

Journée Fédération Française de Diffusion Neutronique & Séminaire Techniques Neutroniques (spectroscopie/petits angles)

Grenoble, 17-18 décembre 2018



Magnétisme quantique dans un composé à chaînes de spins

UFR PhITEM



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UGA & CEA-INAC-MEM, Grenoble



Quantum magnetism in a spin chain compound

- **Introduction**

- **Strongly correlated systems**
- **Classical phase transitions**
- **Conventional 3D vs Quantum 1D antiferromagnets**
- **Motivations for studying $\text{BaCo}_2\text{V}_2\text{O}_8$**

- Neutron scattering study of the $\text{BaCo}_2\text{V}_2\text{O}_8$ spin chain compound

- $\text{BaCo}_2\text{V}_2\text{O}_8$: Crystallographic structure and magnetic model
 - Magnetic structure
 - Magnetic excitations
- } at zero-field and in a transverse magnetic field

- Conclusion and perspectives

- Conclusion: A topological phase transition
- On-going work

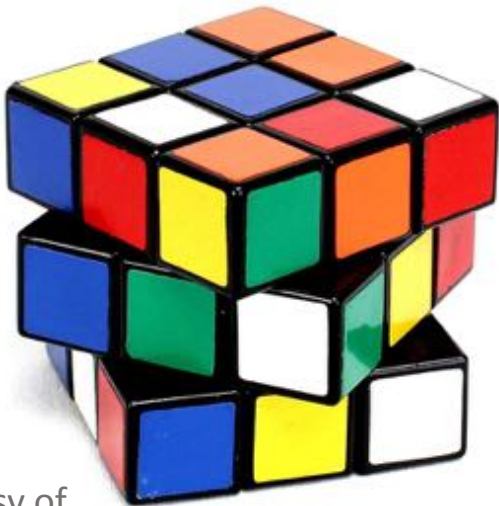
Introduction: Strongly correlated electron systems in 3D

Condensed matter physics → Study of **many-body systems** (Cu: 8.5×10^{22} electrons/cm⁻³)

Strong interactions → **Strongly correlated electron systems:**
collective phenomena = one of the most difficult problem to describe

The Rubik's cube

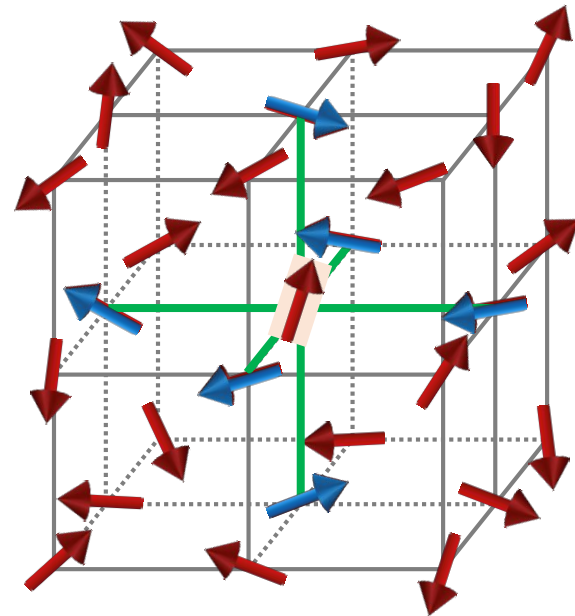
→ 3D correlated (classical) system



Courtesy of
Andrés Felipe Santander-Syro

Magnetic material

→ 3D Strongly correlated electron system



Paramagnet at high T (disordered)

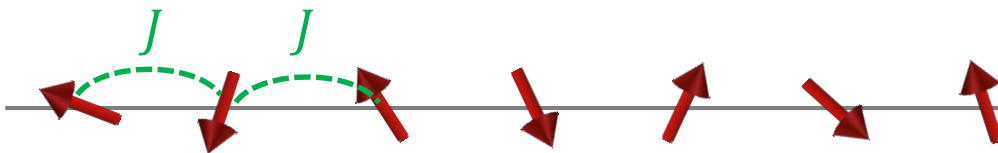
Introduction: Strongly correlated electron systems in 1D

And at one dimension (1D) ?



Courtesy of
Quentin Faure

A simple model: the spin chain!



Strong quantum fluctuations
(especially for low spins)

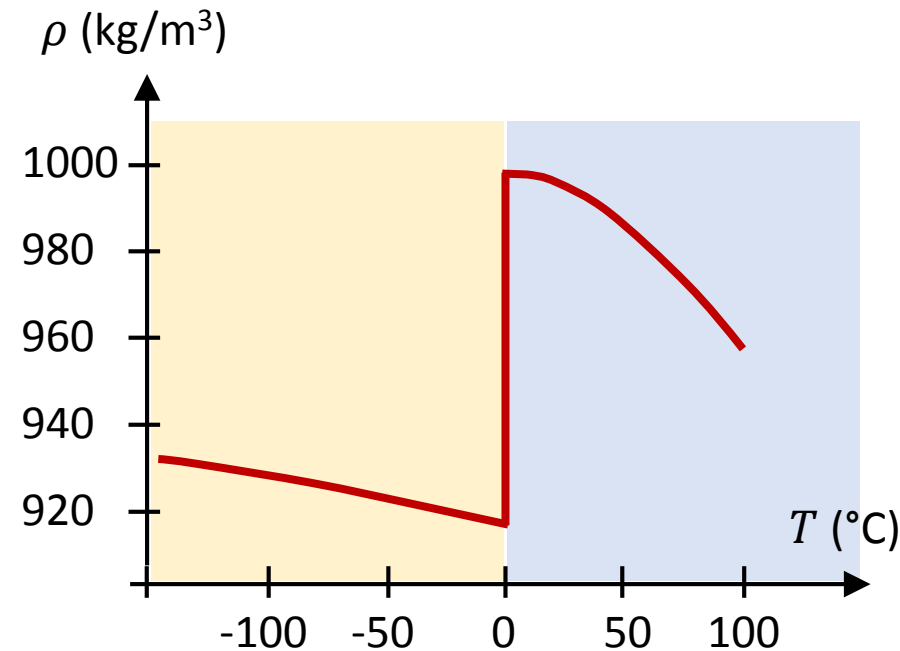
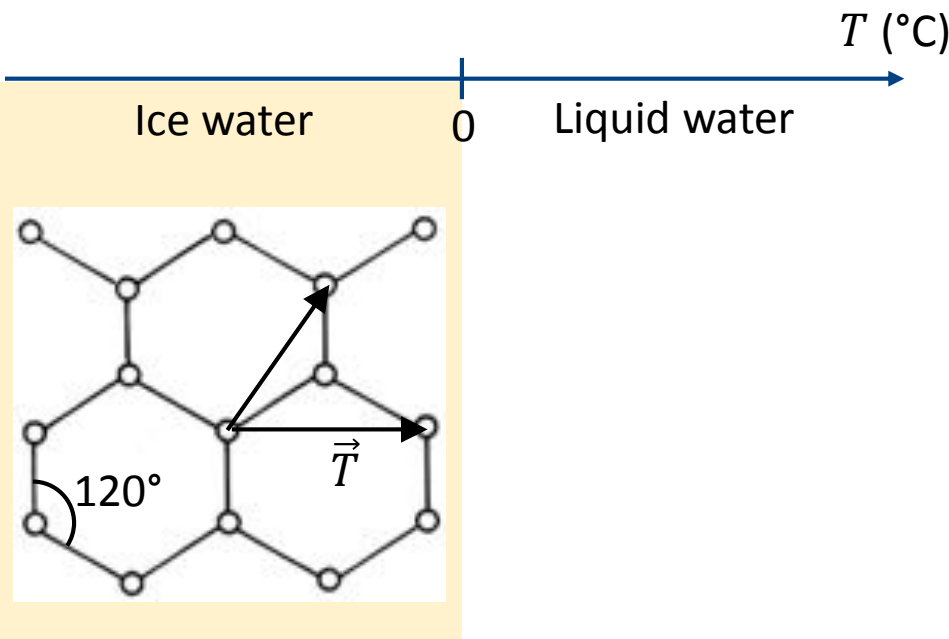
Introduction: Classical phase transition – *Liquid/Solid*

Classical phase transition:

Phase transition between two different phases (phase change) upon cooling / warming

Example 1: water

→ **Long range ordering** (translational & rotational) of the O et H atoms at $T < 0\text{ }^{\circ}\text{C}$ (273 K)



When T increases: ice \rightarrow liquid
Spontaneous symmetry breaking

Order parameter = **mass density ρ**

Introduction: Classical phase transition – *Ferromagnet*

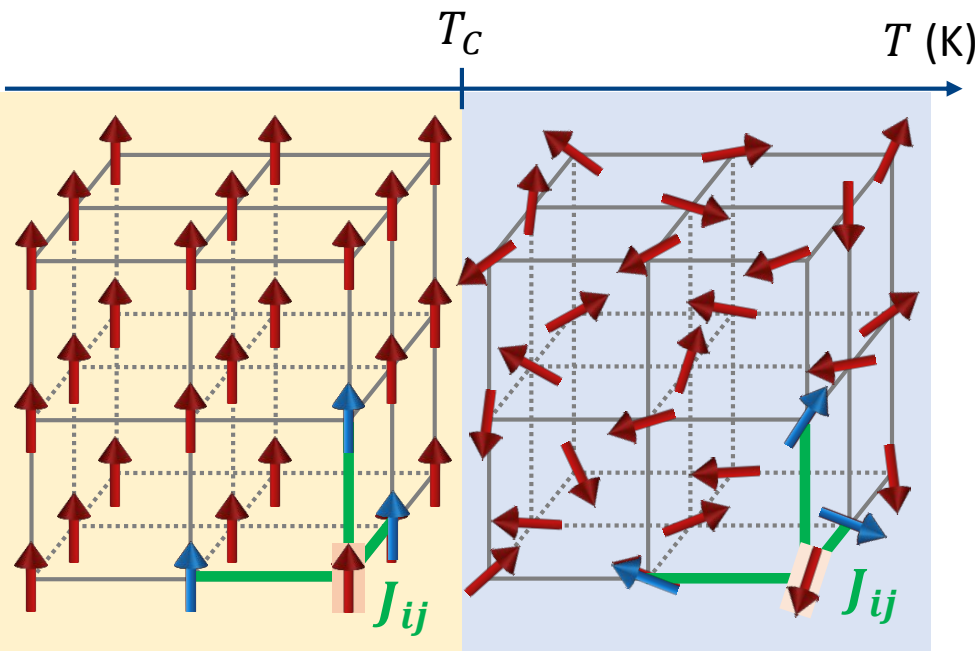
Example 2: conventional 3D ferromagnet

→ **Long range ordering** of the spins at $T < T_C$

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad \text{Hamiltonian}$$

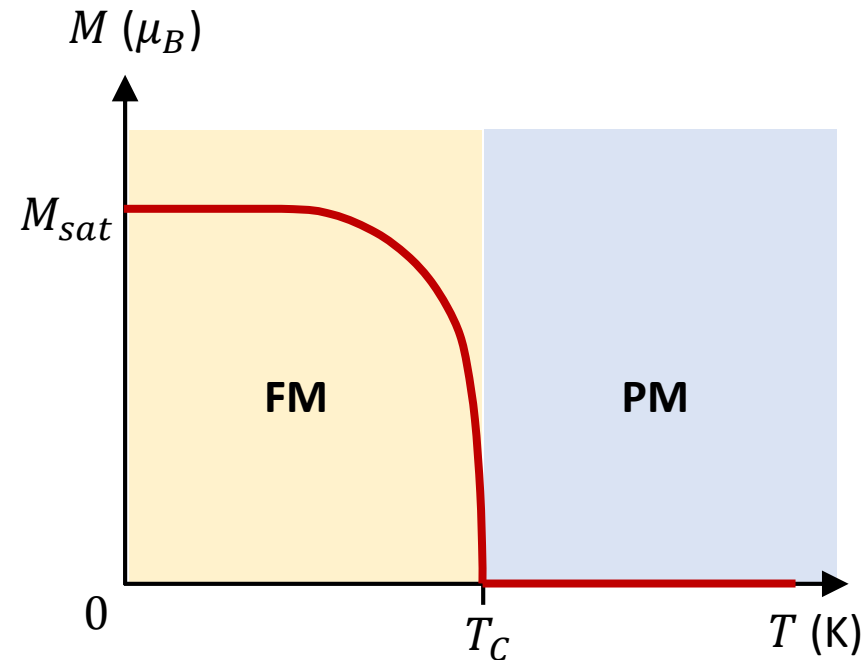
(simplest case)

$$J_{ij} < 0$$



Ferromagnet
(ordered)

Paramagnet
(disordered)



Order parameter = **magnetization M**

Introduction: Classical phase transition – Antiferromagnet

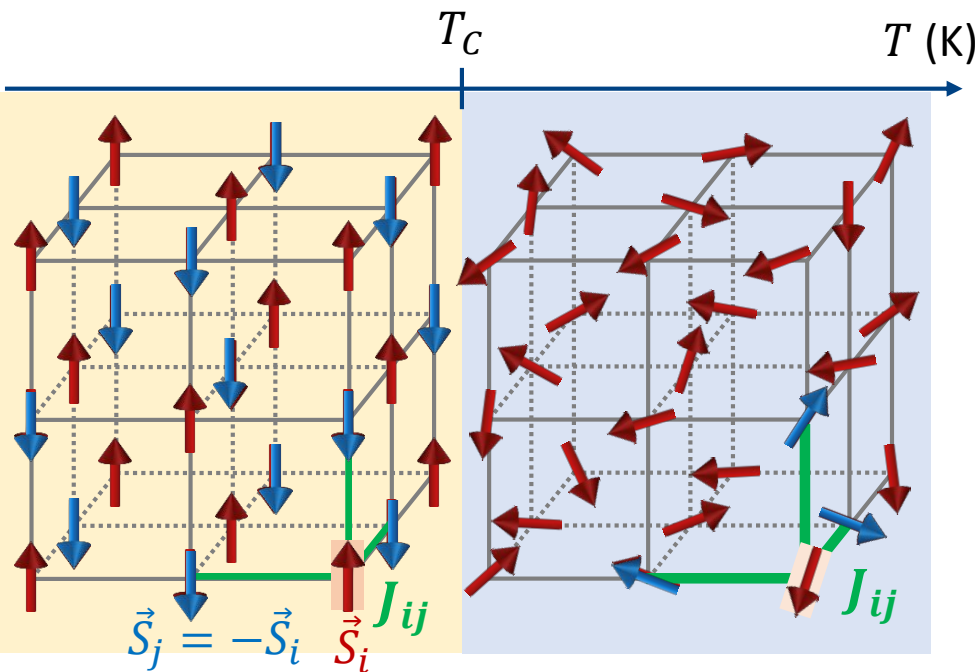
Example 3: conventional 3D antiferromagnet

→ **Long range ordering** of the spins at $T < T_N$

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j \quad \text{Hamiltonian}$$

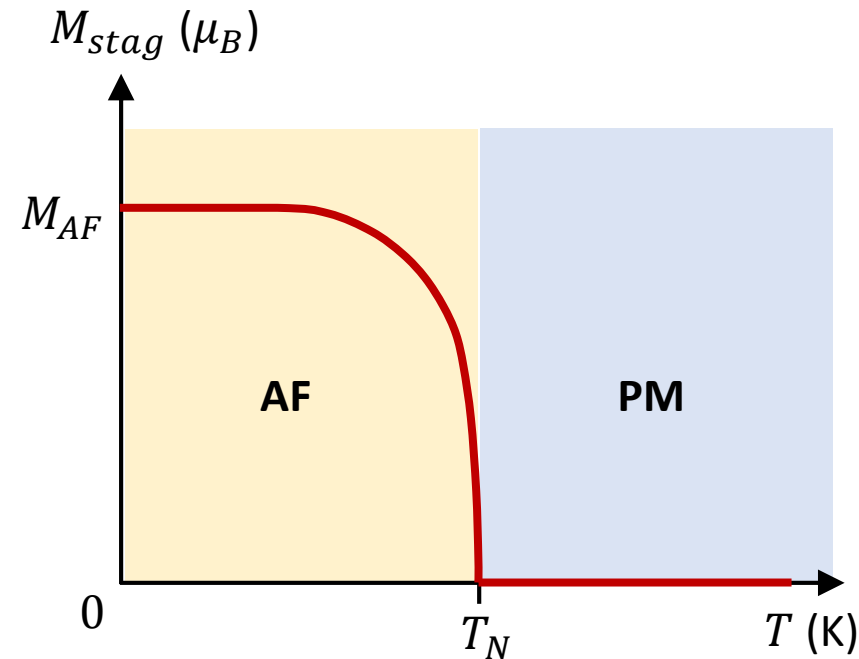
(simplest case)

$$J_{ij} > 0$$



Antiferromagnet
(ordered)

Paramagnet
(disordered)

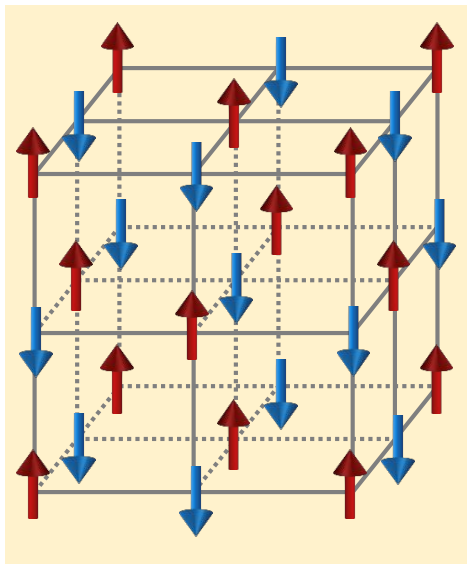
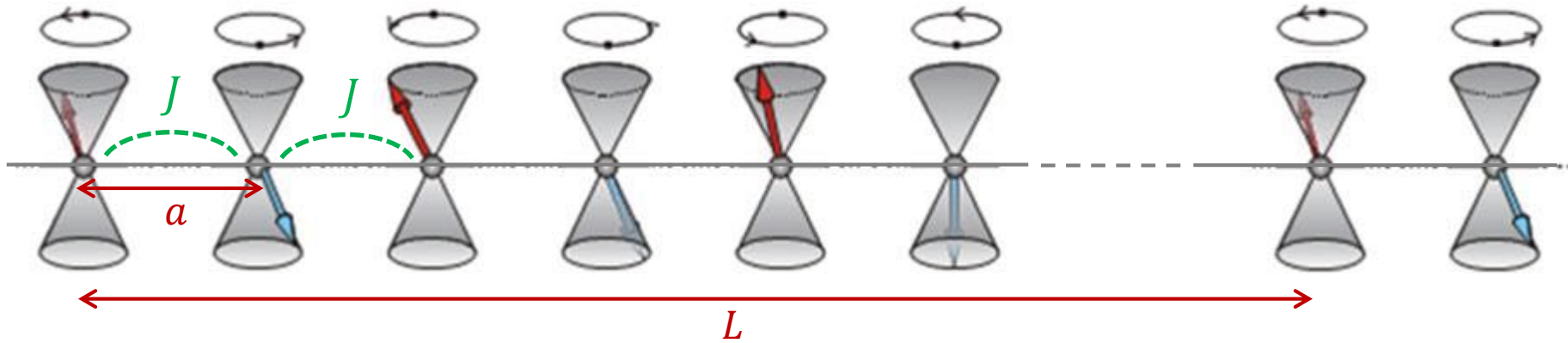


Order parameter = **staggered magnetization M**

Introduction: Magnetic excitations in 3D vs 1D AFs

Example 3: conventional 3D antiferromagnet

→ Magnetic excitations = spin waves = magnons at $T < T_N$

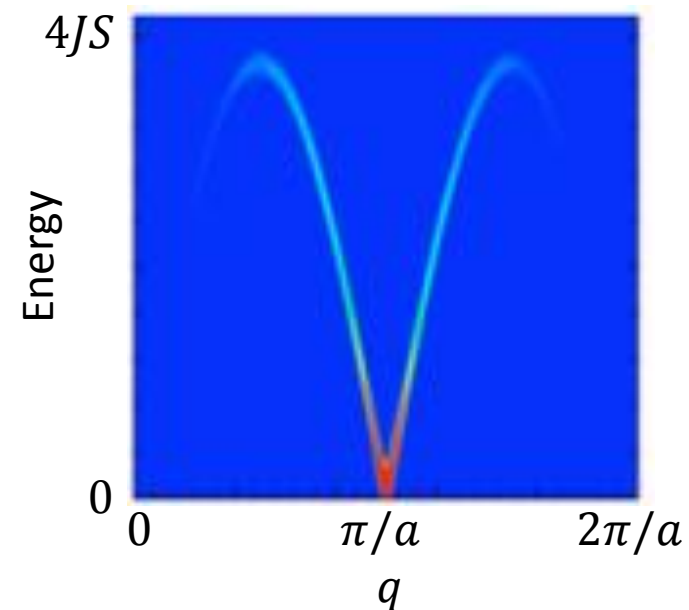


Excitation spectrum:

One well defined dispersion branch

$$E(q) = 4JS |\sin(qa)|$$

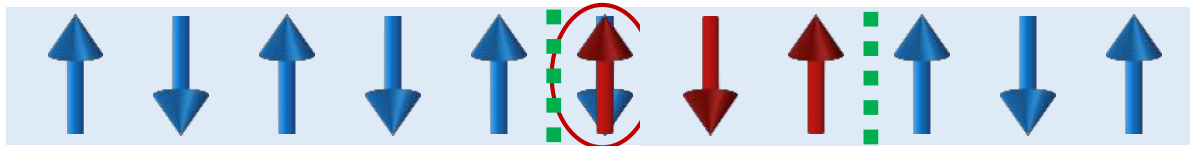
$(q = 2\pi/L)$



Introduction: Magnetic excitations in 1D vs 3D AFs

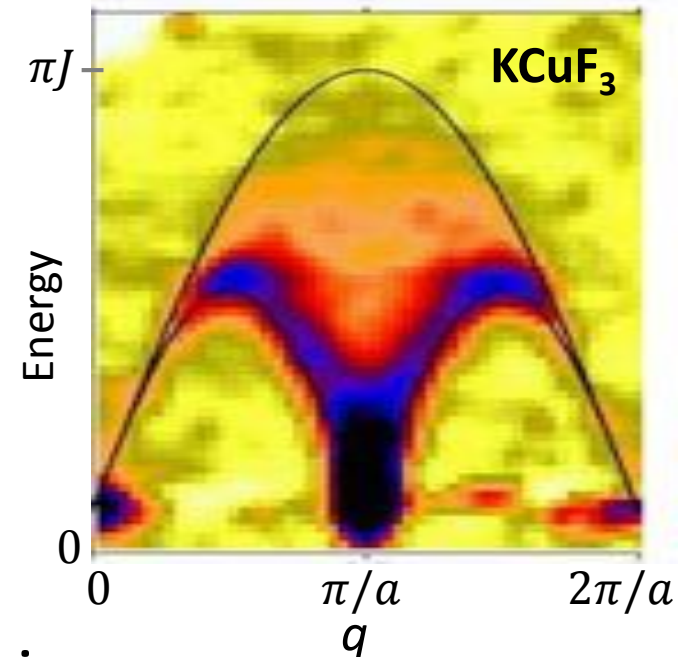
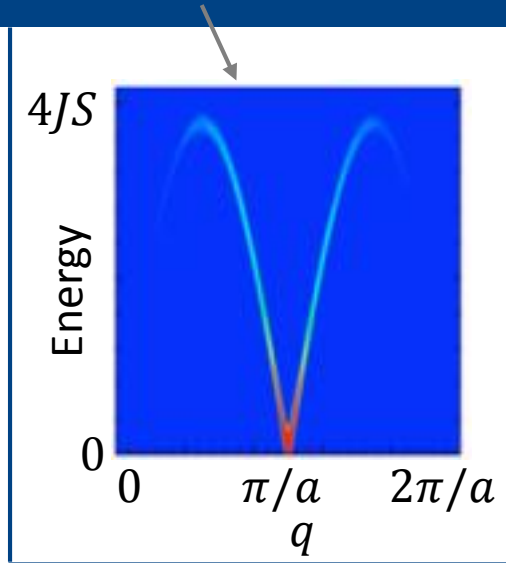
Example 4: quantum 1D antiferromagnet (spin $\frac{1}{2}$ case)

- **No long range ordering down to $T = 0$** (only a quasi AF LRO)
- **Magnetic excitations = deconfined spinons at low T**



spinons \equiv domain walls $\left\{ \begin{array}{l} \text{created in pairs} \\ \text{carry a spin } 1/2 \end{array} \right.$

spinons propagate with no energy cost
 → **ungapped 2-spinon continuum**



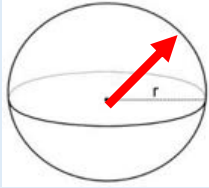
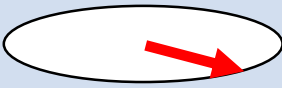
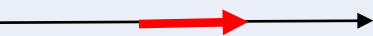
$KCuF_3$: Heisenberg (isotropic) spin $\frac{1}{2}$ chain

Nagler et al., Phys. Rev. B (1991)

Introduction: Motivation for studying $\text{BaCo}_2\text{V}_2\text{O}_8$

- Magnetic anisotropy

$$\mathcal{H} = J \sum_i [\epsilon (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + S_i^z S_{i+1}^z]$$

Heisenberg	Isotropic		$\epsilon = 1$
XY	Planar		$\epsilon \rightarrow +\infty$
Ising	Uniaxial		$\epsilon = 0$

- Spin chains = Playground for studying quantum phase transitions

Phase transition upon the variation of a physical parameter (H, p, \dots) at $T = 0$

- $\text{BaCo}_2\text{V}_2\text{O}_8$: AF effective spin $\frac{1}{2}$ chain with $\left\{ \begin{array}{l} \text{sizeable interchain coupling (quasi-1D)} \\ \text{and weak Ising anisotropy } (\epsilon = 0.5) \end{array} \right.$



Consequences on the static and dynamical properties?

What happens in a magnetic field? \rightarrow topological quantum phase transition

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- Classical phase transitions
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- **Neutron scattering study of the $\text{BaCo}_2\text{V}_2\text{O}_8$ spin chain compound**

- **$\text{BaCo}_2\text{V}_2\text{O}_8$: Crystallographic structure and magnetic properties**
 - **Magnetic structure**
 - **Magnetic excitations**
- } **at zero-field and in a transverse magnetic field**

- Conclusion and perspectives

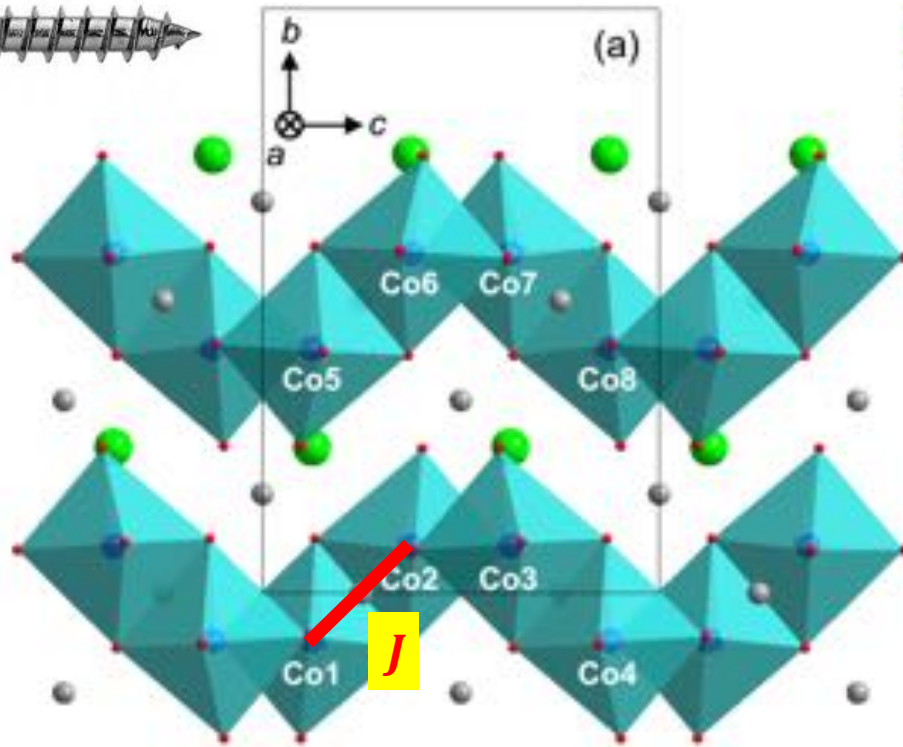
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BaCo₂V₂O₈: an effective spin ½ XXZ quasi-1D AF

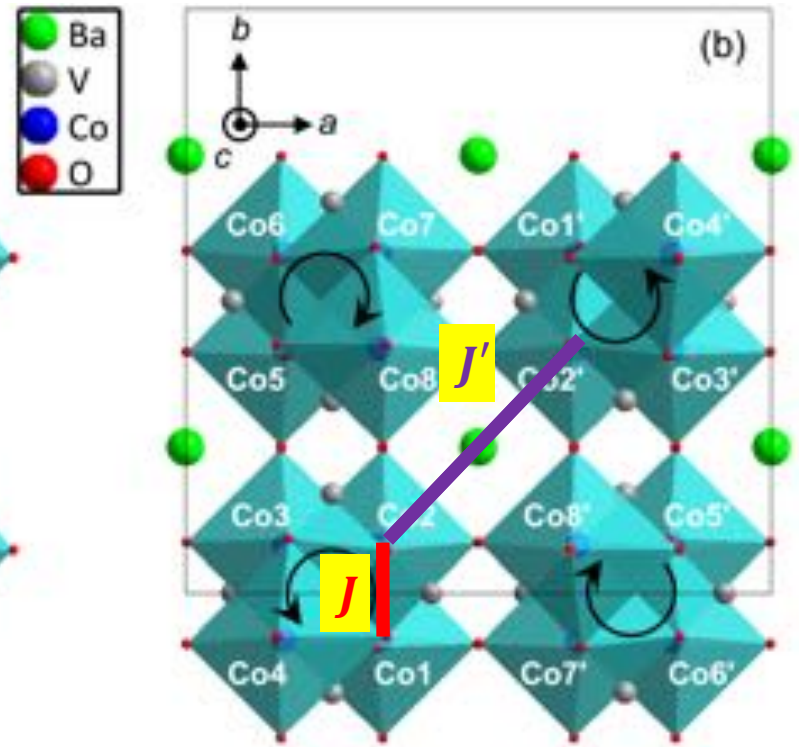
- **Screw chains** of effective spin ½ || **c-axis** $I4_1/acd$ ($a = 12.44 \text{ \AA}$, $c = 8.42 \text{ \AA}$)
R. Wichmann et al., Z. Anorg. Allg. Chem. (1986)
- **Ising-like anisotropy** (XXZ): $\epsilon \sim 0.5$ ($Z \equiv c$)
- **Non-negligible inter-chain interactions** (quasi-1D)

$$\mathcal{H} = J \sum_i [\epsilon (S_i^a S_{i+1}^a + S_i^b S_{i+1}^b) + S_i^c S_{i+1}^c]$$

$$J' \ll J$$



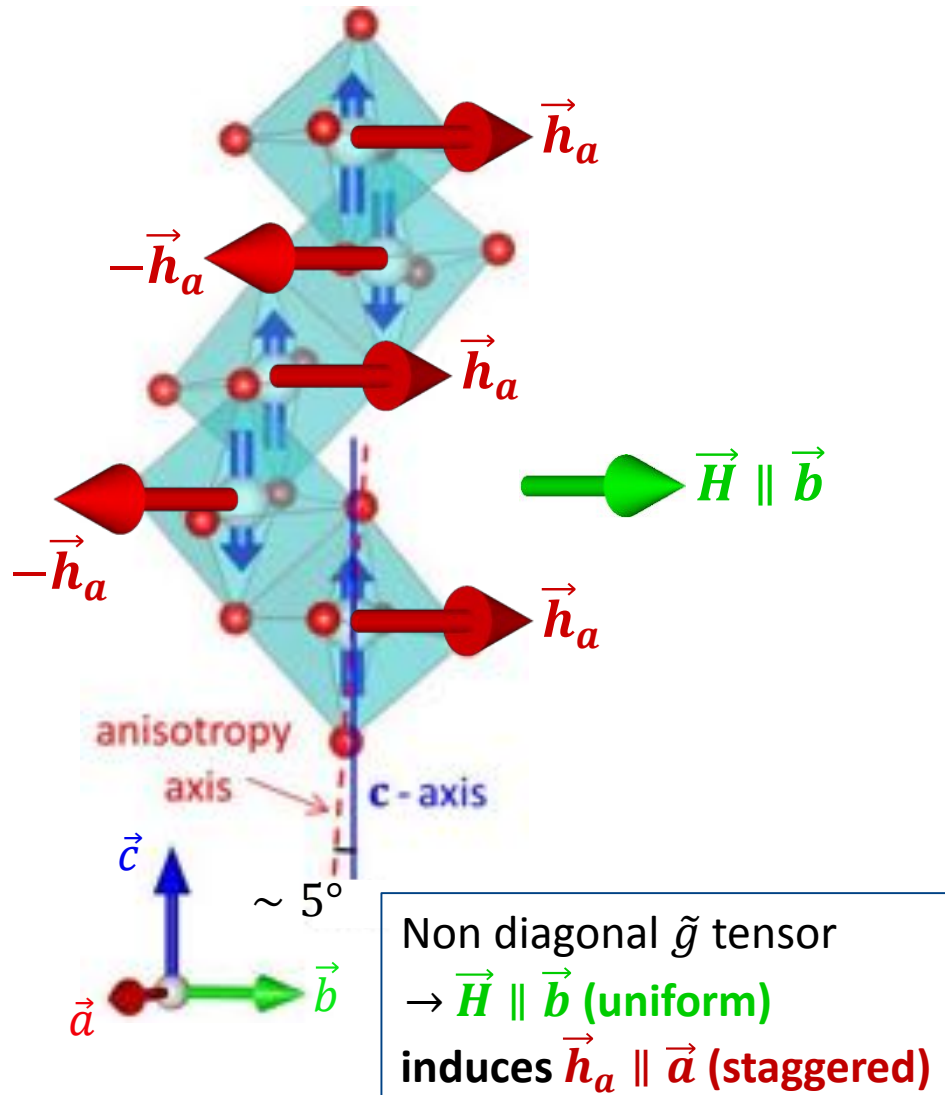
Intrachain interaction: J AF



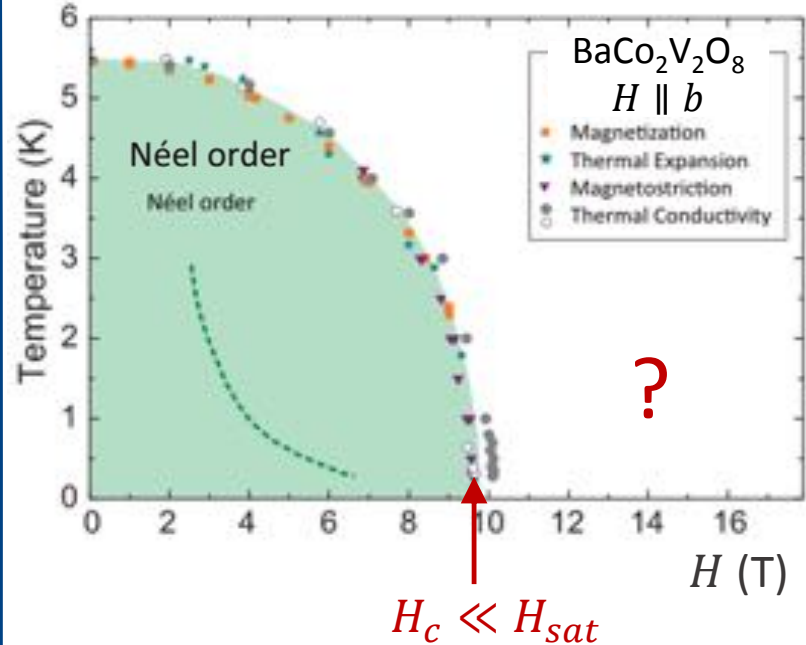
Dominant interchain interaction: J' AF

BaCo₂V₂O₈ in a transverse magnetic field $\vec{H} \parallel \vec{b}$

• Crystallographic peculiarities



• Macroscopic measurements



S. K. Niesen et al., Phys. Rev. B (2013)

Nature of the phase transition and of the phase above?

Neutron diffraction set up

- **Crystal synthesis:**

Floating zone method @ **Institut Néel**, Grenoble
P. Lejay et al., Journ. Cryst. Growth (2001)



- **Single-crystal diffractometer D23 @ ILL**

$\lambda = 1.28 \text{ \AA}$

Technical support: *Pascal Fouilloux*

$H = 0$: Orange cryostat

$H \parallel b$: 12 T vertical field cryomagnet



DIFFRACTION = elastic scattering ($\Delta E = 0$)

- **Bragg peaks positions:**

periodicity of the magnetic structure

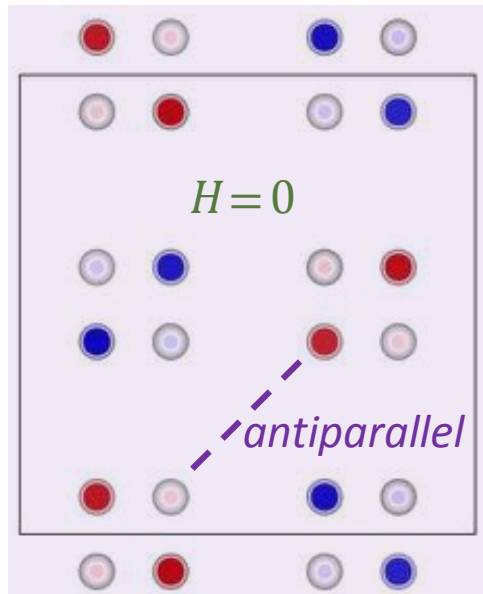
- **Bragg peak intensities:**

Arrangement (directions + amplitude)
of the magnetic moments in the unit cell

Magnetic ordering below and above H_c

$$H = 0$$

$$\vec{k} = (1,0,0)$$

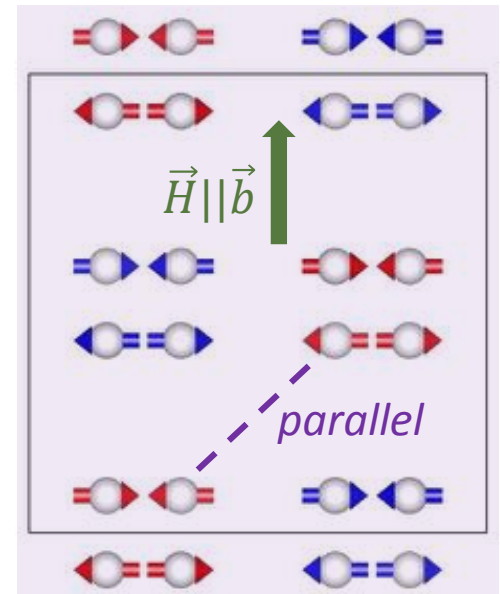


*E. Canévet et al.,
Phys Rev B (2013)*

$$m_c = 2.3 \mu_B/\text{Co}^{2+}$$

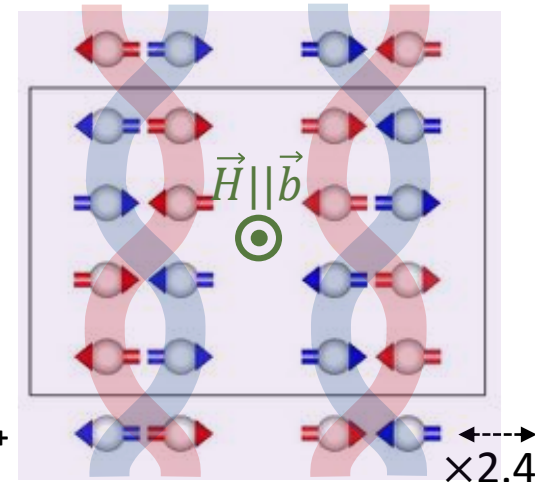
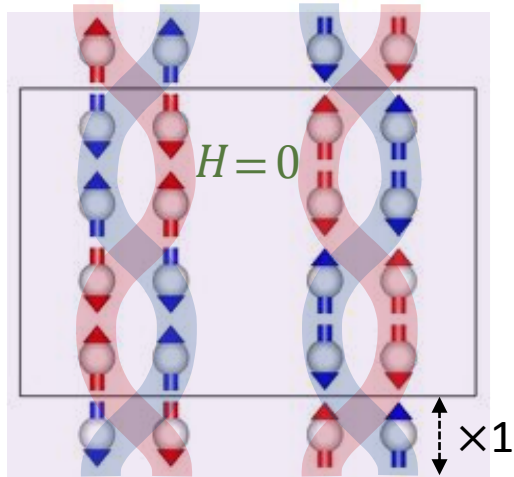
$$H = 12 \text{ T}$$

$$\vec{k}' = (0,0,0)$$

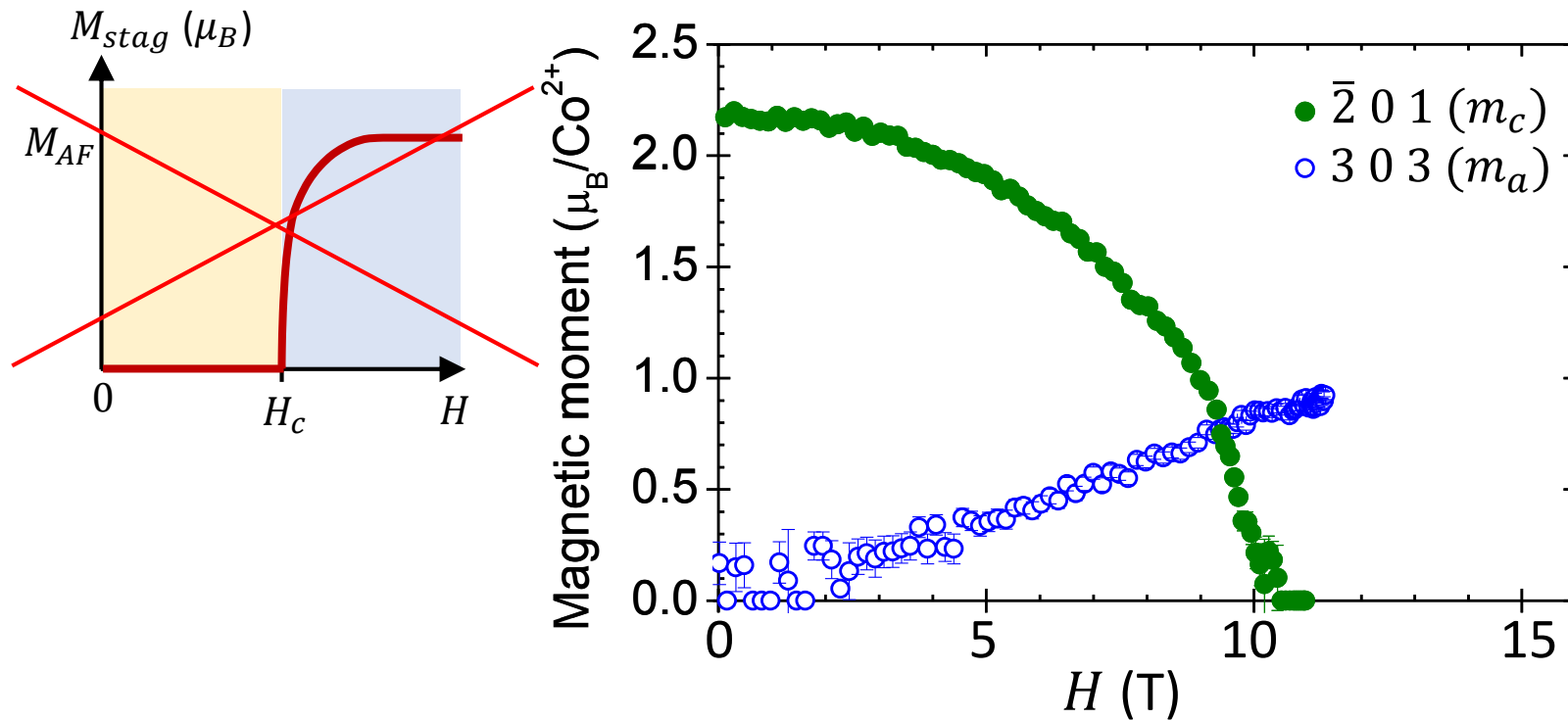


*Q. Faure et al.,
Nature Phys. (2018)*

$$m_a = 0.4 \mu_B/\text{Co}^{2+}$$



Magnetic field dependence of m_c and m_a



Staggered m_c : typical behavior of an order parameter

Staggered m_a : unusual behavior

⇒ **Unconventional quantum phase transition**

→ field-induced AF order along a stabilized by the **effective staggered field h_a** induced by H_b

Inelastic neutron scattering set-up

- Cold neutron Triple-Axis Spectrometers (TAS) **ThALES** and **IN12** @ ILL

$k_f = 1.3 \text{ \AA}^{-1}$; scattering plane (\vec{a}^*, \vec{c}^*) ; orange cryostat (0 T) & 12 T vertical field cryomagnet

Technical support: *Eric Villard, Bruno Vettard*

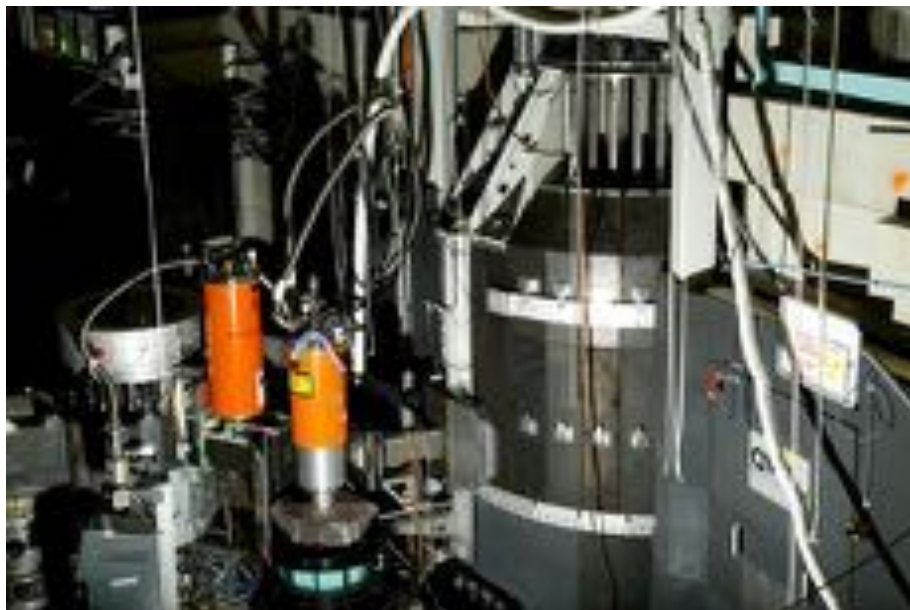
Local contacts: *Martin Boehm, Stéphane Raymond*

Measurement of $S(\vec{Q}, \omega)$ with $\begin{cases} \vec{Q} = \vec{k}_i - \vec{k}_f \\ \hbar\omega = (E_i - E_f) \end{cases}$



Magnetic excitations → determination of J, J', ϵ, \dots

Neutrons "measure"
spin fluctuations $\perp \vec{Q}$



ThALES, non polarized neutrons

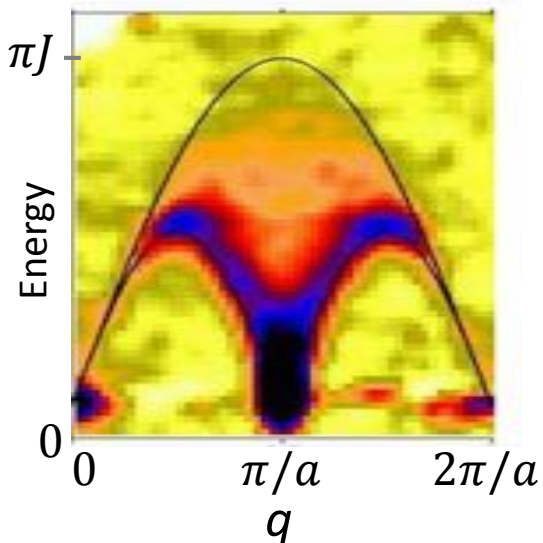


IN12, (un)polarized neutrons at (0 T) 12 T

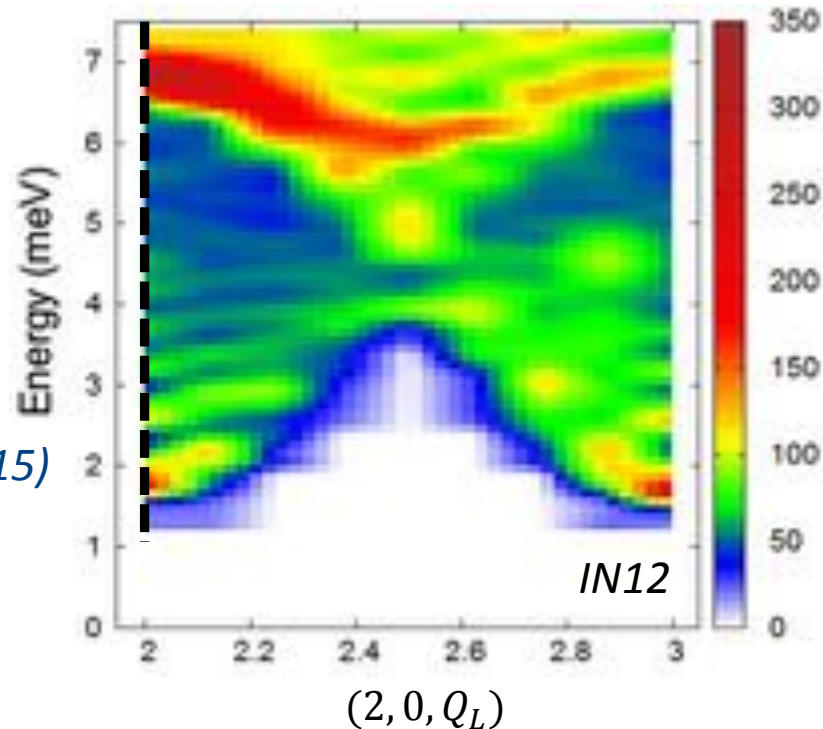
Zero-field magnetic excitations

1D Heisenberg spin 1/2 AF

BaCo₂V₂O₈, quasi-1D Ising-like effective spin 1/2 AF

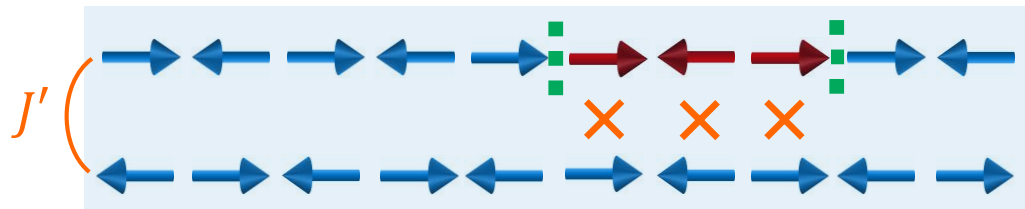


*B. Grenier et al.,
Phys. Rev. Lett. (2015)*

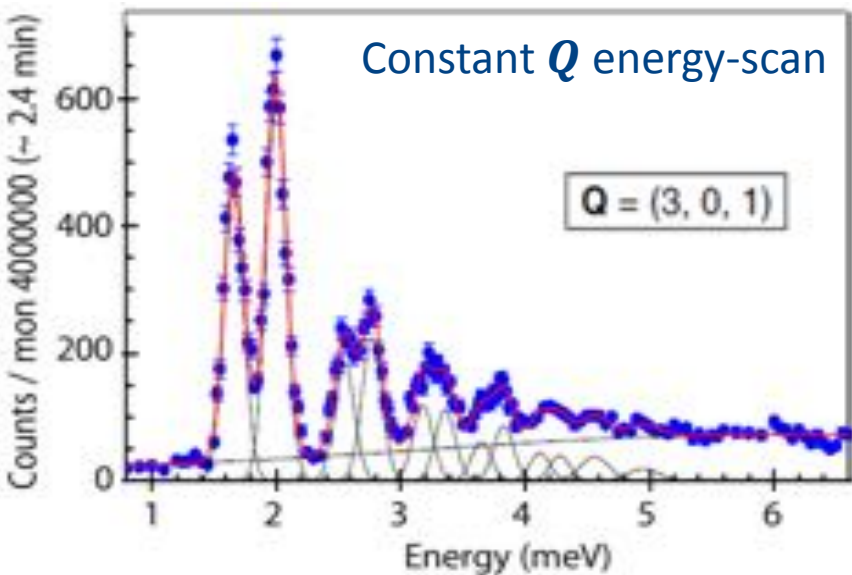


• Gap (~ 1.8 meV) ← **Ising-like** anisotropy

• Discretization ← **Confined spinons** ← J'

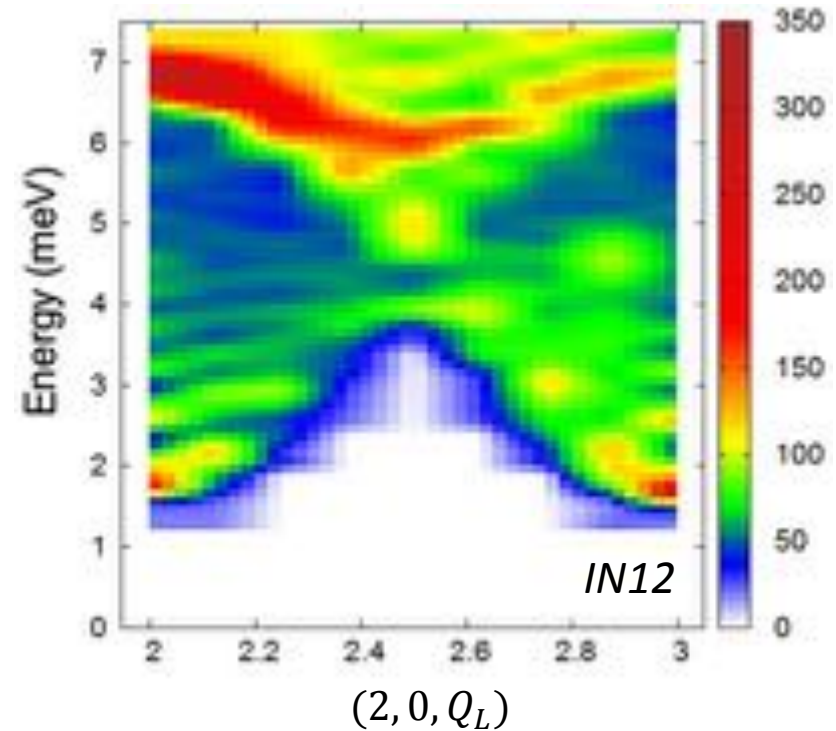
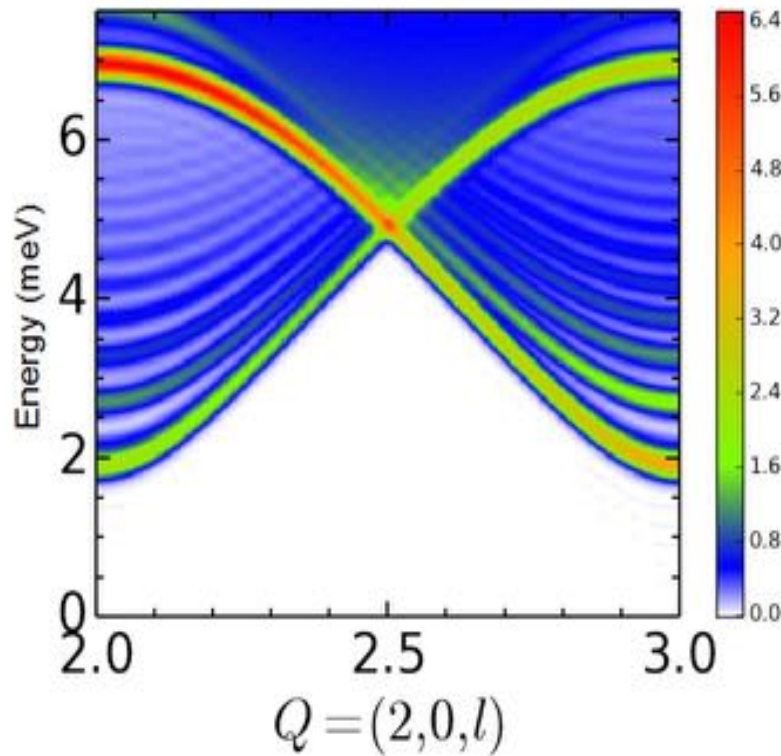


H. Shiba, Prog. Theor. Phys. (1980)



Zero-field magnetic excitations

$\text{BaCo}_2\text{V}_2\text{O}_8$, quasi-1D Ising-like effective spin $\frac{1}{2}$ AF

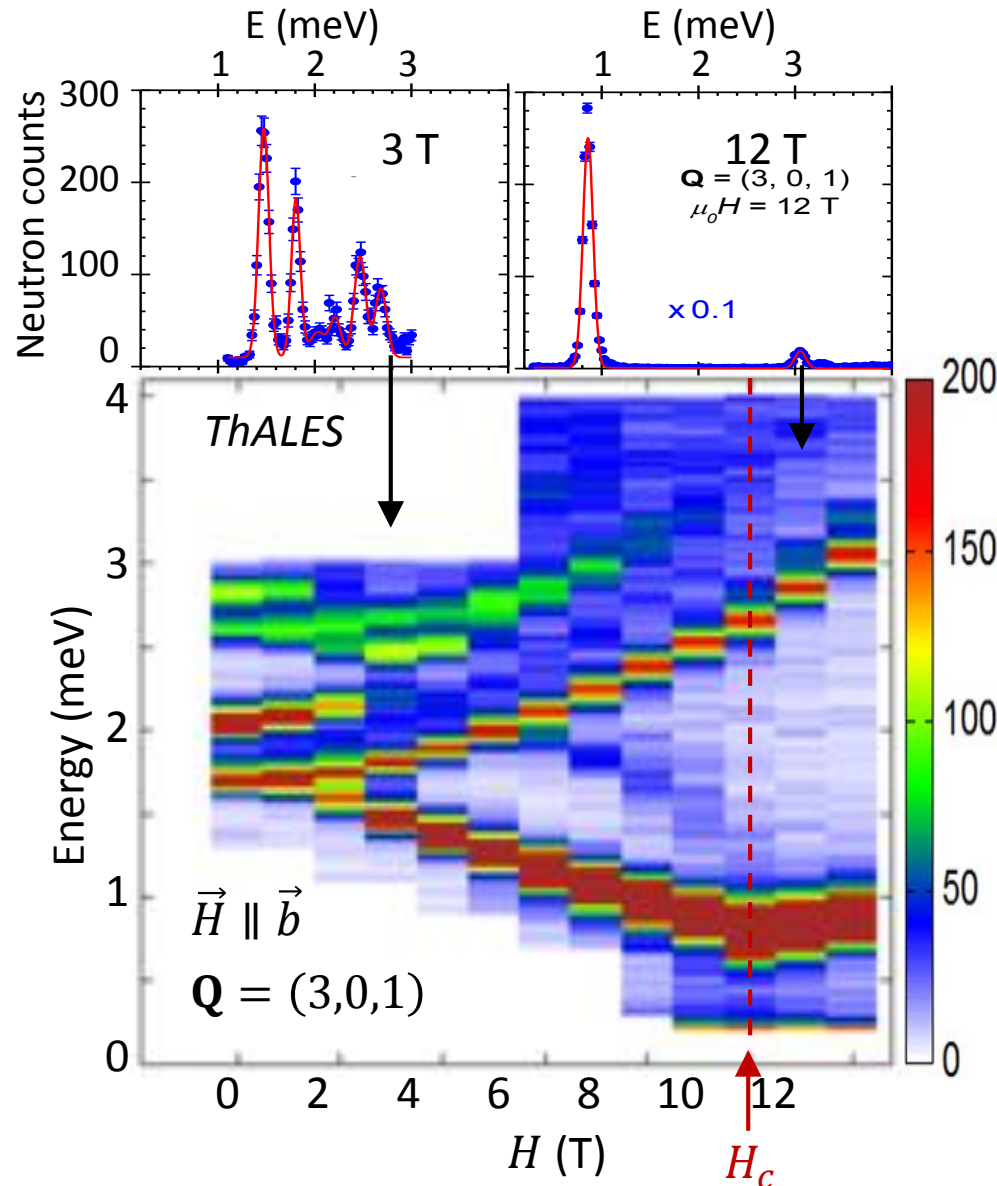


Shintaro Takayoshi and **Thierry Giamarchi**
DQMP, University of Geneva, Switzerland

Infinite Time Evolution Block Decimation (iTEBD)

$J = 5.8 \text{ meV}, \epsilon = 0.53, J' = 0.16 \text{ meV}$

Magnetic excitations in a transverse magnetic field

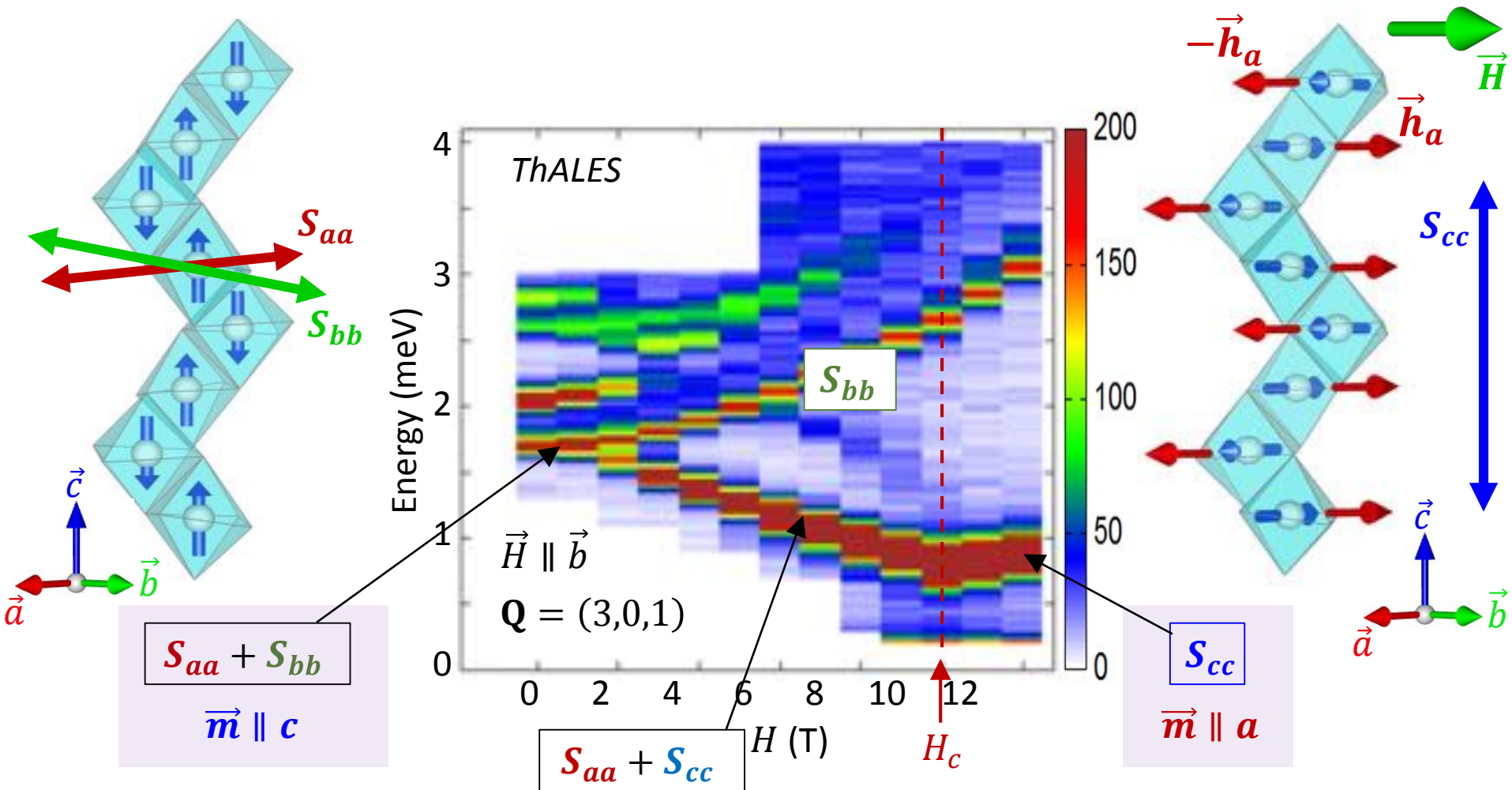


Q. Faure et al.,
Nature Phys. (2018)

Magnetic excitations in a transverse magnetic field

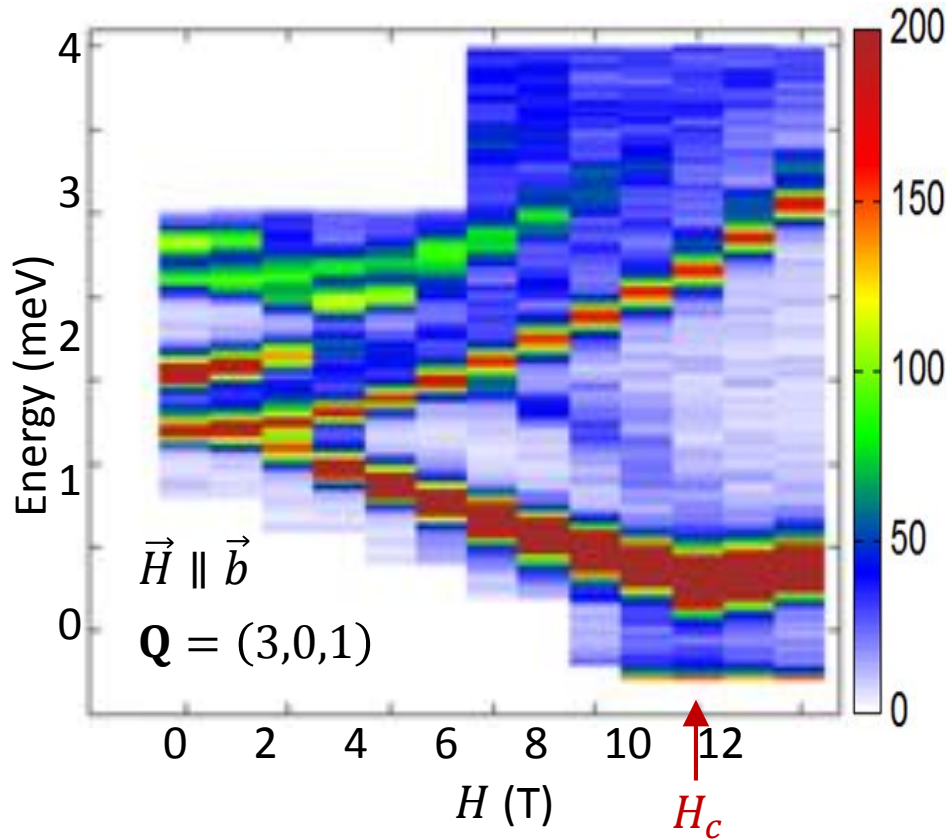
Polarized neutrons (IN12): separation between fluctuations $\parallel \vec{b}$ (S_{bb}) and $\perp \vec{b}$ (S_{aa} and S_{cc})

Anisotropy of the magnetic neutron scattering ($S_{\alpha\alpha} \perp \vec{Q}$): separation between S_{aa} and S_{cc}



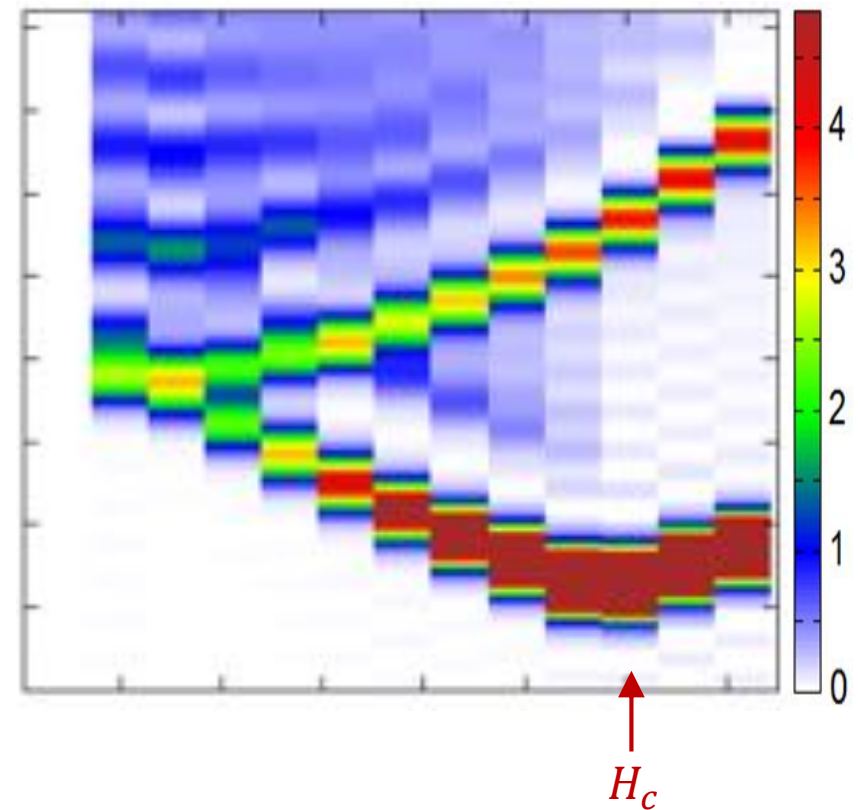
Magnetic excitations in a transverse magnetic field

Experiment (ThALES)



Theory (iTEBD)

Shintaro Takayoshi and Thierry Giamarchi



Q. Faure et al., Nature Phys. (2018)

S. Takayoshi, Phys. Rev. B (2018)

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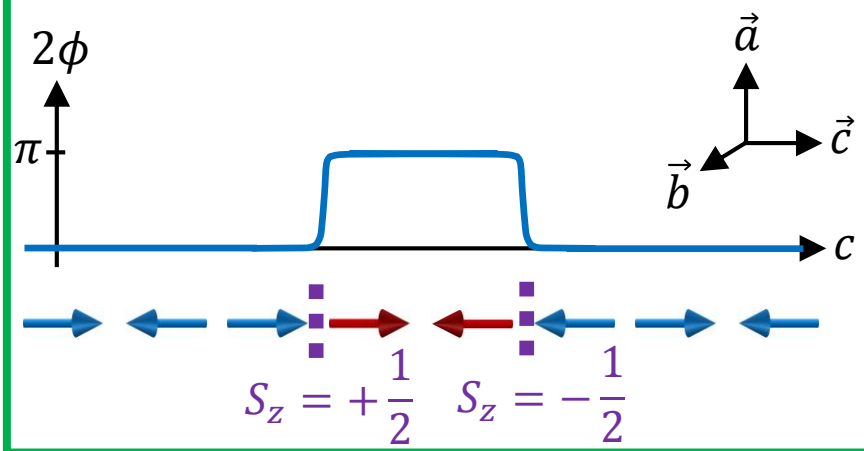
- **Conclusion and perspectives**

- **Conclusion: A topological phase transition**
- **On-going work**

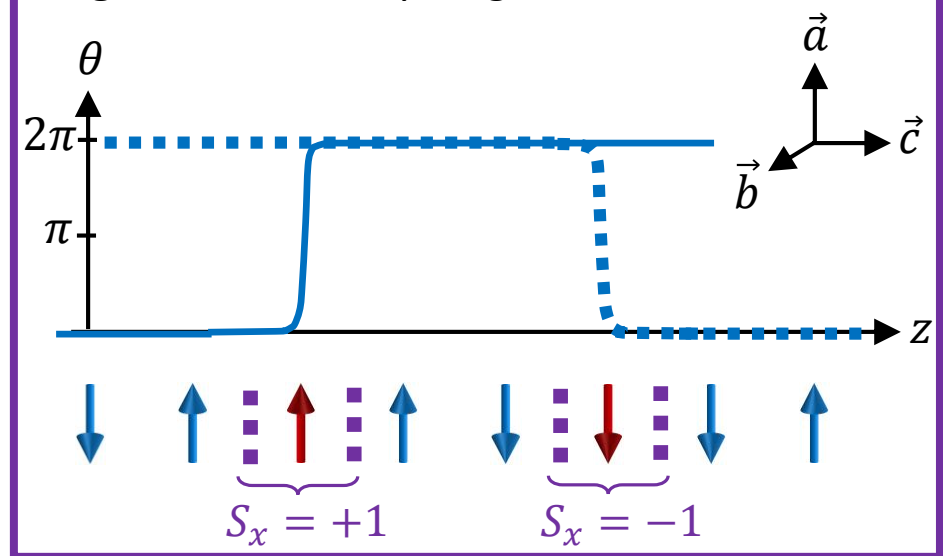
Conclusion: Topological quantum phase transition

- **Numerical calculations:** exact diagonalization (Q. Faure) & iTEBD (S. Takayoshi & T. Giamarchi)
→ **phase transition induced by the staggered field**
- **Field theory** (S. Takayoshi & T. Giamarchi)
Competition Ising anisotropy (low H) / staggered field (high H)
→ **competition between two dual topological excitations**

Low field: topological excitations = spinons



High field: dual topological excitations



BaCo₂V₂O₈ = first realization of the double sine Gordon model

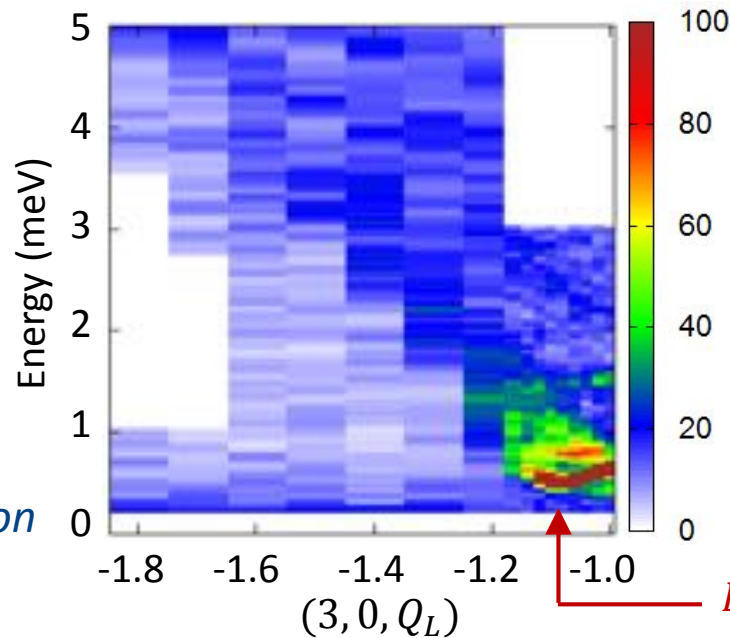
On-going work / Perspectives

- **Magnetic field || chains:**

Incommensurate dynamics
(Tomonaga Luttinger liquid theory)

TASP, PSI

Technical support: *M. Bartkowiak*
Local contacts: *J. S. White, M. Månsson*

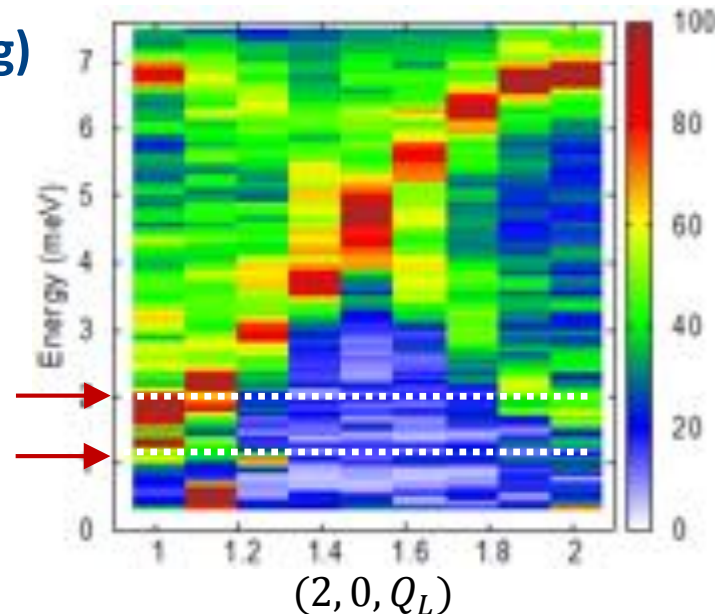


- **Doping by non magnetic impurities (Mg)**

Chain cuts → **flat modes**

IN12, ILL

Technical support: *B. Vettard*
Local contact: *S. Raymond*



Acknowledgments



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Thank you for attention