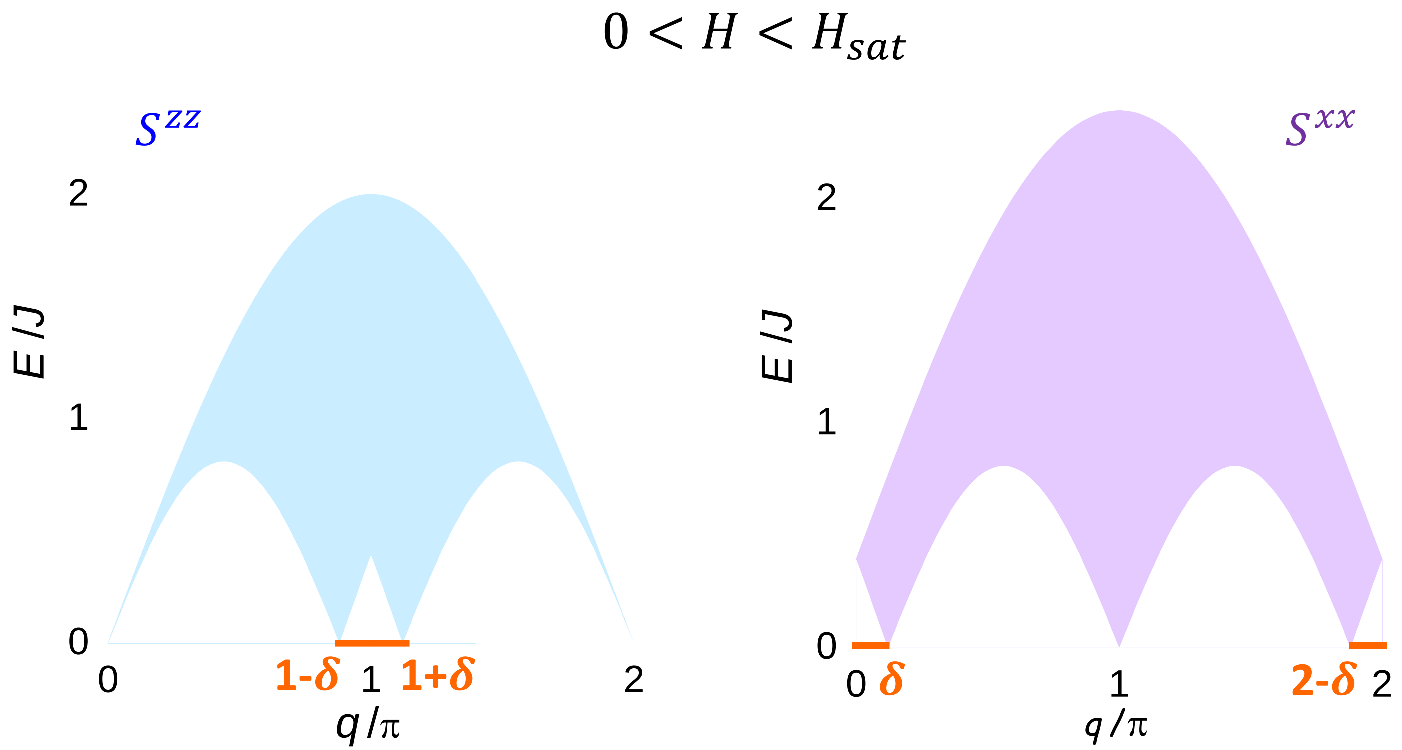
$\mathbf{\Delta = 1}$: most of the systems ($KCuF_3$, CuSO4· 5D2O, CuPzN …)

$\mathbf{\Delta = 10}$: $CsCoX_3$ (X=Br, Cl) extensively studied in 70's and 80's → $H_c \simeq 75$ T

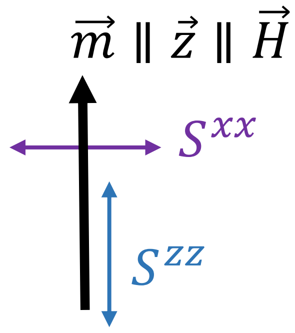
$\Delta = 2$: **$BaCo_2V_2O_8$** Kimura *et al.*, PRL (2008) → $H_c \simeq 4$ T → **easily reachable with neutron scattering experiments**

Introduction: *Heisenberg antiferromagnetic spin 1/2 chains*





$\boldsymbol{H = 0}$: **ungapped** two-spinon continuum ⇔ TLL spin-dynamics



$\vec{\boldsymbol{H}} \parallel \vec{\boldsymbol{z}}$ (**TLL phase:** $0 < H < H_{sat}$): **Incommensurability** $\boldsymbol{\delta}$ develops with $\delta = 2\pi\langle S^z\rangle \propto H$

- Around $\boldsymbol{q = \pi}$ for **longitudinal** $\boldsymbol{S^{zz}}$ fluctuations
- Around $\boldsymbol{q = 0}$ and $\boldsymbol{2\pi}$ for **transverse** $\boldsymbol{S^{xx}}$ fluctuations

G. Müller, PRB (1981)

Introduction on $BaCo_2V_2O_8$

- crystallographic structure
- magnetic structures in a longitudinal field
- zero-field magnetic excitations

$BaCo_2V_2O_8$: *Crystallographic structure*

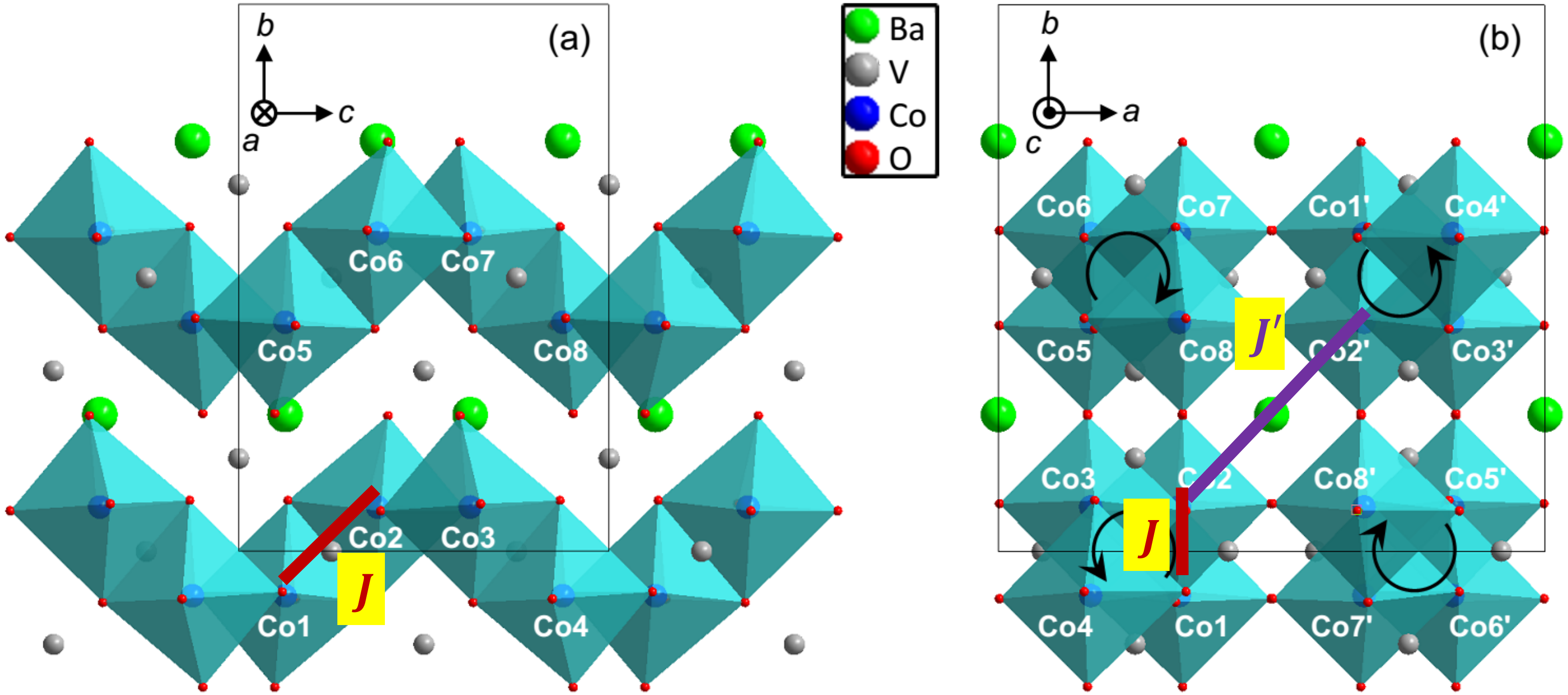
- **Screw chains of effective spin 1/2 ∥ *c*-axis** (tetragonal space group)

- **Ising-like AF 1D model with $\Delta \sim 2$; Easy-axis $z = c$ chain axis** $(J_z \sim 2J_x \sim 2J_y)$
  S. Kimura *et al.*, J. Phys.: Conf. Series (2006) & JPSJ (2013)

XXZ Hamiltonian

$$\mathcal{H}_{XXZ} = J\sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta\, S_i^z S_{i+1}^z\right)$$

- **Non-negligible inter-chain interactions** (quasi-1D)
  → AF LRO at $T < 5.6$ K



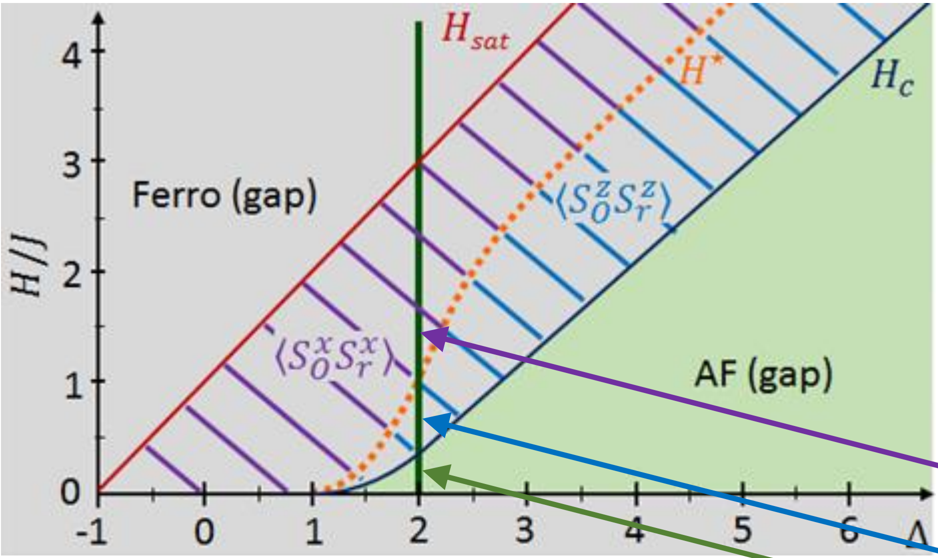
$x \equiv a$
$y \equiv b$
$z \equiv c$

$J' \ll J$

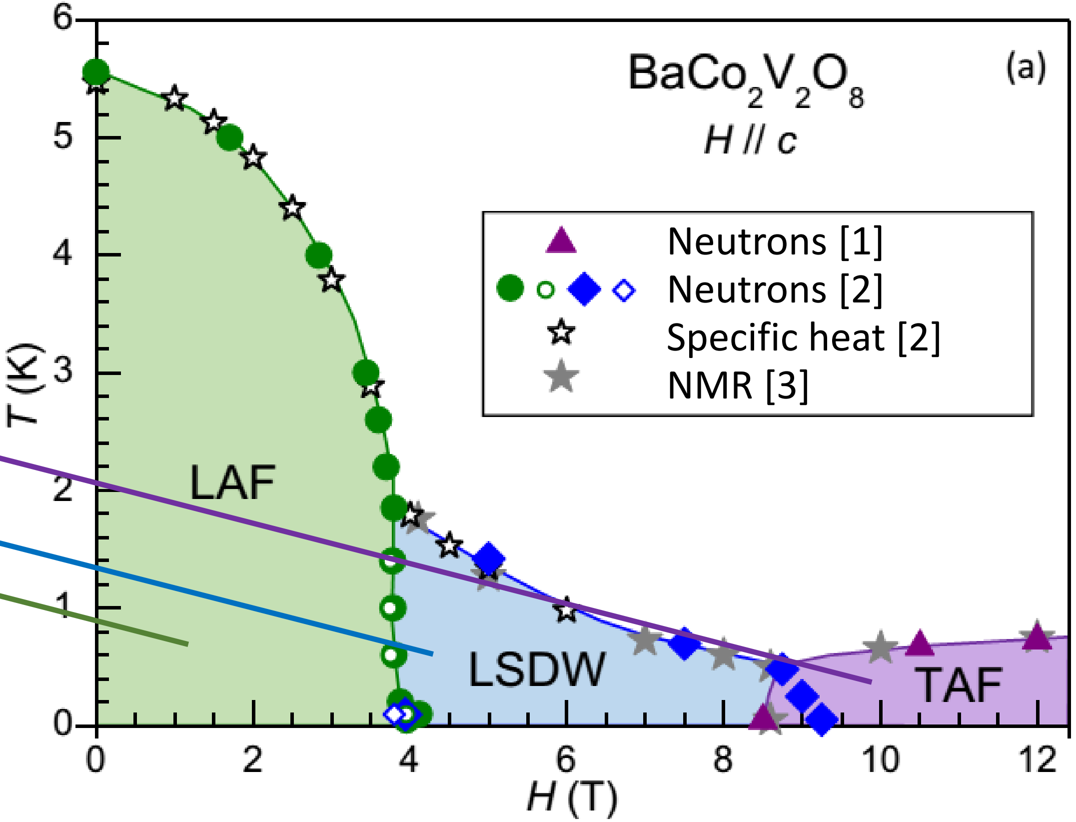
Intrachain interaction: ***J*** AF

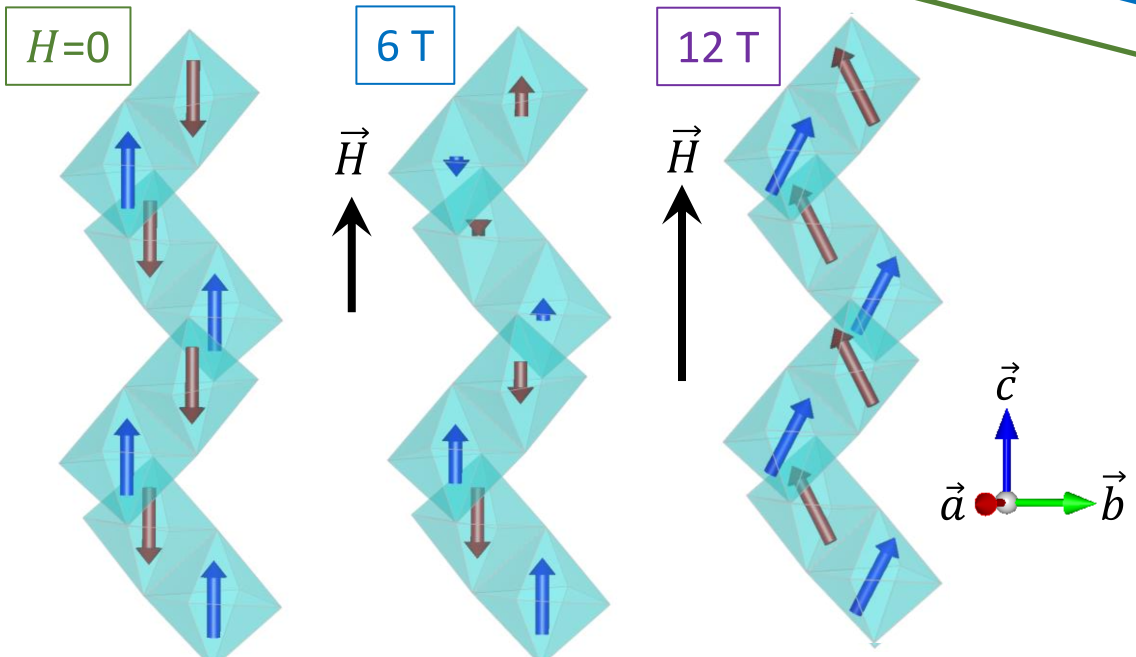
Relevant interchain interaction: ***J'*** diagonal, AF

$BaCo_2V_2O_8$: *Magnetic structures for H ∥ c*



Single crystal diffraction on D23 @ ILL





$\vec{k}_{AF} = (1,0,0)$ $\vec{k}_{LSDW} = (1,0,\delta)$ $\vec{k}_{AF} = (1,0,0)$

LAF: Longitudinal AF ($\vec{m}_{AF} \parallel \vec{c}$)

LSDW: Longitudinal Spin Density Wave ($\vec{m}_{IC} \parallel \vec{c}$)

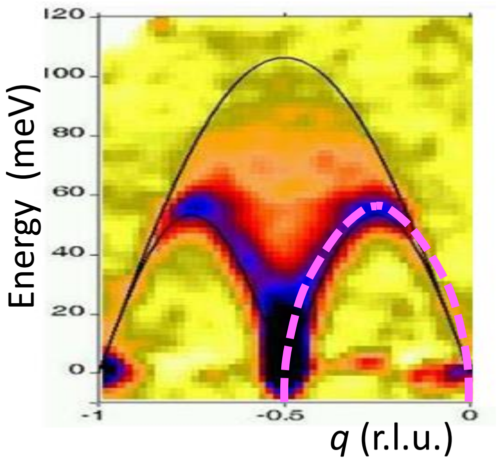
TAF: canted Transverse AF ($\vec{m}_{AF} \parallel \vec{a}$)

[1] B. Grenier *et al.*, PRB (2015); [2] E. Canévet *et al.*, PRB (2013);
[3] M. Klanjšek *et al.*, PRB (2015)

$BaCo_2V_2O_8$: *Zero-field spinon excitations*

- **Heisenberg 1D AF $KCuF_3$:**

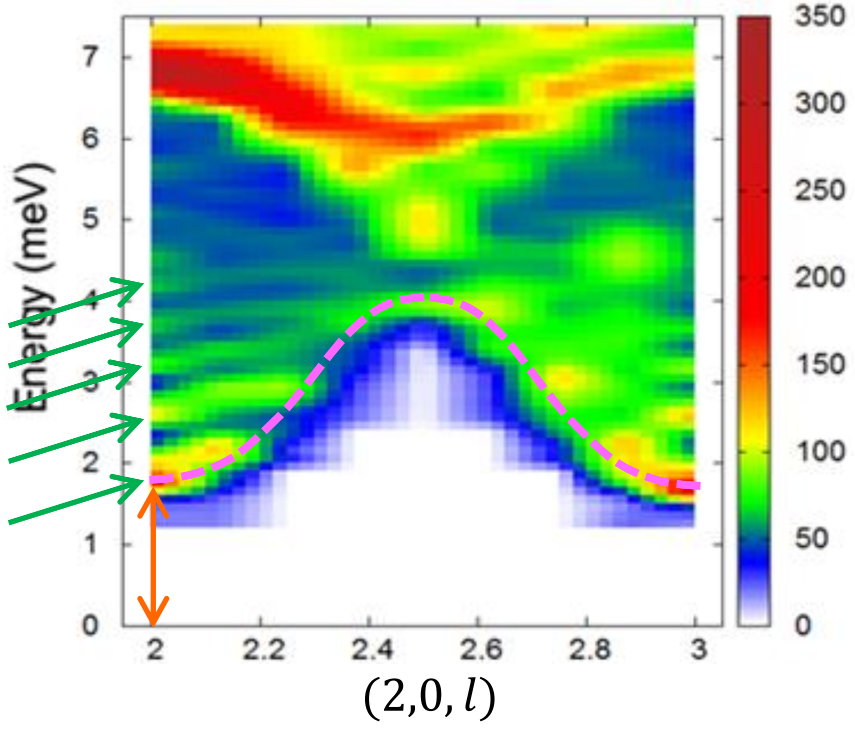
Deconfined spinons



B. Grenier *et al.*, PRL (2015)

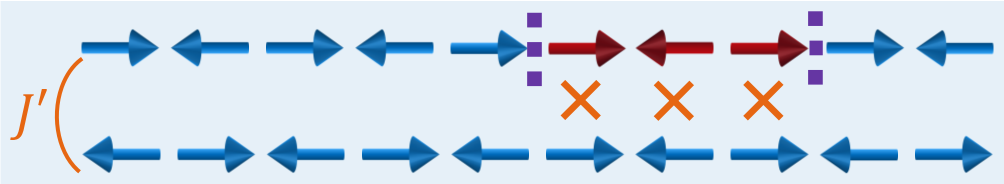
- **Ising-like quasi-1D AF $BaCo_2V_2O_8$**

Inelastic neutron scattering on IN12 @ ILL

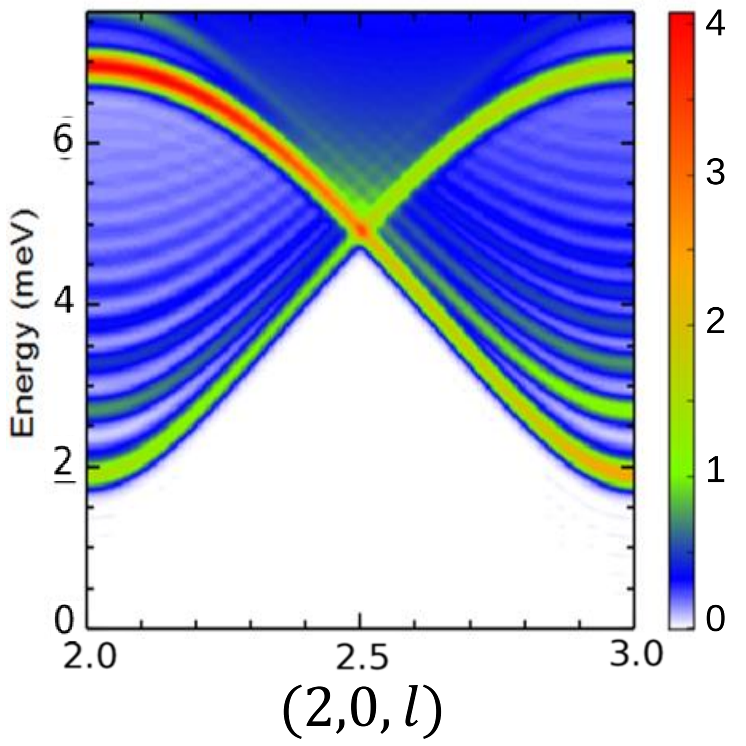


Gap ← **Ising-like** anisotropy

Discretization ← **Confined spinons** ← J'



Numerics: TEBD + mean field (S. Takayoshi and T. Giamarchi)



$J = 5.8$ meV, $\Delta = 1.89$, $J' = 0.17$ meV

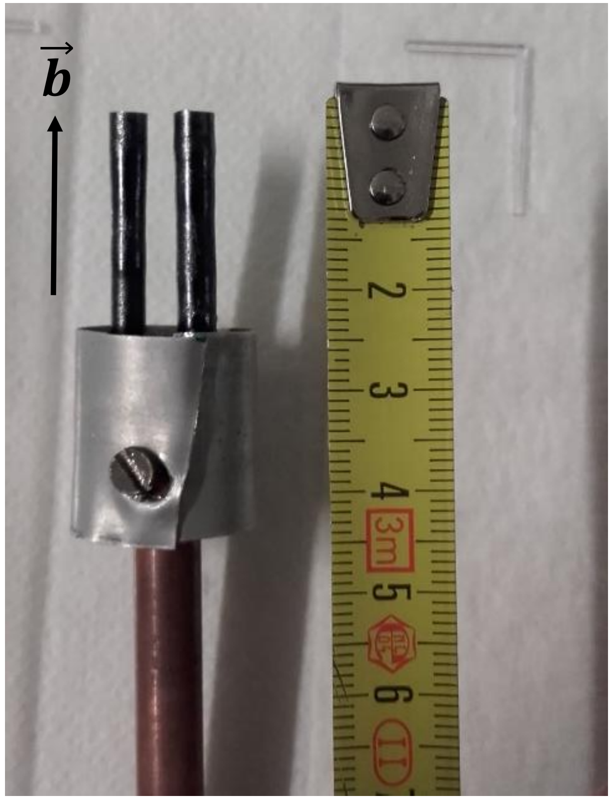
Q. Faure, S. Takayoshi *et al.*, Nature Physics (2018)

Spin dynamics of $BaCo_2V_2O_8$ in a longitudinal field

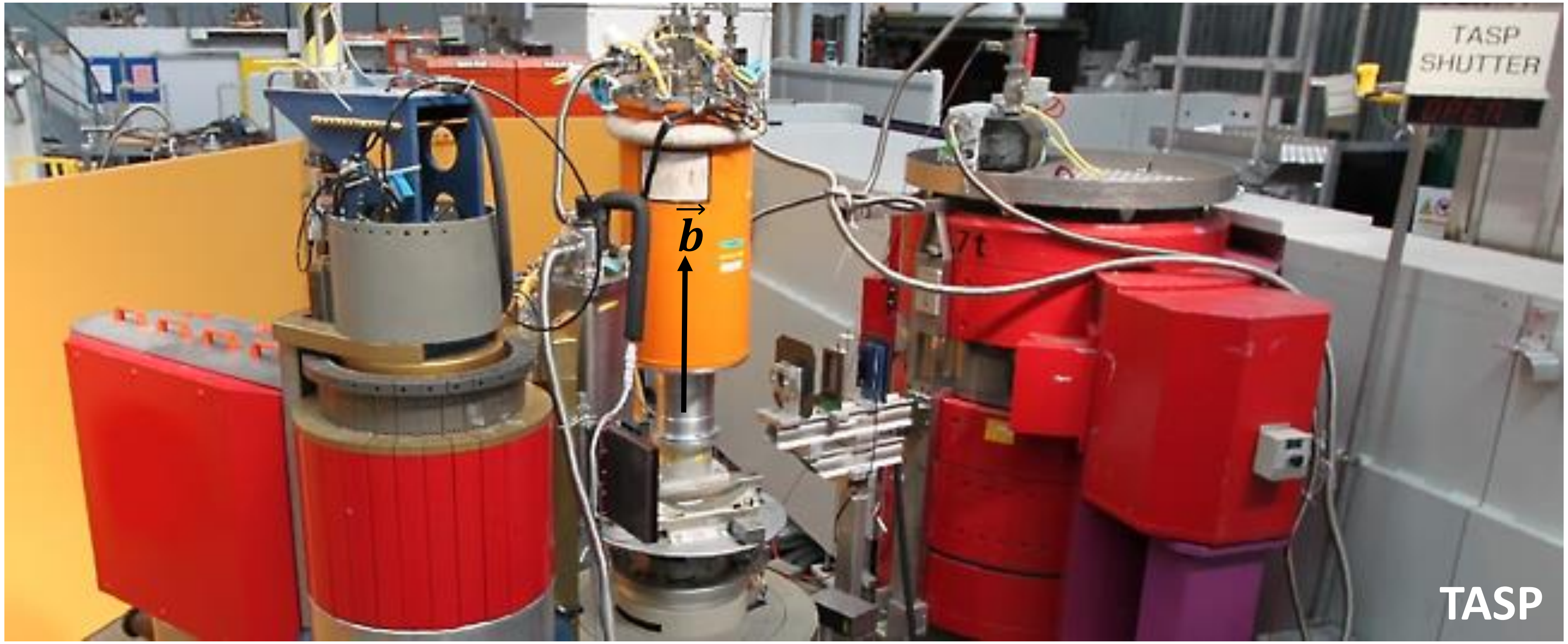
1- in the LSDW phase (up to 6.8 T, on TASP)
2- across LSDW – TAF phase transition (up to 10 T, on IN5)

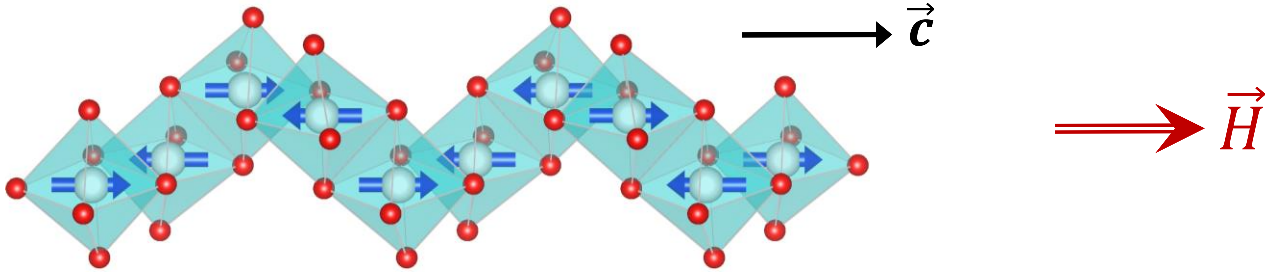
Spin dynamics in a longitudinal field: *experimental set-up 1*

2 co-aligned single-crystals with $\vec{c}$ **horizontal**



Three-axis spectrometer **TASP** @ PSI, Villigen (Switzerland) with **6.8 T horizontal cryomagnet** + dilution

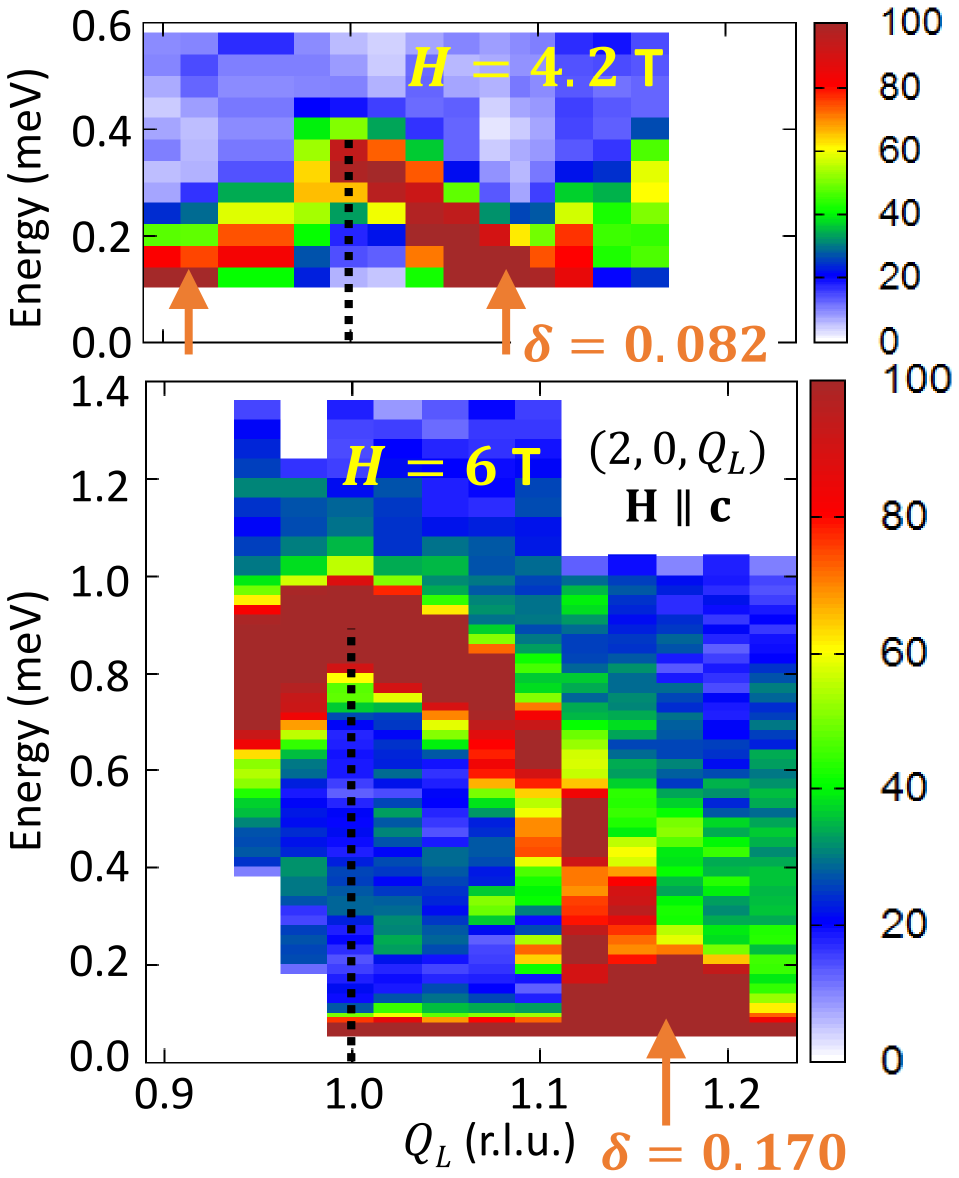


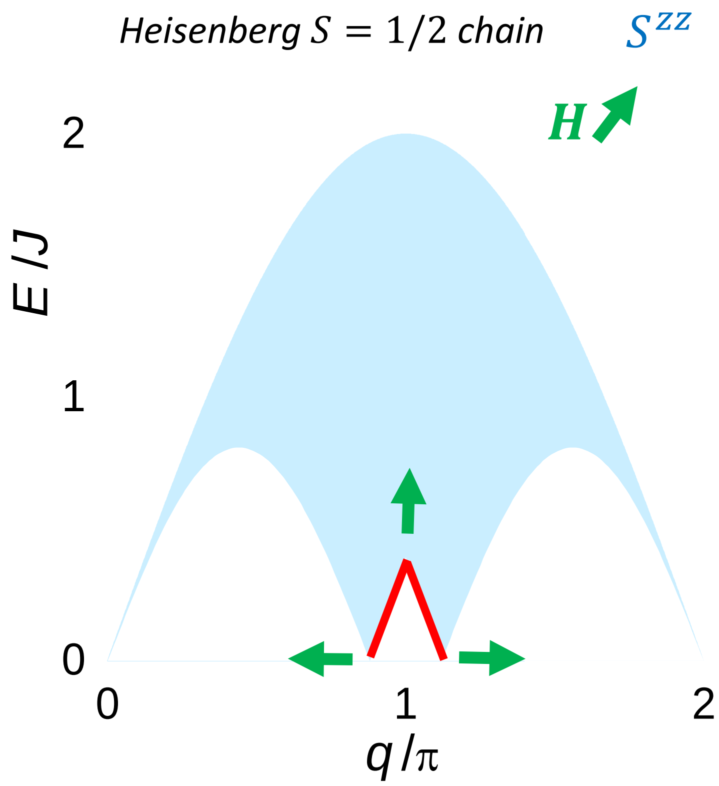


Q. Faure, S. Takayoshi *et al.*, PRL 2019

$BaCo_2V_2O_8$: *spin dynamics in the field-induced LSDW phase*

- **INS intensity maps** around the AF position Q = (2,0,1): **field dependence**





Minima of energy at the IC positions $Q_L = 1 \pm \delta$
(and local maximum at $Q_L = 1$)

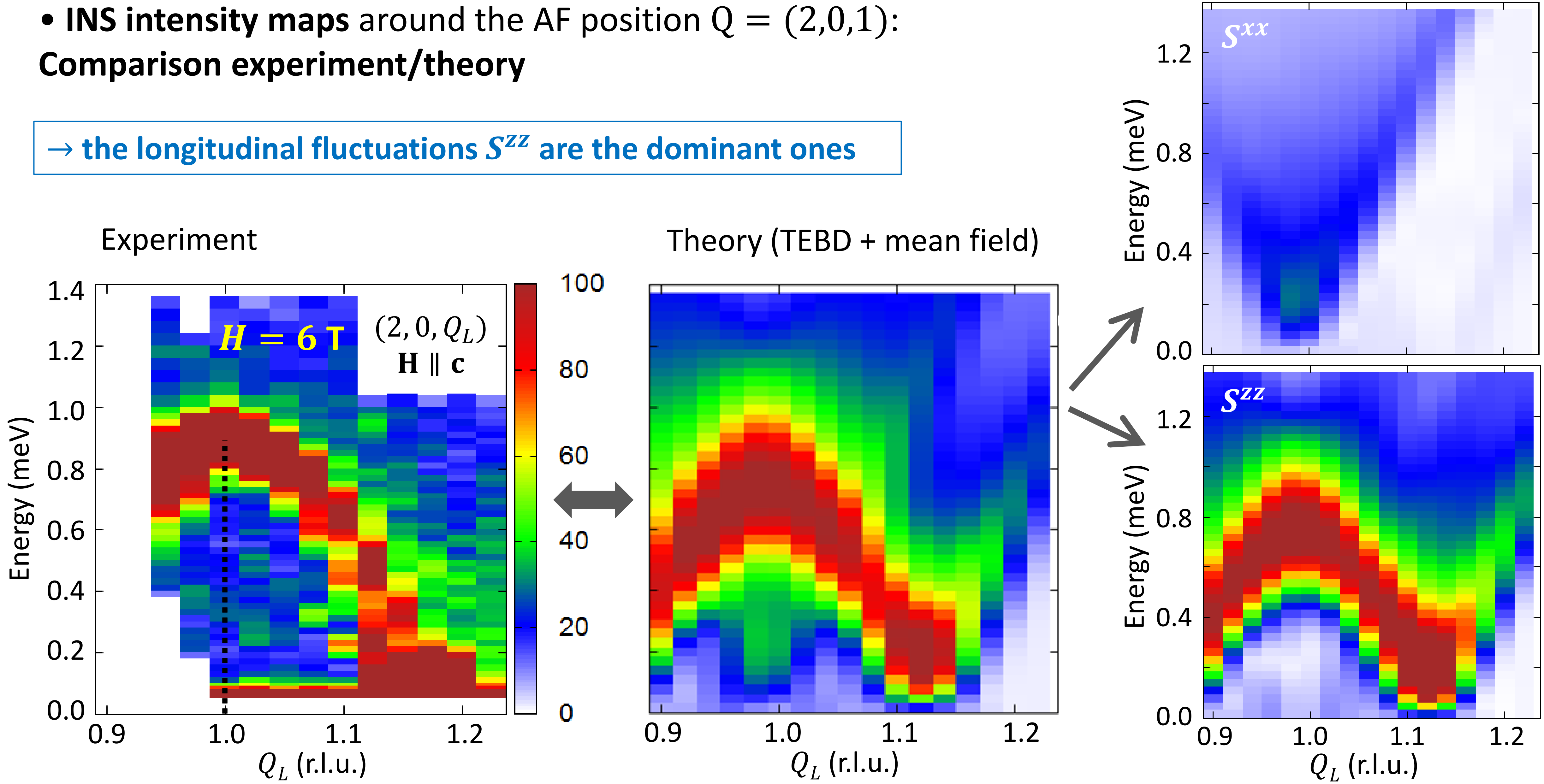
δ increases when H increases
⇒ **the maximum of energy** at $Q_L = 1$ also increases

$BaCo_2V_2O_8$: *spin dynamics in the field-induced LSDW phase*

- **INS intensity maps** around the AF position Q = (2,0,1):

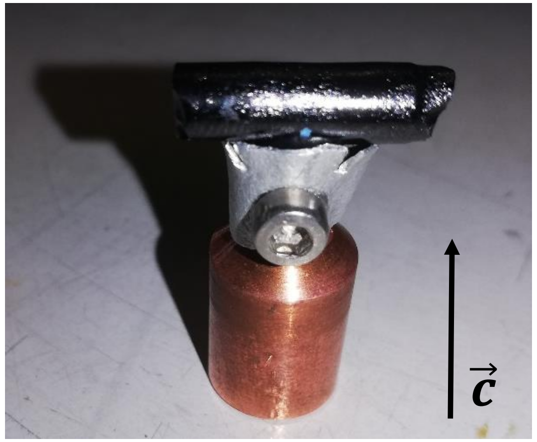
Comparison experiment/theory

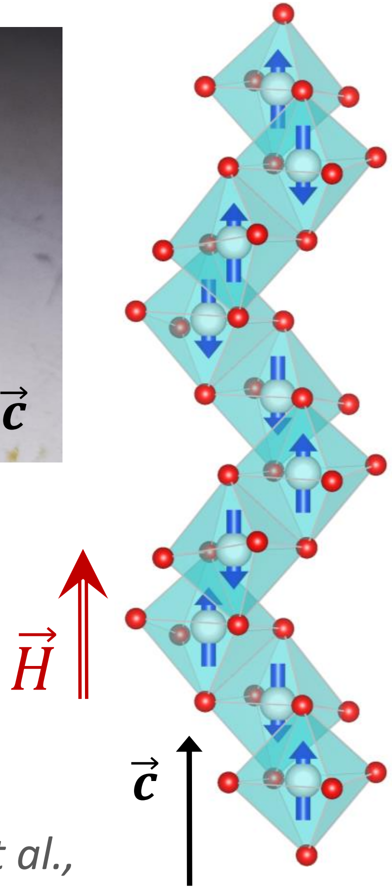
→ **the longitudinal fluctuations S^{zz} are the dominant ones**



Spin dynamics in a longitudinal field: *experimental set-up 2*

1 single-crystal
with $\vec{c}$ **vertical**





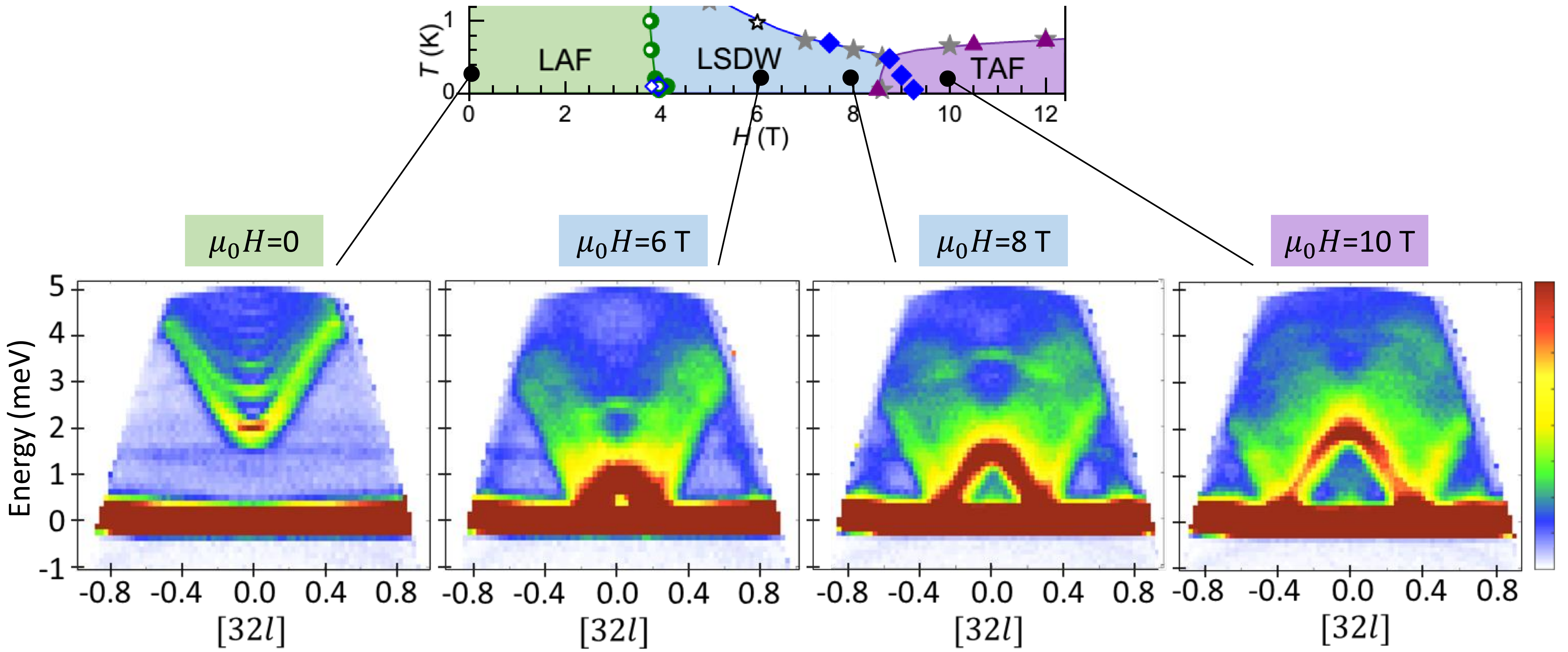
S. Takayoshi, Q. Faure *et al.*,
arXiV:2302.03833v1,
to appear in PRR

Time-Of-Flight spectrometer **IN5** @ ILL, Grenoble
with **vertical 10 T cryomagnet + dilution**

$BaCo_2V_2O_8$: *spin dynamics across the LSDW – TAF phase transition* | IN5

$\lambda = 3.4$ Å

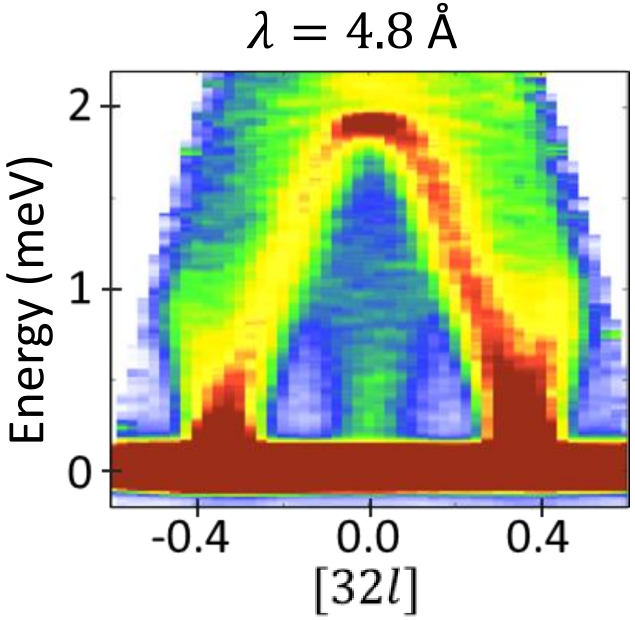
$T = 50$ mK

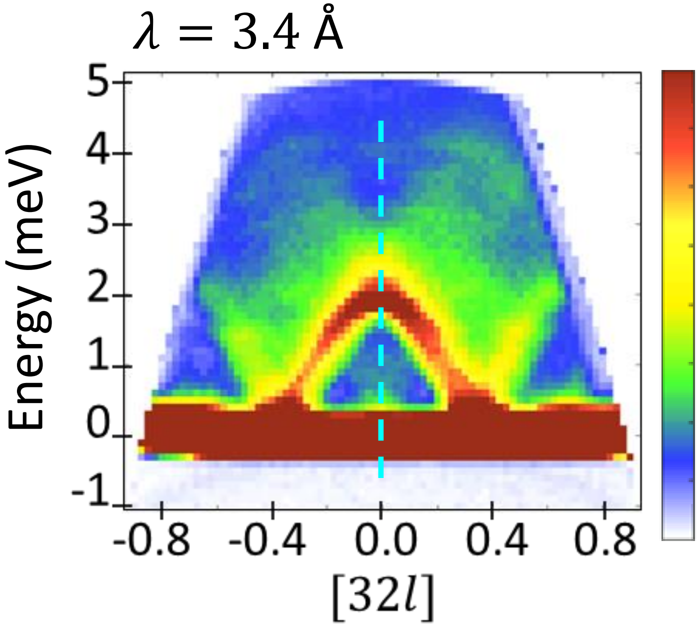


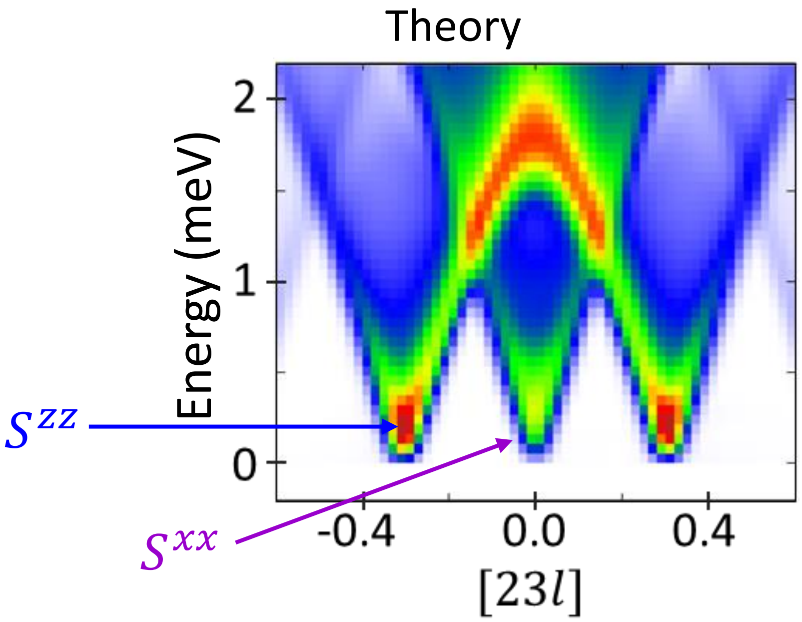
$BaCo_2V_2O_8$: *spin dynamics across the LSDW – TAF phase transition* | IN5

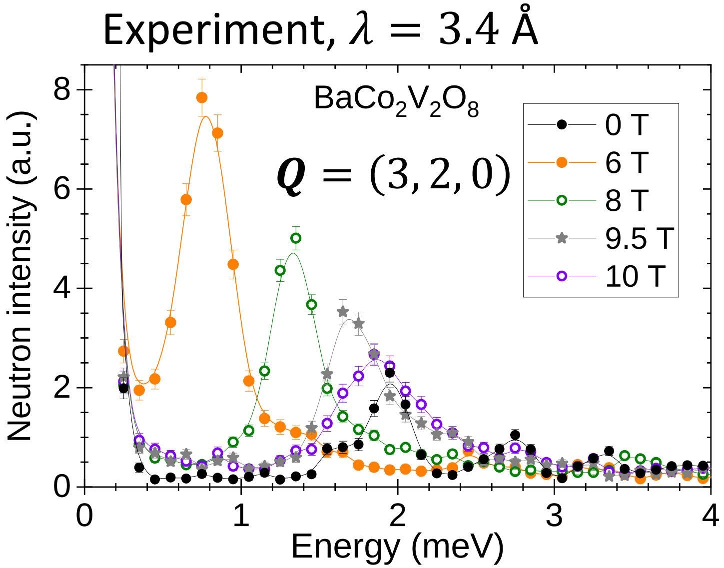
$\mu_0 H$=10 T

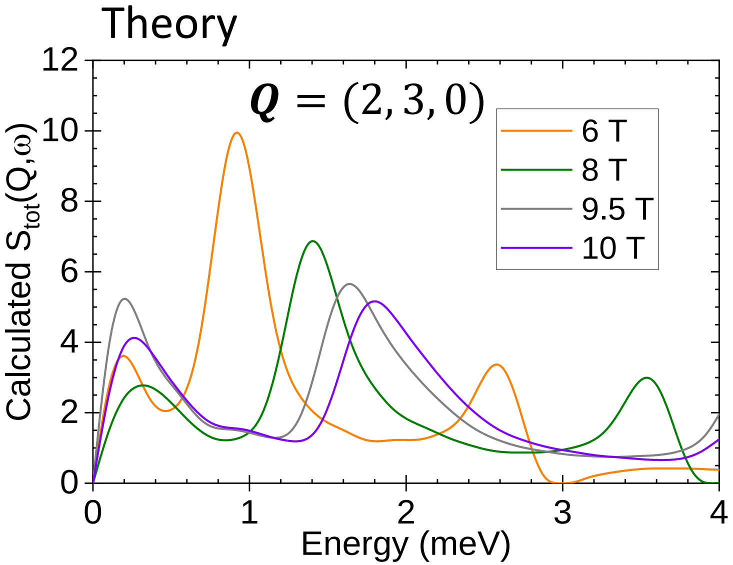
T = 50 mK





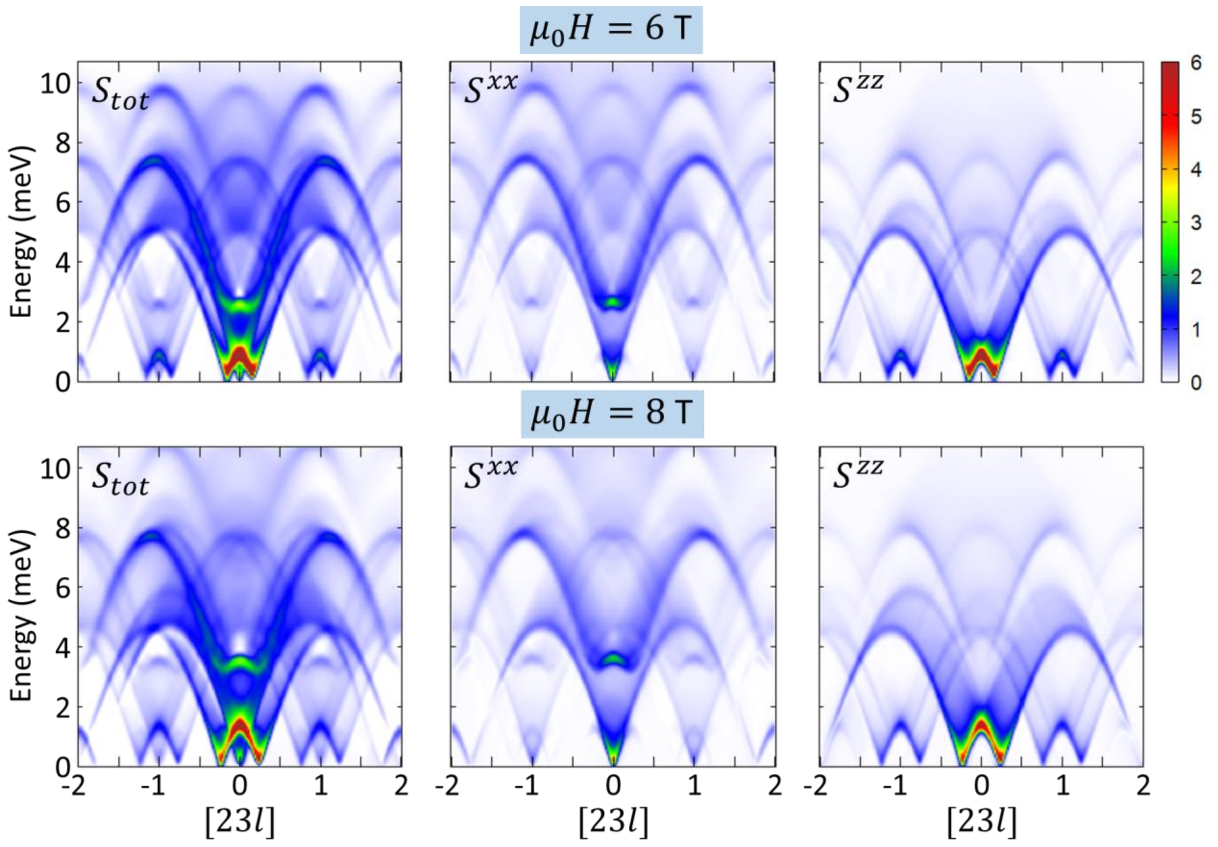


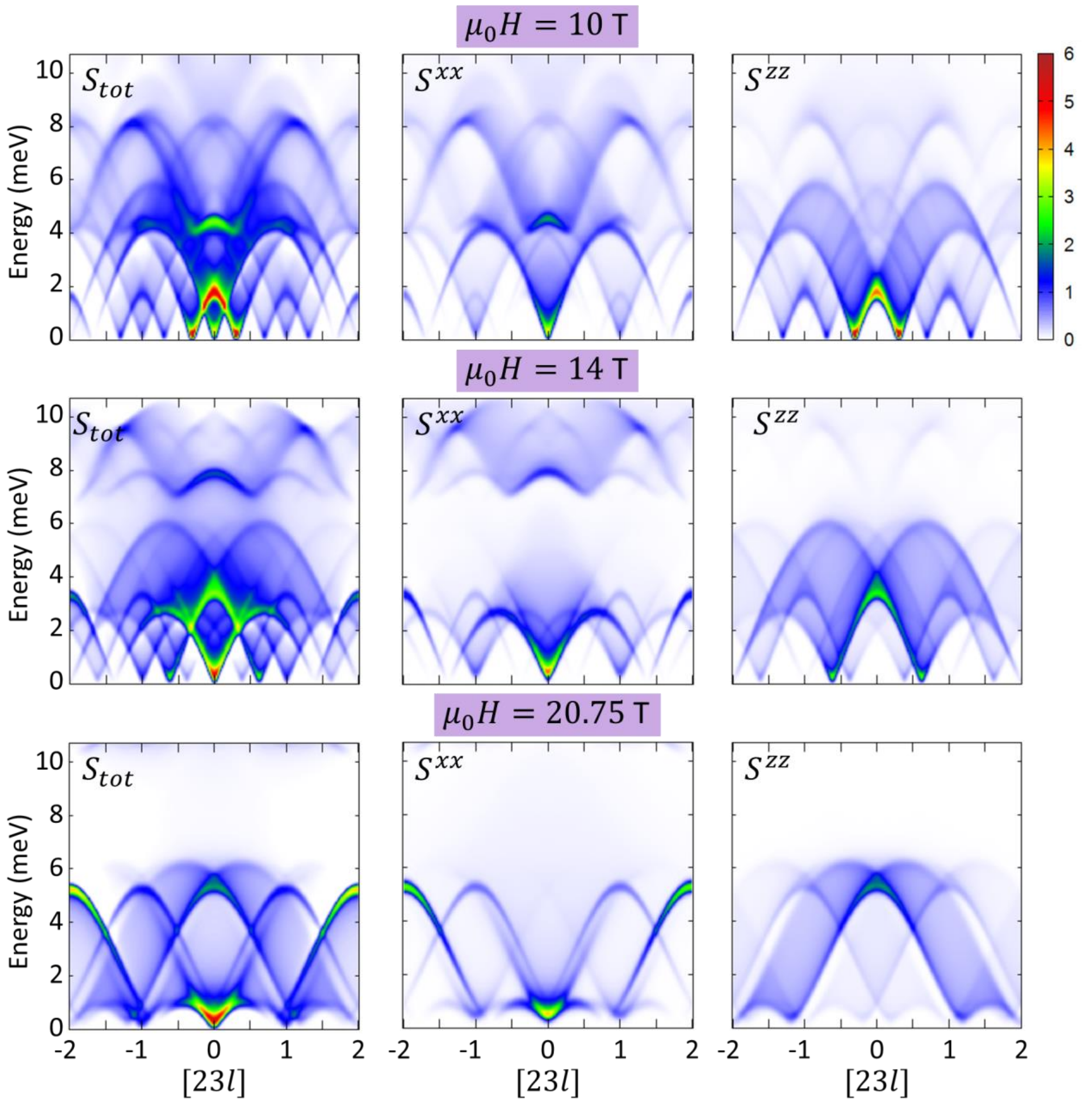




$BaCo_2V_2O_8$: *spin dynamics across the LSDW – TAF phase transition*

TEBD calculations in the LSDW and TAF phases
(S. Takayoshi and T. Giamarchi)





Conclusion

$BaCo_2V_2O_8$ in a longitudinal field ($H \parallel c$):

Quantum phase transition from Néel to LSDW phase described by the **XXZ model**

Clear **Tomonaga-Luttinger liquid** (TLL) signatures are observed in both the LSDW and TAF phases.

- Incommensurate dynamics in both phases, with a dominance of the longitudinal excitations:
  - in the LSDW phase
  - and in the low-field region of the TAF phase

- At higher field, the transverse excitations dominate

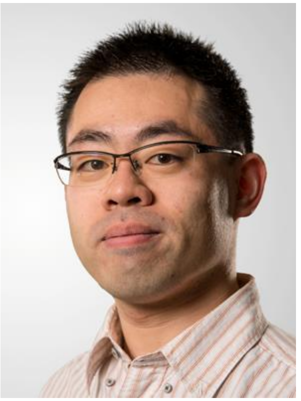
Fingerprint of TLL quantum dynamics in Ising-like chain observed for the first time

Shintaro Takayoshi, Quentin Faure, Virginie Simonet, Béatrice Grenier, Sylvain Petit, Jacques Ollivier, Pascal Lejay, Thierry Giamarchi
arXiV:2302.03833v1, to appear in PRR

Acknowledgments

Quentin FAURE
(Ph-D 2015-2018)
UGA, CEA-IRIG & Inst. Néel,
Grenoble, France

now at LLB, CEA-Saclay



Shintaro TAKAYOSHI
(Post-doc 2017-2019)
DQMP, Univ. Geneva,
Geneva, Switzerland

now at Konan univ., Kobe, Japan

Sylvain PETIT	LLB, CEA – Saclay, France
Virginie SIMONET	Institut Néel, Grenoble, France
Pascal LEJAY	Institut Néel, Grenoble, France
Stéphane RAYMOND, Louis-Pierre REGNAULT	CEA-IRIG, Grenoble, France
Jacques OLLIVIER	ILL, Grenoble, France
Christian RÜEGG, Martin MÅNSSON **Gregory S. TUCKER, Jonathan S. WHITE**	PSI, Villigen, Switzerland
Thierry GIAMARCHI	DQMP, Univ. Geneva, Switzerland

Thank you for your attention