



Low-Dimensional Spin Systems and Quantum Magnetism

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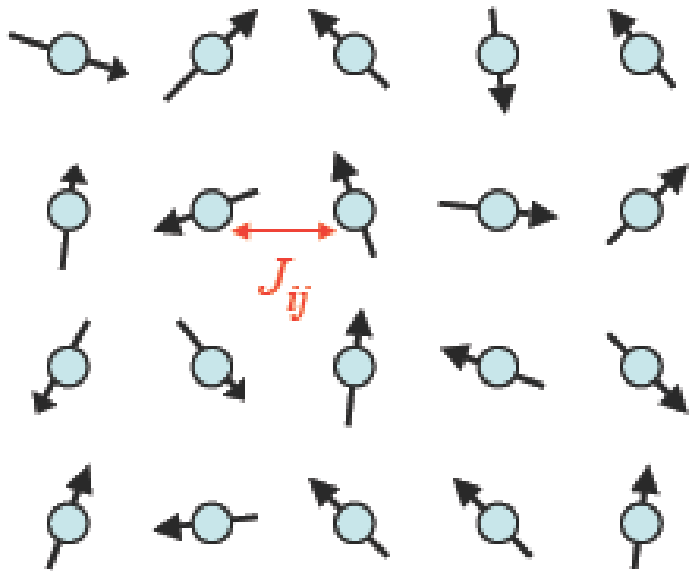
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INDIAN ACADEMY OF SCIENCES, 84th Annual Meeting, BHU-Varanasi
Nov 1- 3, 2018

Magnetic Phase Transitions

An ordered configuration of magnetic moments with a long correlation length

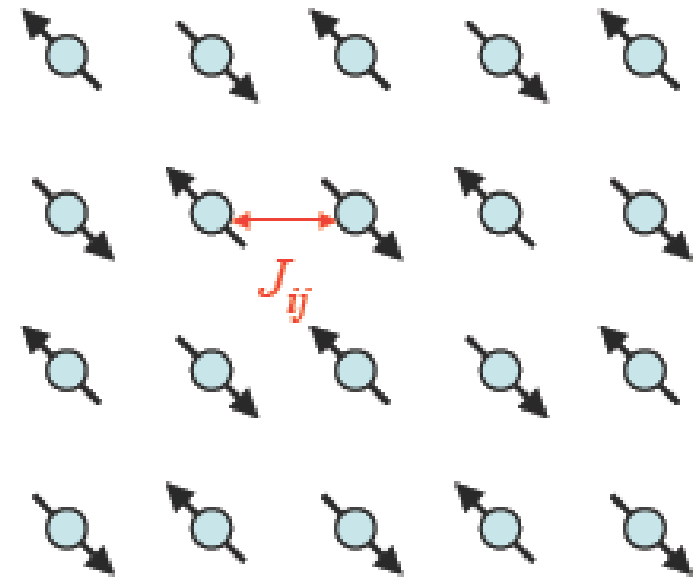
Disordered State:



$$\langle S \rangle = 0$$

$k_B T$ vs. Exchange Energy

Ordered State:



$$\langle S \rangle \neq 0$$

Absence or Presence of a LRO at a Finite T

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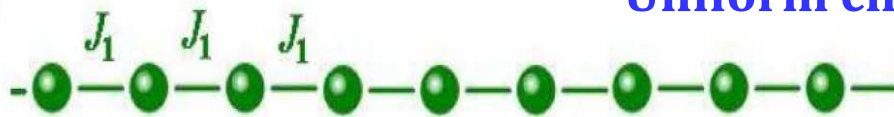
N. D. Mermin[†] and H. Wagner[‡]

Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York

| Spin/Space | $d = 1$ | $d = 2$ | $d = 3$ |
|------------|---------|---------|---------|
| Ising | X | Yes | Yes |
| XY | X | Yes? | Yes |
| Heisenberg | X | X | Yes |

→ Theorem of Mermin and Wagner

Uniform chain



dimer spin-chain

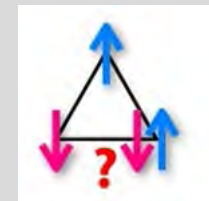


trimer spin-chain



Frustration with NN interactions

Ising



Heisenberg/XY



square

4 NN

honeycomb

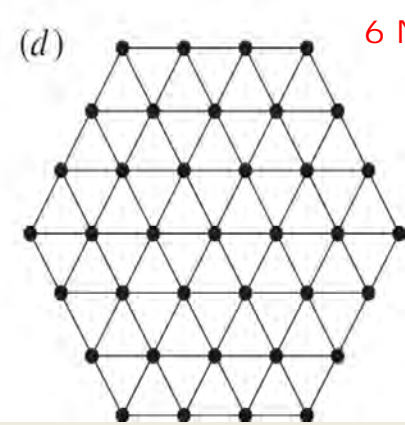
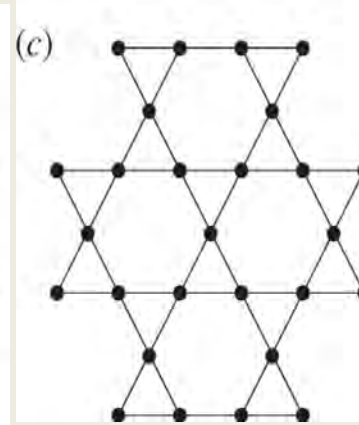
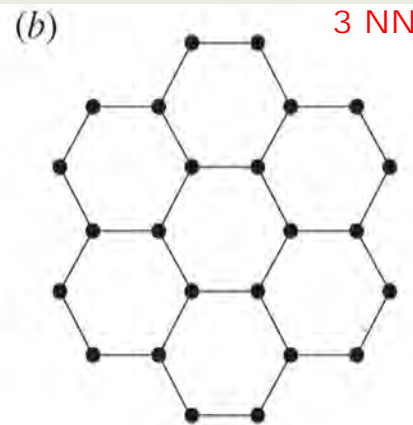
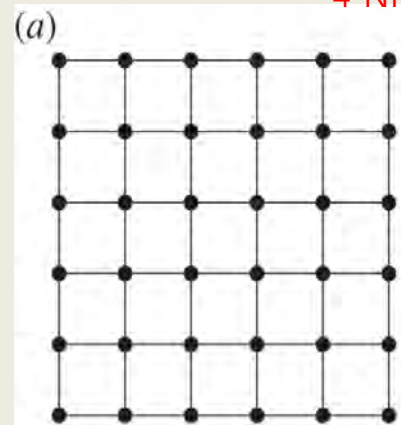
3 NN

Kagome

4 NN

triangular

6 NN

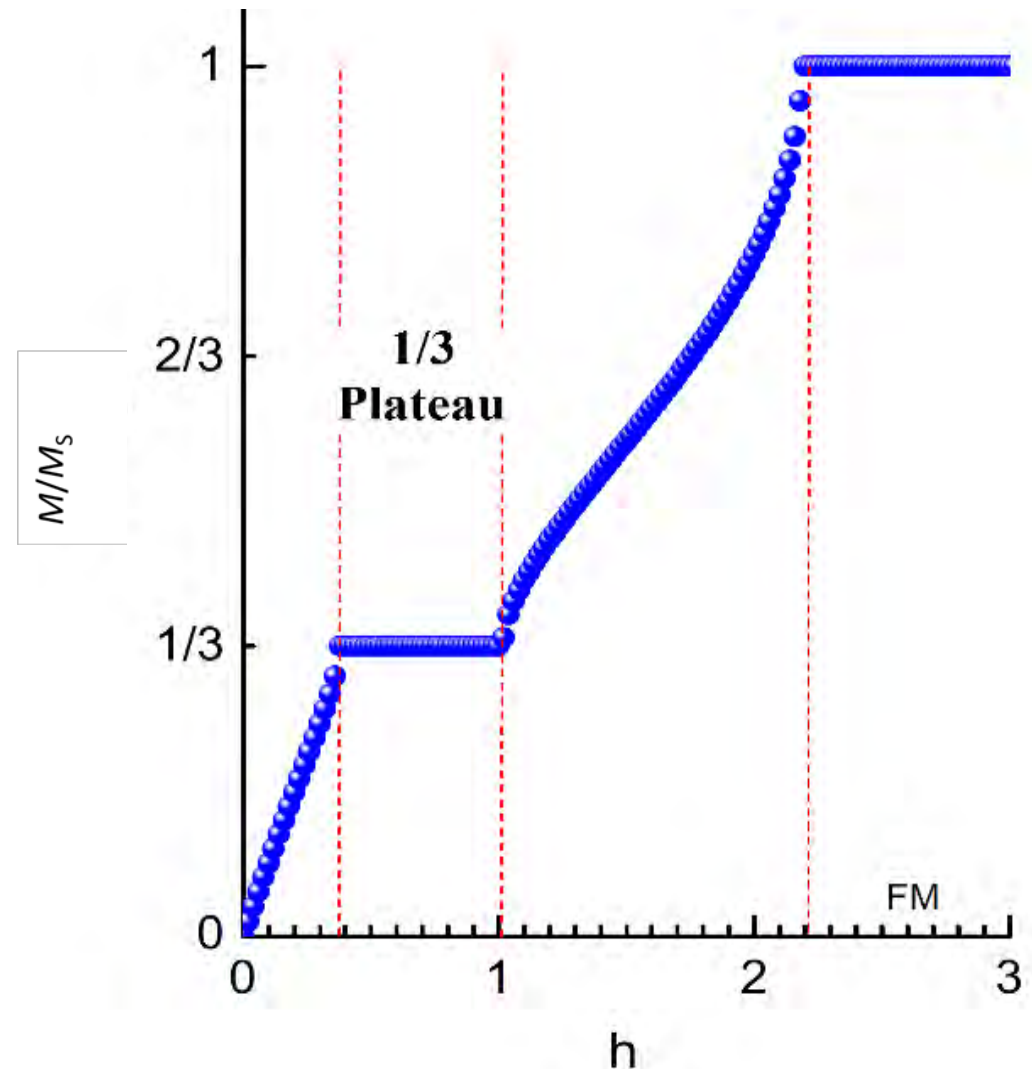


Magnetic properties dictated by the nature of exchange interactions

Quantum Fluctuations

Quantum Phase Transitions

Quantum Magnetization Plateau



Review Article:

APPLIED PHYSICS REVIEWS 4, 031303 (2017)

APPLIED PHYSICS REVIEWS

Neutron scattering of advanced magnetic materials

S. M. Yusuf^{a)} and Amit Kumar

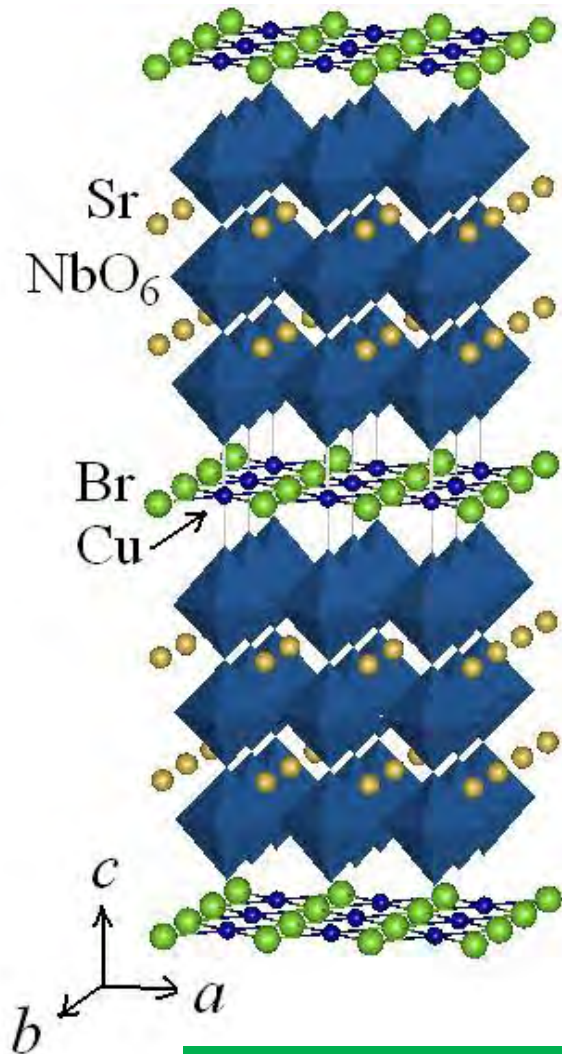
Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400 085, India

(Received 23 February 2017; accepted 9 June 2017; published online 16 August 2017)

^{a)}Email: smyusuf@barc.gov.in

Square-lattice spin system $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$

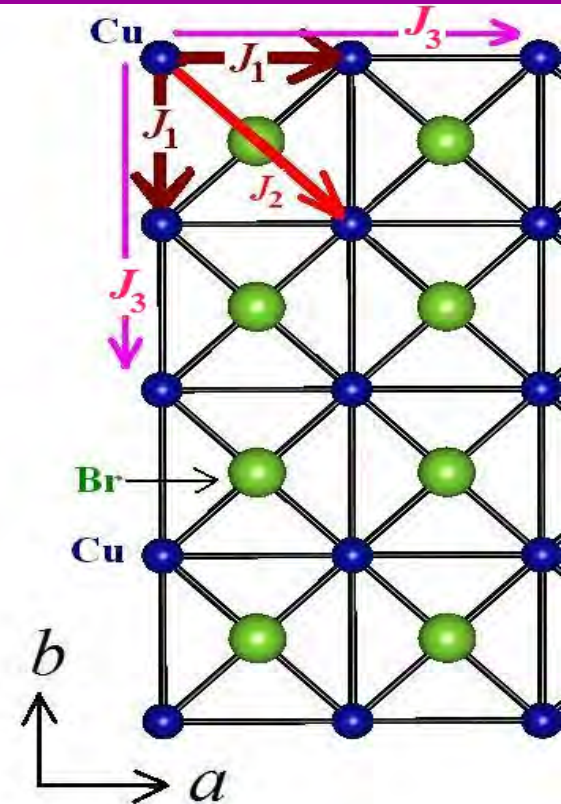
Layered Crystal Structure Square-lattice Spin $\frac{1}{2}$ System



Tetragonal

$P4/mmm$

**$a = 3.888(1) \text{ \AA}$
 $c = 15.947(1) \text{ \AA}$**



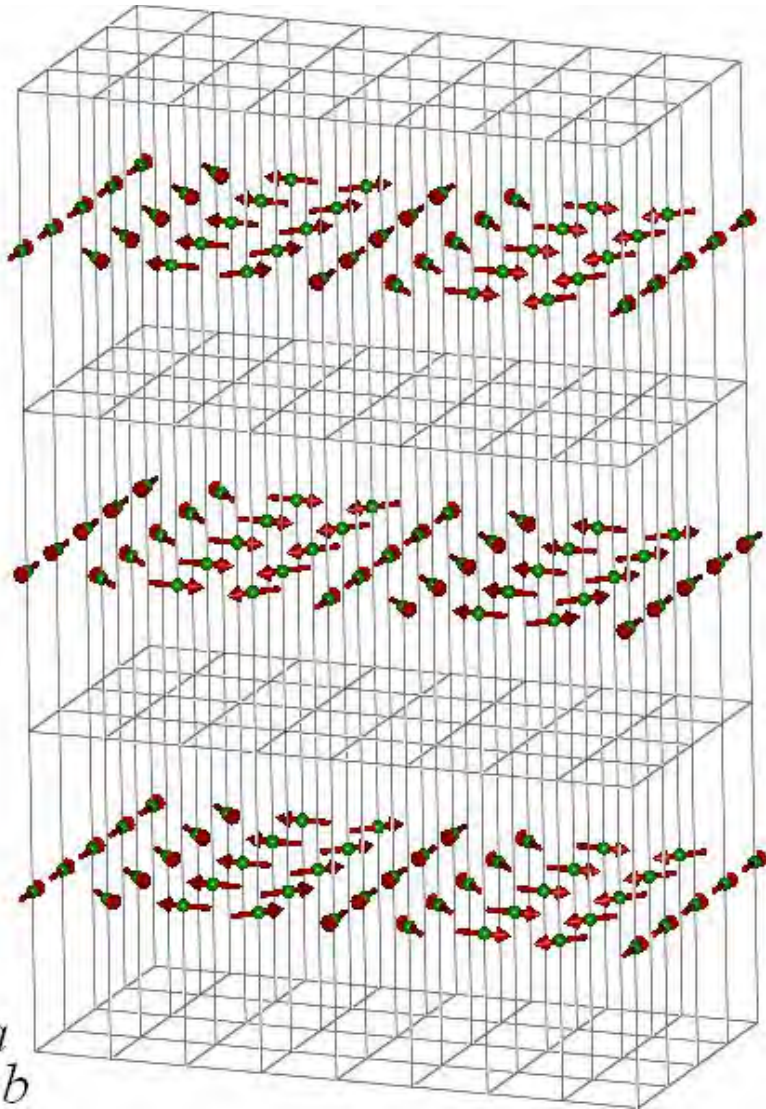
S. M. Yusuf, A. K. Bera, et al.
Phys. Rev. B 84, 064407 (2011)

C Ritter, S M Yusuf, et al.
Phys. Rev. B 88, 104401 (2013)

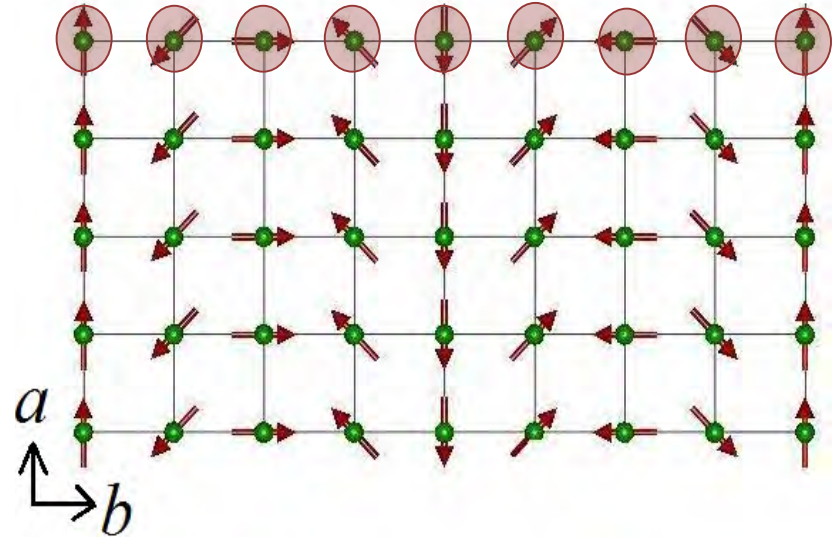
Square-lattice spin system $(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$

Commensurate in-plane Spiral Order

$$k = (0 \ 3/8 \ 1/2) \ 4a \times 8b$$



$4a \times 8b \times 3c$



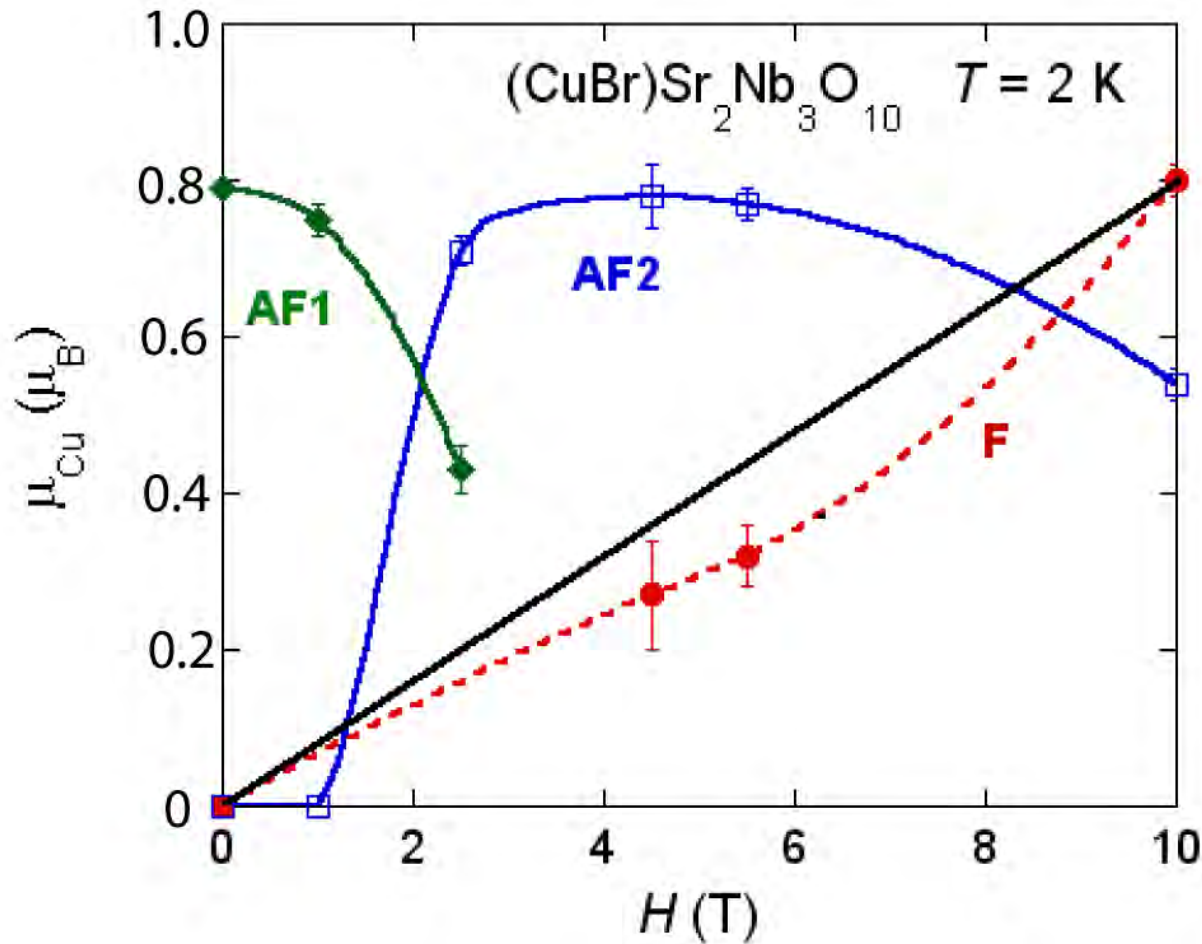
Cu^{2+} : $0.79(7) \mu_B$ at 2 K

Quantum fluctuations.

2D $S = 1/2$ AFM square lattice: $\sim 0.6 \mu_B$

S. M. Yusuf, et al.

Phys. Rev. B 84, 064407 (2011)



Helical antiferro
AF1, with $\kappa = [0 \ 3/8 \ 1/2]$

Second AFM, AF2,
with $\kappa = [0 \ 1/3 \sim 0.46]$

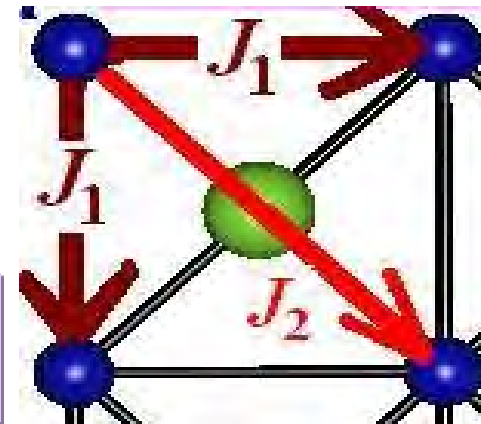
Simple ferro phase with
 $\kappa = [0 \ 0 \ 0]$

S. M. Yusuf, A. K. Bera, et al.
Phys. Rev. B 84, 064407 (2011)

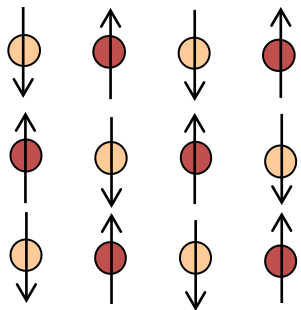
C Ritter, S M Yusuf, et al.
Phys. Rev. B 88, 104401 (2013)

$S = 1/2$ Square-lattice

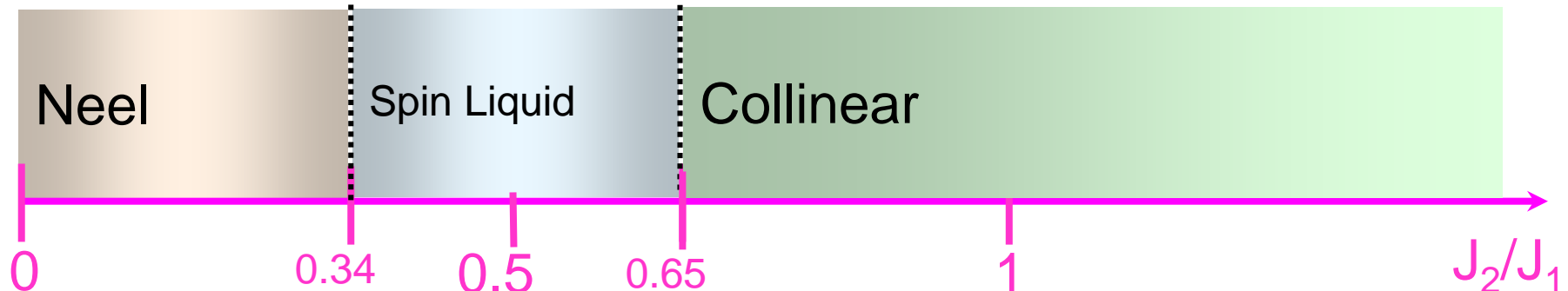
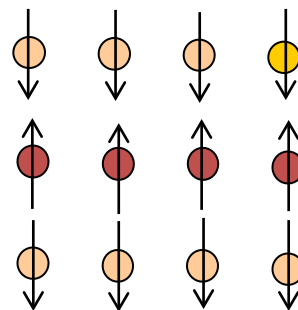
At $T = 0$ K



All four nearest neighbour spins are antiparallel



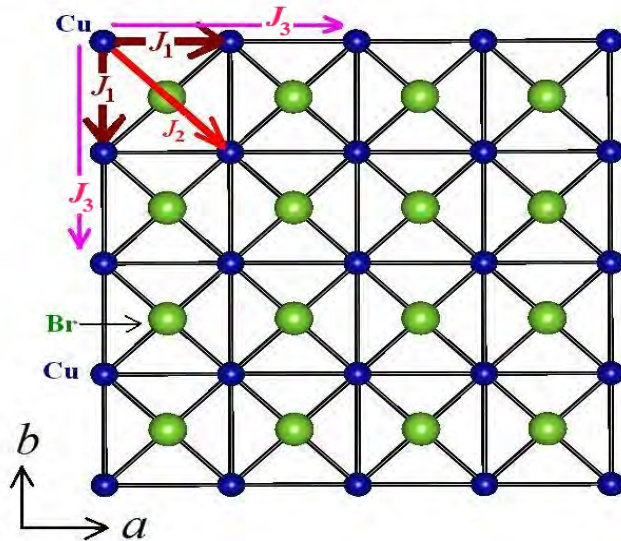
Antiparallel coupling of FM spin chains



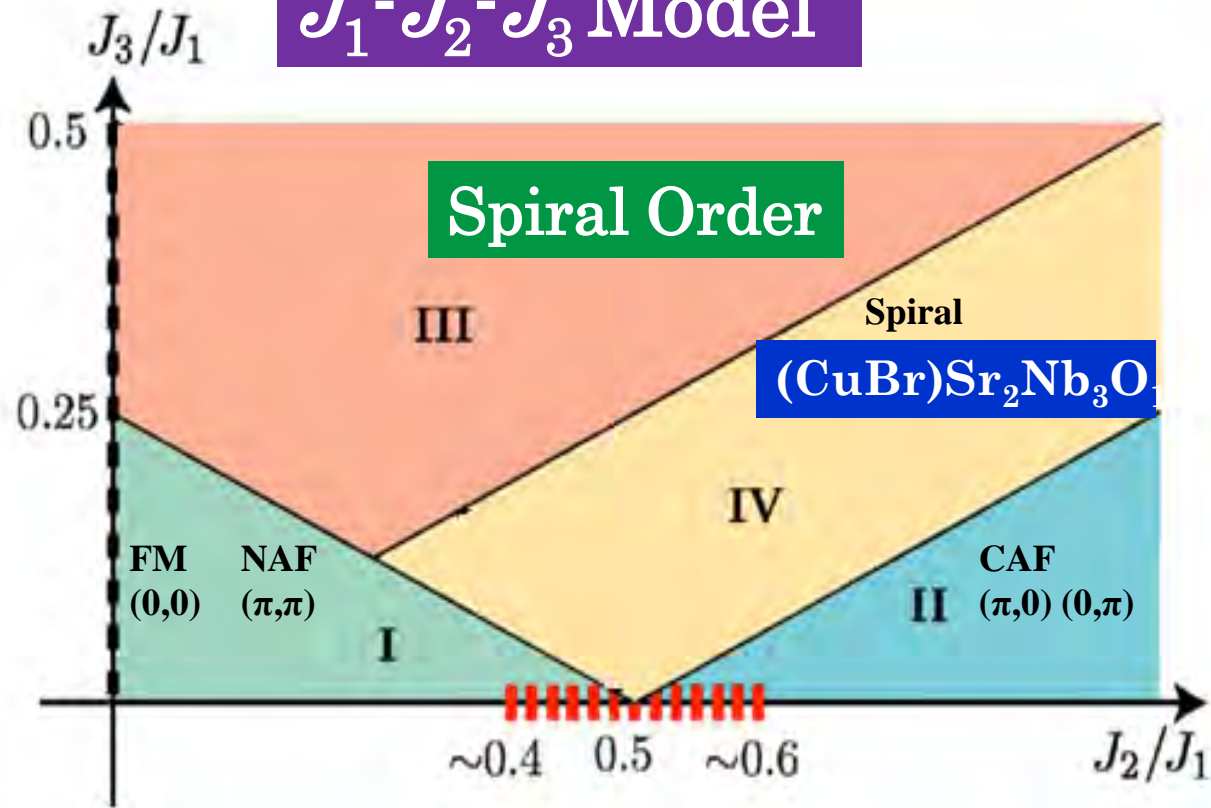
Schmalfuß et al., Phys. Rev. Lett. 97, 157201 (2006)

Square-lattice System

J_1 - J_2 - J_3 Model



$(\text{CuBr})\text{Sr}_2\text{Nb}_3\text{O}_{10}$



S. M. Yusuf, et al,
Phys. Rev. B84,064407(2011)

C Ritter, S M Yusuf, et al.
Phys. Rev. B 88, 104401 (2013)

Cu^{2+} : $0.79(7) \mu_B$ at 2 K

Quantum fluctuations
2D $S = \frac{1}{2}$ AFM square lattice: $\sim 0.6 \mu_B$

Our Research on Haldane chain compound

PHYSICAL REVIEW B **86**, 024408 (2012)

Quantum phase transition from a spin-liquid state to a spin-glass state in the quasi-one-dimensional spin-1 system $\text{Sr}_{1-x}\text{Ca}_x\text{Ni}_2\text{V}_2\text{O}_8$

A. K. Bera and S. M. Yusuf*

Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India

(Received 21 September 2011; revised manuscript received 16 June 2012; published 9 July 2012)

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¹N. D. Mermin and H. Wagner, *Phys. Rev. Lett.* **17**, 1133 (1966).

²H. A. Bethe, *Z. Phys.* **71**, 205 (1931).

³H. J. Schulz, *Phys. Rev. Lett.* **77**, 2790 (1996).

⁴D. A. Tennant, T. G. Perring, R. A. Cowley, and S. E. Nagler, *Phys. Rev. Lett.* **70**, 4003 (1993).

⁵R. Caciuffo, L. Paolasini, A. Sollier, P. Ghigna, E. Pavarini, J. van den Brink, and M. Altarelli, *Phys. Rev. B* **65**, 174425 (2002).

⁶D. C. Dender, D. Davidovic, D. H. Reich, C. Broholm, K. Lefmann, and G. Aeppli, *Phys. Rev. B* **53**, 2583 (1996).

⁷F. D. M. Haldane, *Phys. Rev. Lett.* **50**, 1153 (1983).

⁸F. D. M. Haldane, *Phys. Lett.* **93A**, 464 (1983).

²⁶L.-P. Regnault, I. A. Zaliznyak, and S. V. Meshkov, *J. Phys.: Condens. Matter* **5** L677 (1993).

²⁷B. Pahari, K. Ghoshray, A. Ghoshray, T. Samanta, and I. Das, *Physica B* **395**, 138 (2007).

²⁸M. D. Mukadam, S. M. Yusuf, P. Sharma, and S. K. Kulshreshtha, *J. Magn. Magn. Mater.* **269** 317 (2004).

²⁹D. Petit, L. Fruchter, and I. A. Campbell, *Phys. Rev. Lett.* **83**, 5130 (1999).

³⁰J. R. L. de Almeida and D. J. Thouless, *J. Phys. A* **11**, 983 (1978).

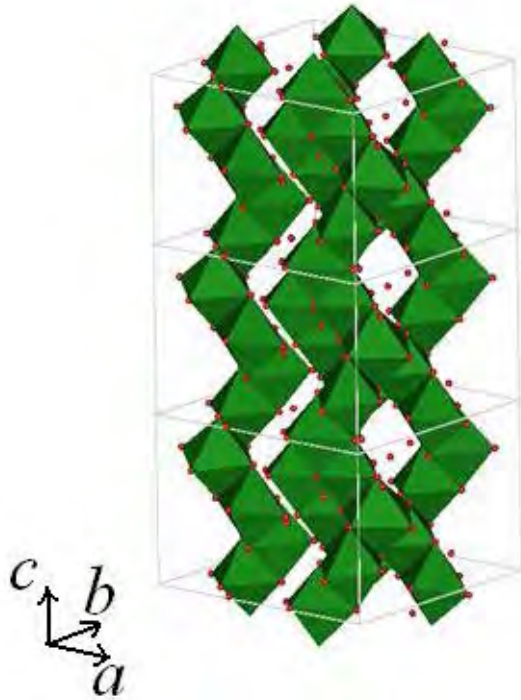
³¹Z. He, T. Taniyama, T. Kyomen, and M. Itoh, *Phys. Rev. B* **72**, 172403 (2005).

³²S. Friedemann, T. Westerkamp, M. Brando, N. Oeschler, S. Wirth,

Quantum Spin-chain Systems: $\text{Sr}_{1-x}\text{Ca}_x\text{Ni}_2\text{V}_2\text{O}_8$

A. K. Bera and S. M. Yusuf

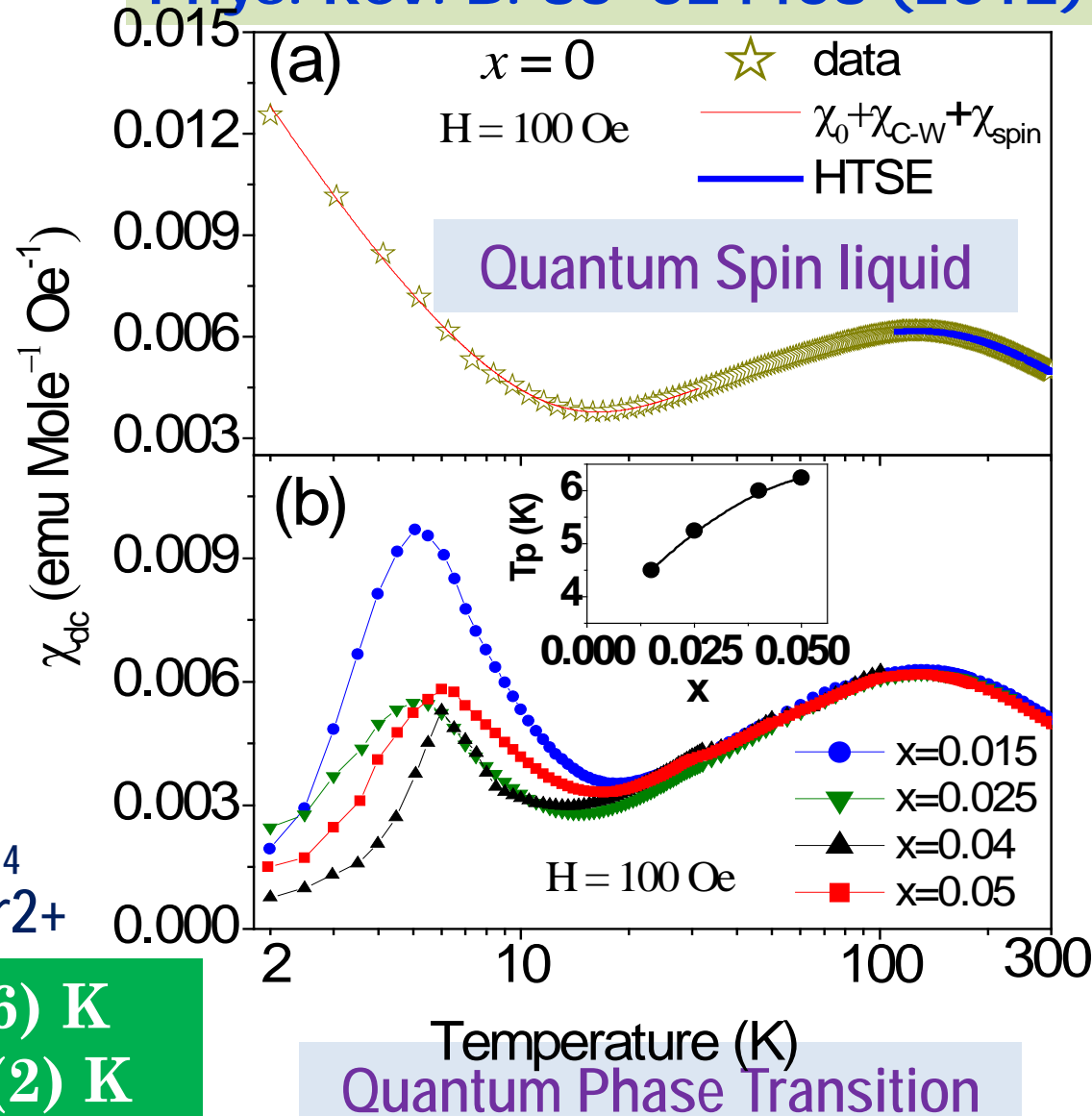
Phys. Rev. B. 86 024408 (2012)



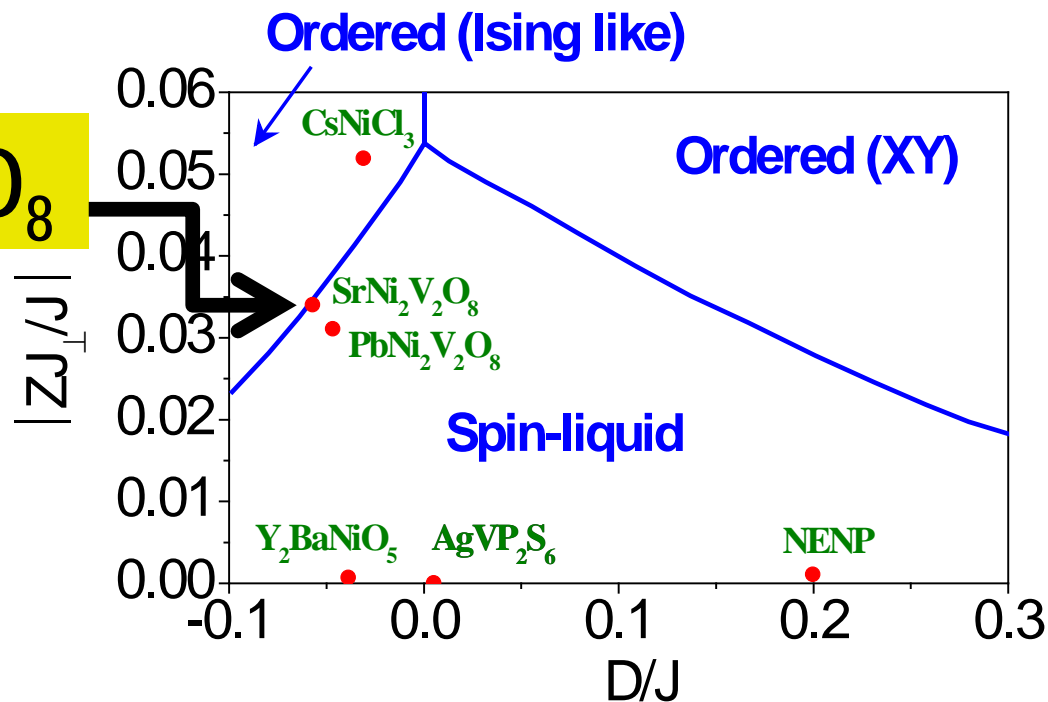
Screw chains of edge-shared NiO_6 (Ni^{2+} ; $3d^8$, $S=1$) octahedra along c-axis.
Separated by nonmagnetic VO_4 (V^{5+} ; $3d^0$, $S=0$) tetrahedra & Sr^{2+}

$$\Delta_{\text{gap}} = 26.6(6) \text{ K}$$

$$J/k_B = 106.4(2) \text{ K}$$



Sakai-Takahashi Phase Diagram for weakly coupled 1D spin-chain with $S = 1$



J_{\perp} = inter-chain interaction

J = intra-chain interaction

D = single ion anisotropy

Possibility of Quantum Phase Transition

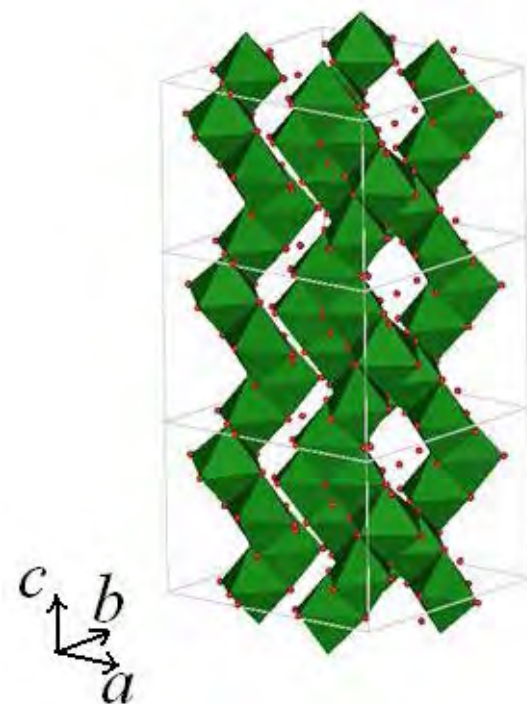
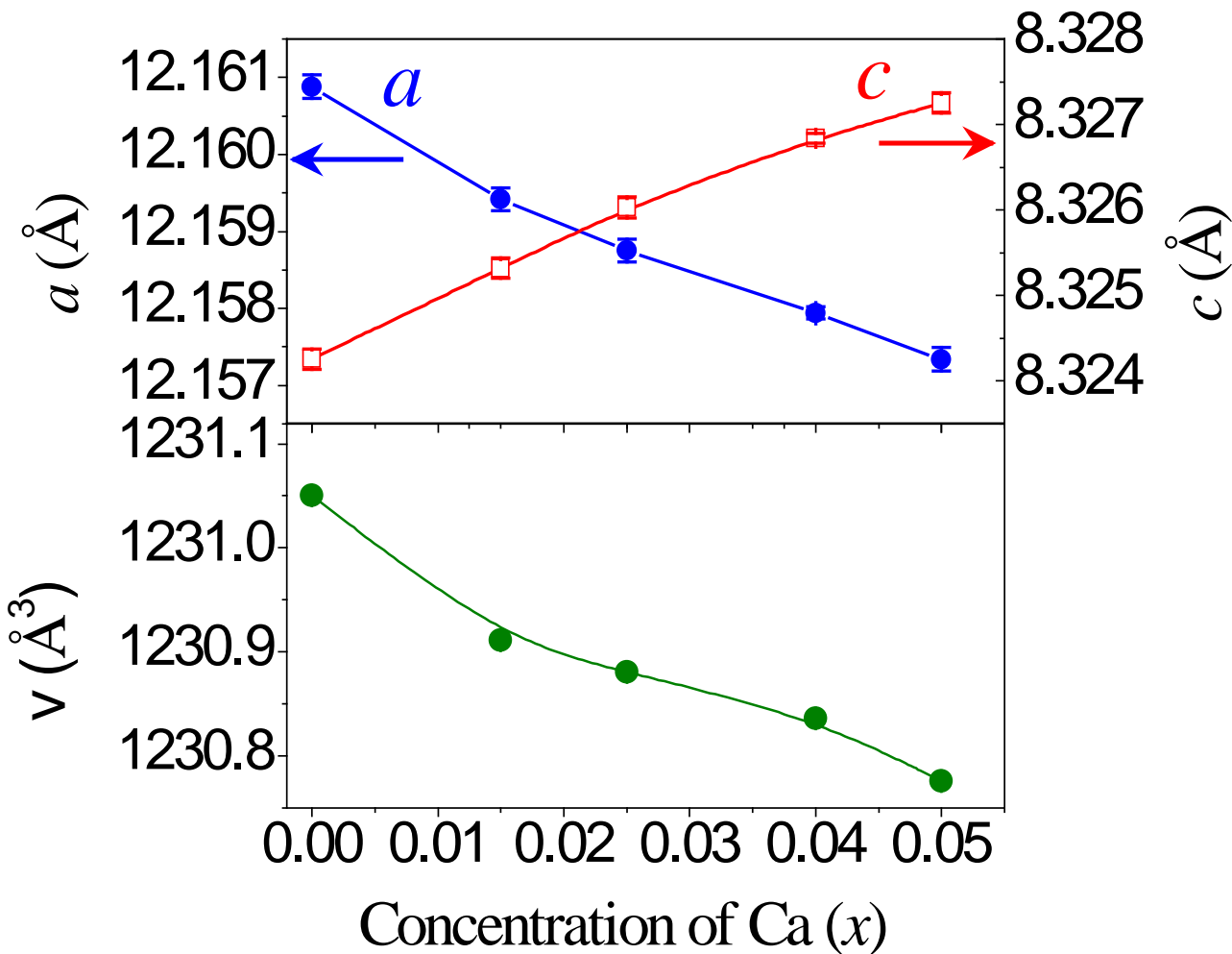
- Enhancement of J_{\perp}
- and/or Reduction in D

$\text{SrNi}_2\text{V}_2\text{O}_8$, $|D/J| = |(-0.56 \text{ meV}) / (106.4 \text{ K} = 9.17 \text{ meV})| = 0.06$

Concentration dependent Lattice Parameter



Sr^{2+} : 1.26 Å
 Ca^{2+} : 1.12 Å



Decrease in the distances
between screw chains

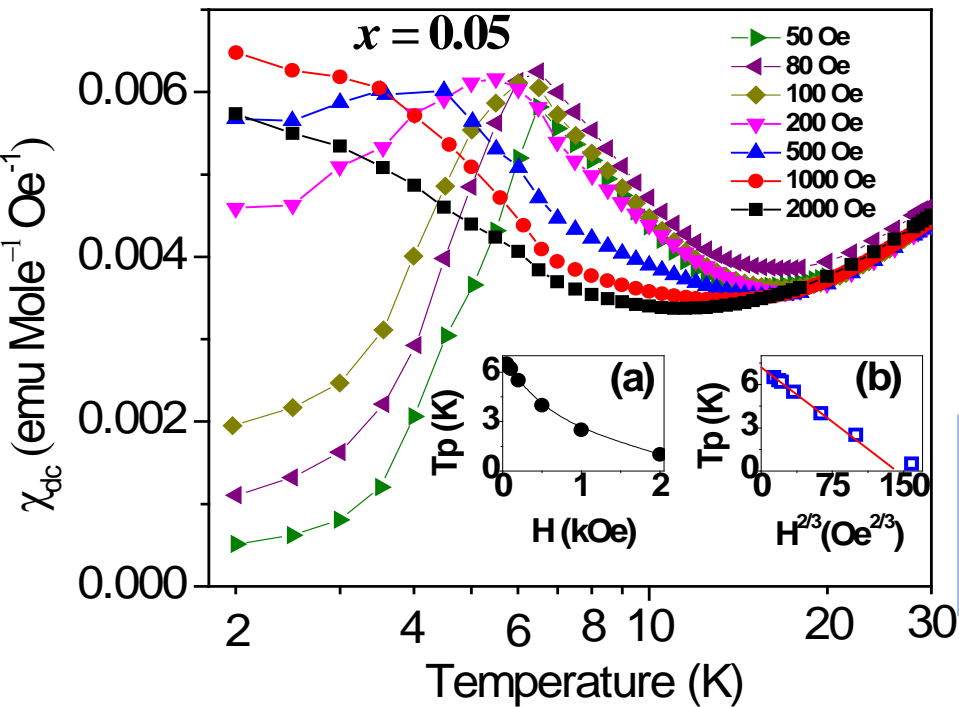
Spin-chain System $\text{Sr}_{1-x}\text{Ca}_x\text{Ni}_2\text{V}_2\text{O}_8$

$\text{Sr}_{0.95}\text{Ca}_{0.05}\text{Ni}_2\text{V}_2\text{O}_8$

dc susceptibility

De Almeida -Thouless (AT)-type Phase boundary

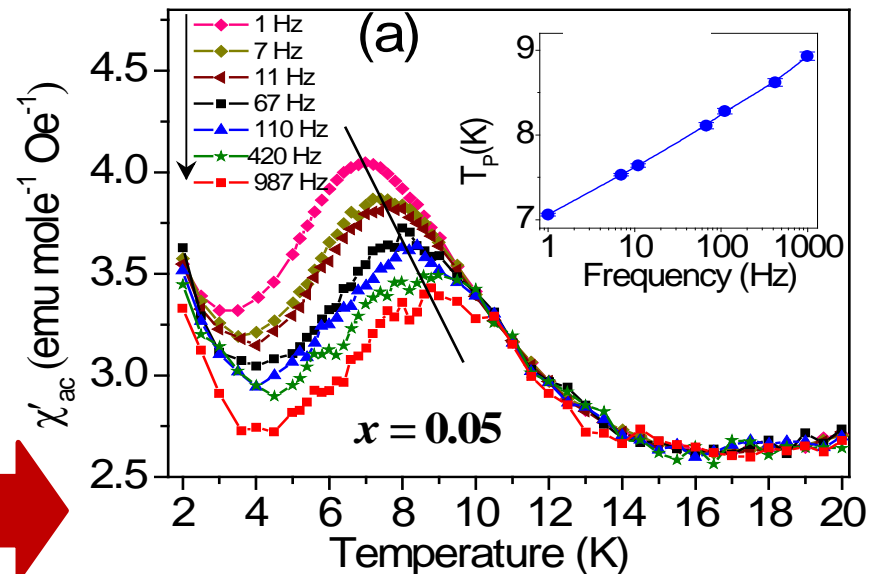
$T_g(0) = 7.6 \pm 0.1 \text{ K}$, $\beta = 1.47 \pm 0.03$
 $\beta = 3/2$, predicted by the mean field theory
 for Ising spin-glass systems



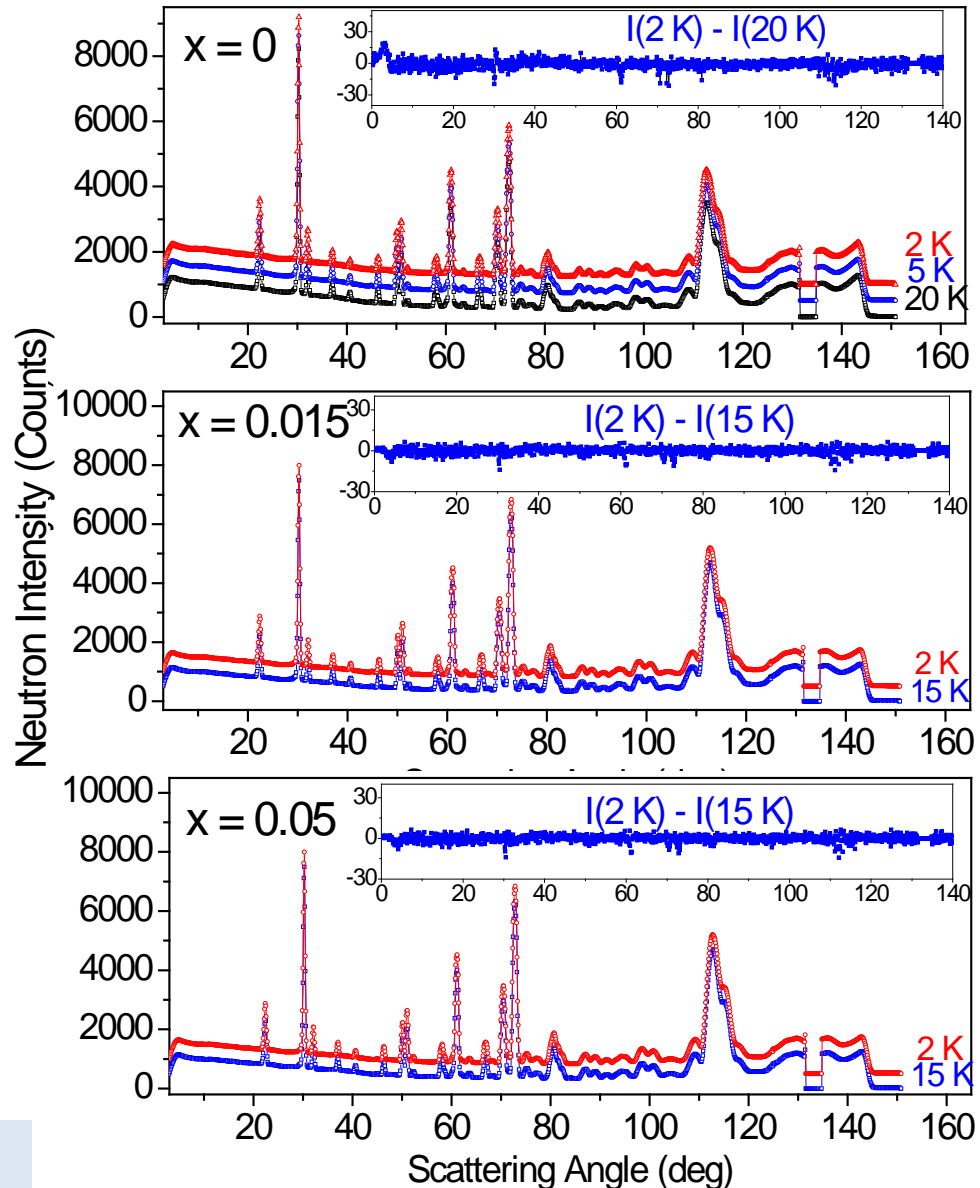
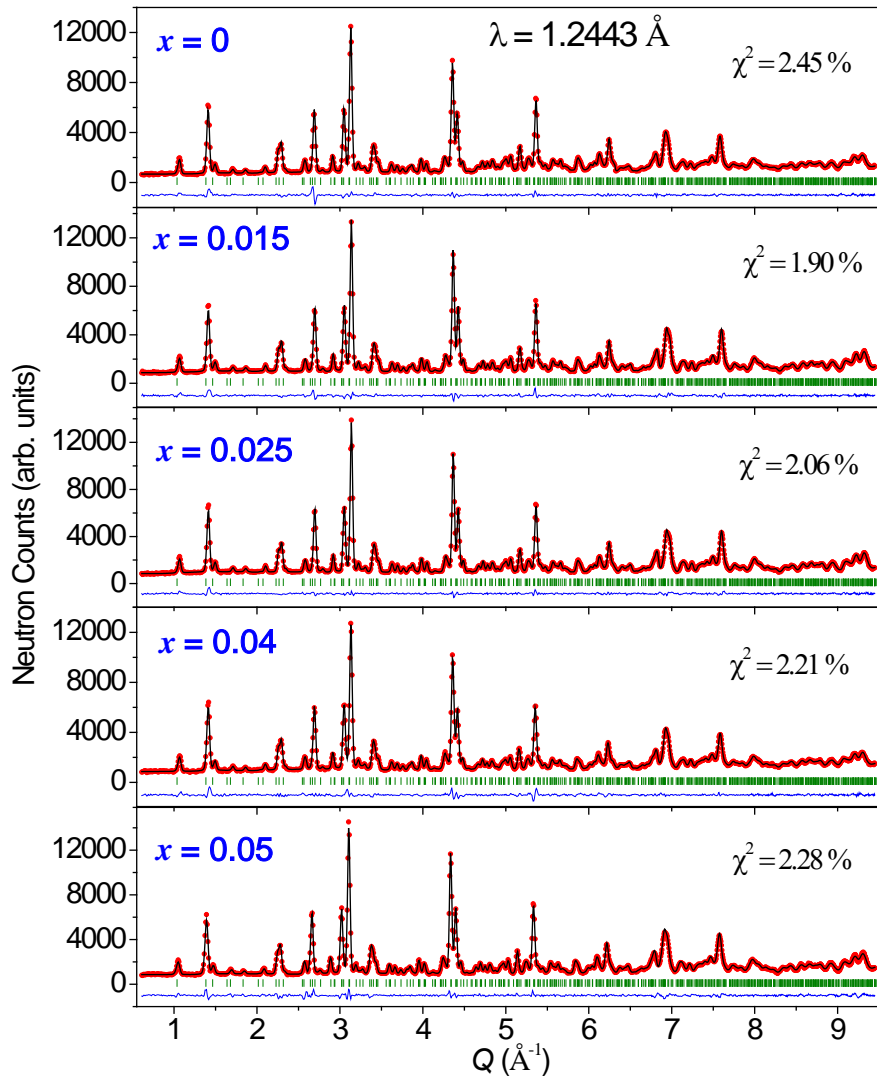
$$H(T_g) \propto \left[1 - \frac{T_g(H)}{T_g(0)} \right]^\beta$$

A. K. Bera and S. M. Yusuf
 Phys. Rev. B. 86 024408 (2012)

ac susceptibility



Neutron diffraction of $\text{Sr}_{1-x}\text{Ca}_x\text{Ni}_2\text{V}_2\text{O}_8$



A. K. Bera and S. M. Yusuf
Phys. Rev. B. 86 024408 (2012)

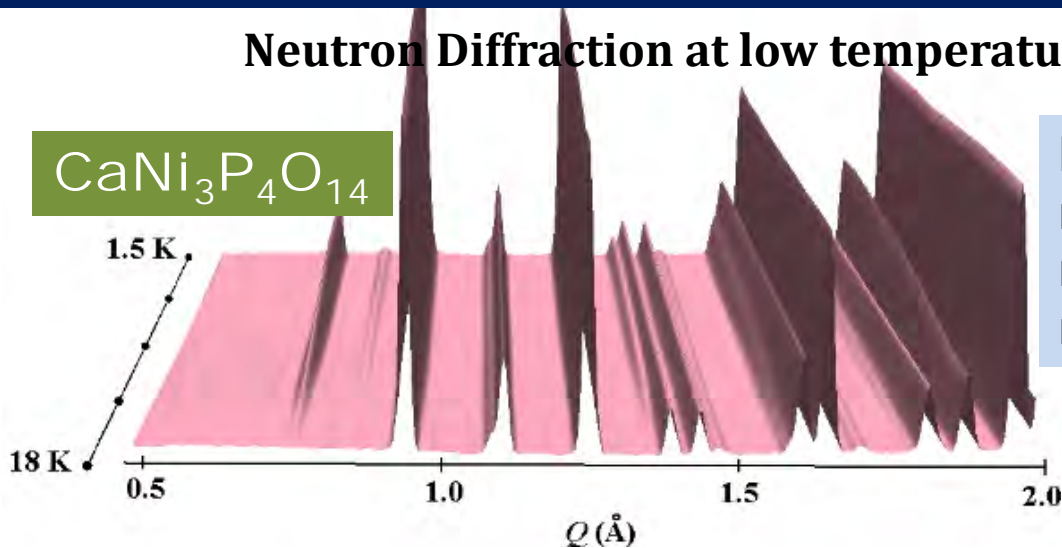
Quantum Phase Transition

Quasi-1D $S=1$ trimmer chain $\text{CaNi}_3\text{P}_4\text{O}_{14}$

Neutron Diffraction at low temperatures

Magnetic Ground State

$\text{CaNi}_3\text{P}_4\text{O}_{14}$



NiO_6 octahedra, forming zigzag chains,
connected by two corner shared PO_4 tetrahedra

Ni(1) site:

$$m_a = -0.13 \pm 0.06 \mu_B$$

$$m_b = 0.18 \pm 0.10 \mu_B$$

$$m_c = 1.92 \pm 0.04 \mu_B$$

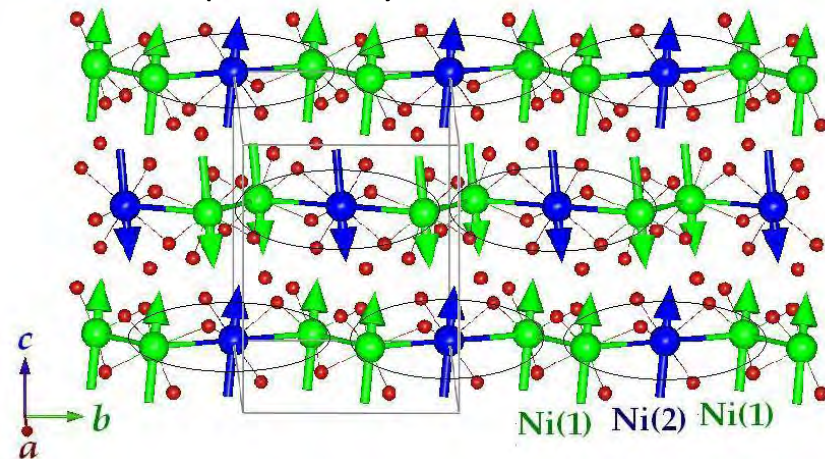
Ni(2) site:

$$m_a = 0.16 \pm 0.10 \mu_B$$

$$m_b = 0.18 \pm 0.10 \mu_B$$

$$m_c = 2.01 \pm 0.06 \mu_B$$

$\text{Ni}^{2+} (3d^8, S=1)$

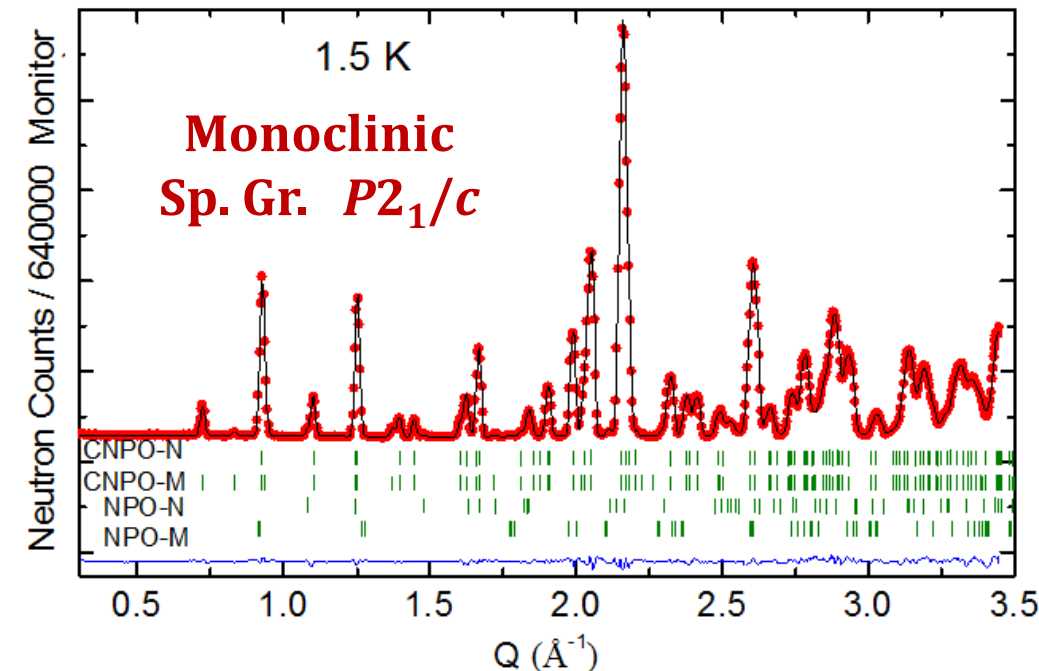


AFM long-range ground state

$$a = 7.3091(8) \text{ \AA}, \quad b = 7.5574(9) \text{ \AA}$$

$$c = 9.3545(11) \text{ \AA}, \quad \beta = 111.989(7)^\circ$$

Monoclinic
Sp. Gr. $P2_1/c$

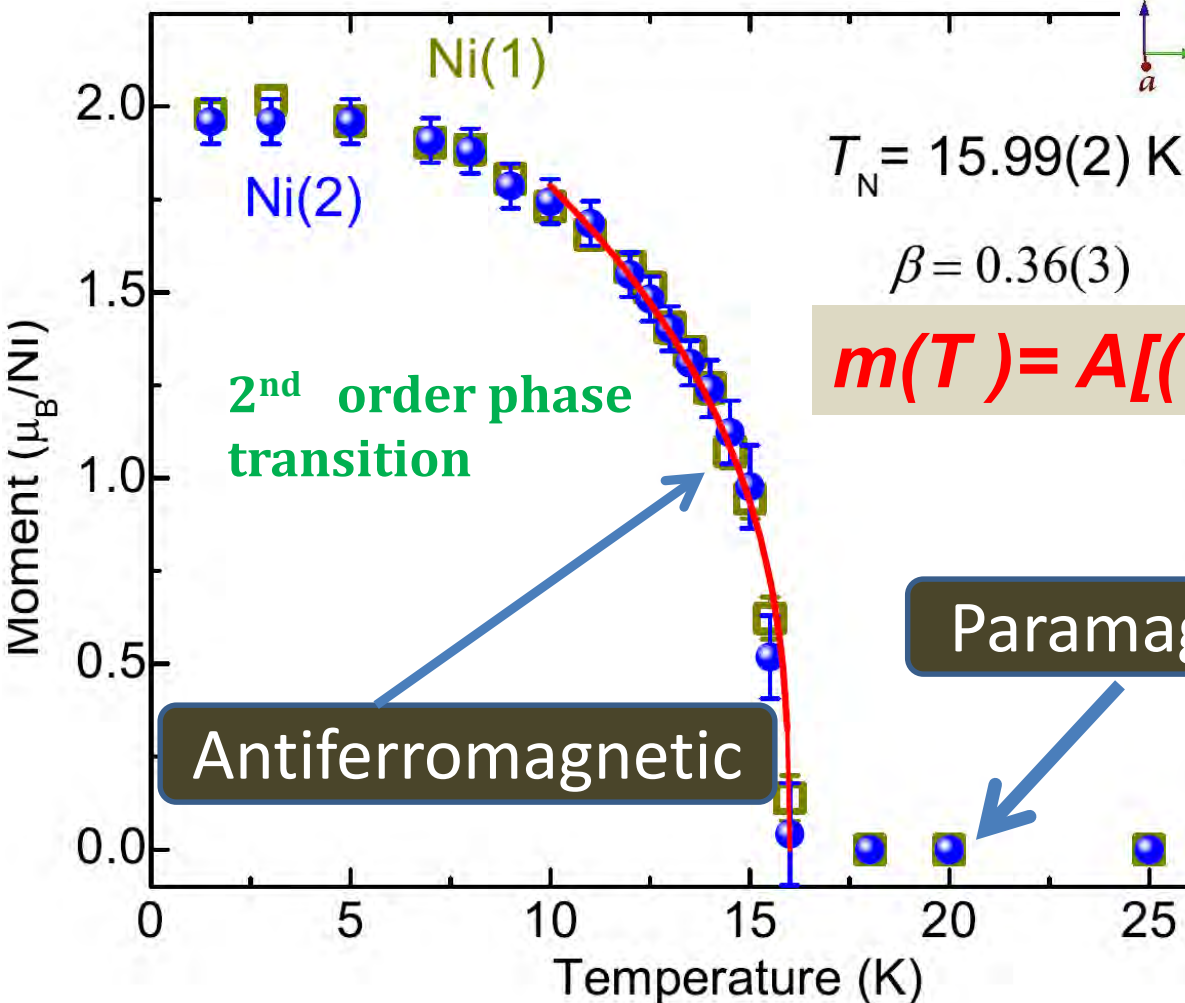
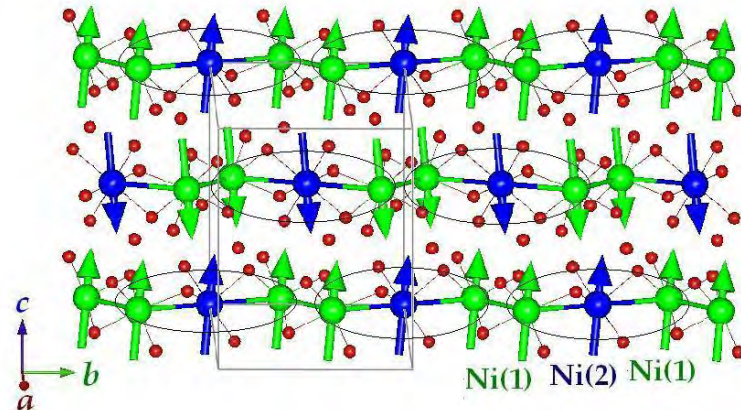


**A. K. Bera, S. M. Yusuf *et. al.*,
Phys. Rev. B 93, 184409 (2016)**



Neutron diffraction

Ni^{2+} ($3d^8$, $S = 1$)



Paramagnetic

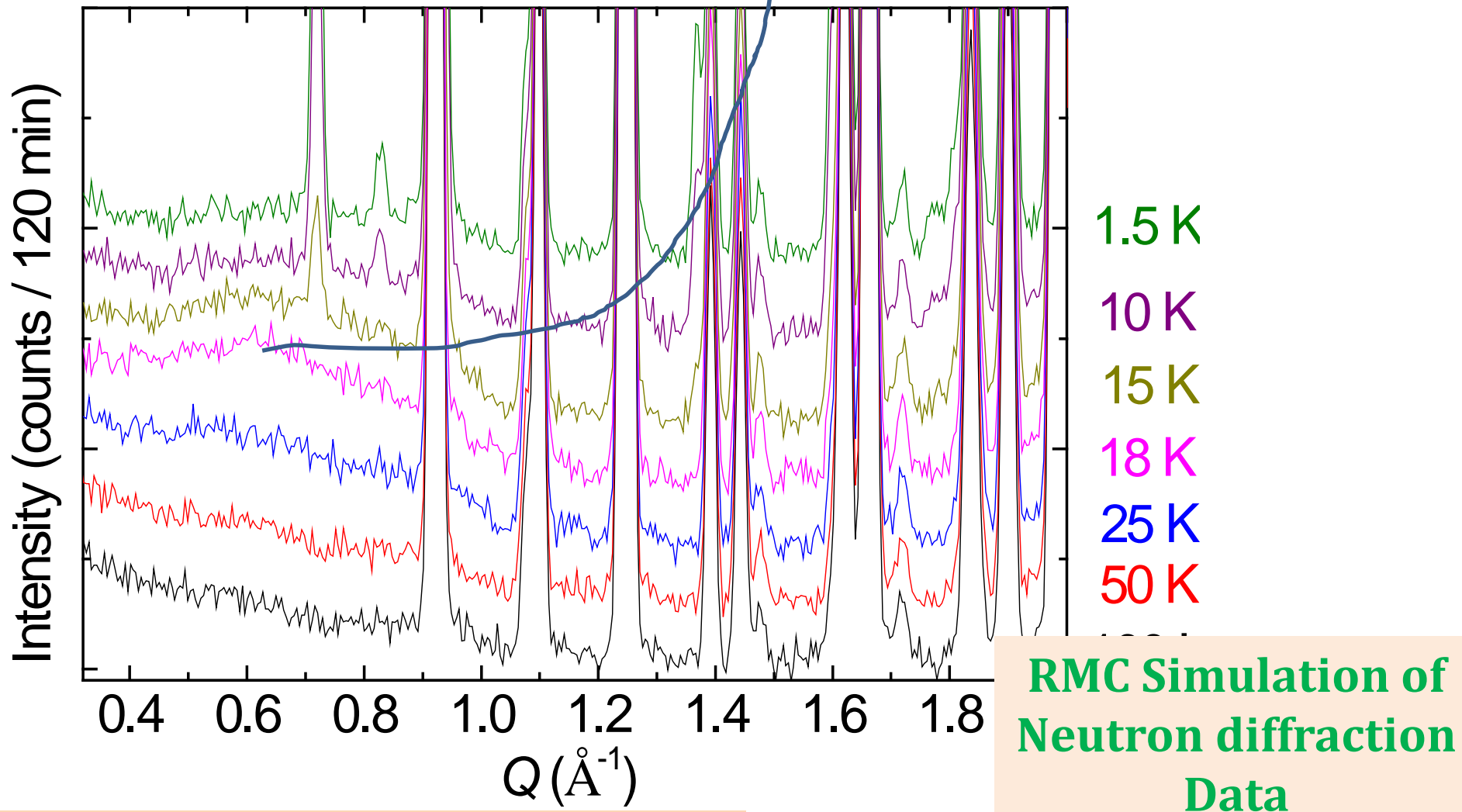
Antiferromagnetic

A. K. Bera, S. M. Yusuf *et al.*,
Phys. Rev. B 93, 184409 (2016)

Antiferromagnetic Neel Temperature, $T_N = 15.99 \text{ K}$

Neel Temp = 15.99 K

Short-range magnetic ordering

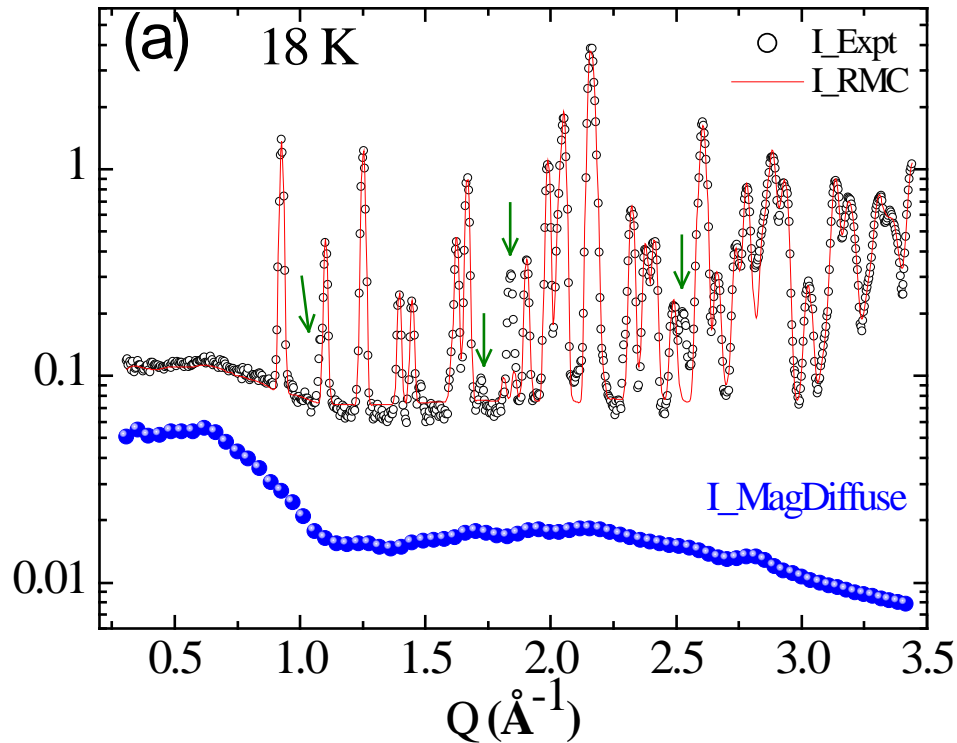
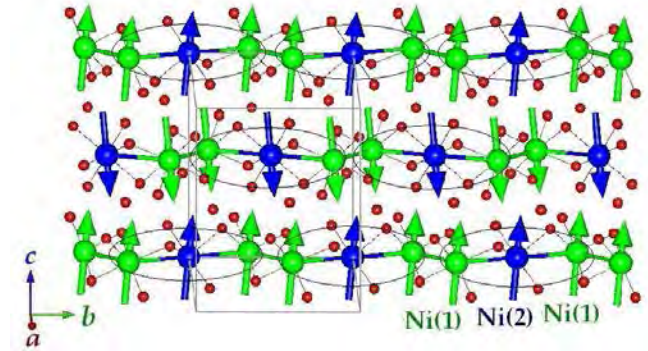


A. K. Bera, S. M. Yusuf, *et al.*
Phys. Rev. B 95, 094424 (2017)

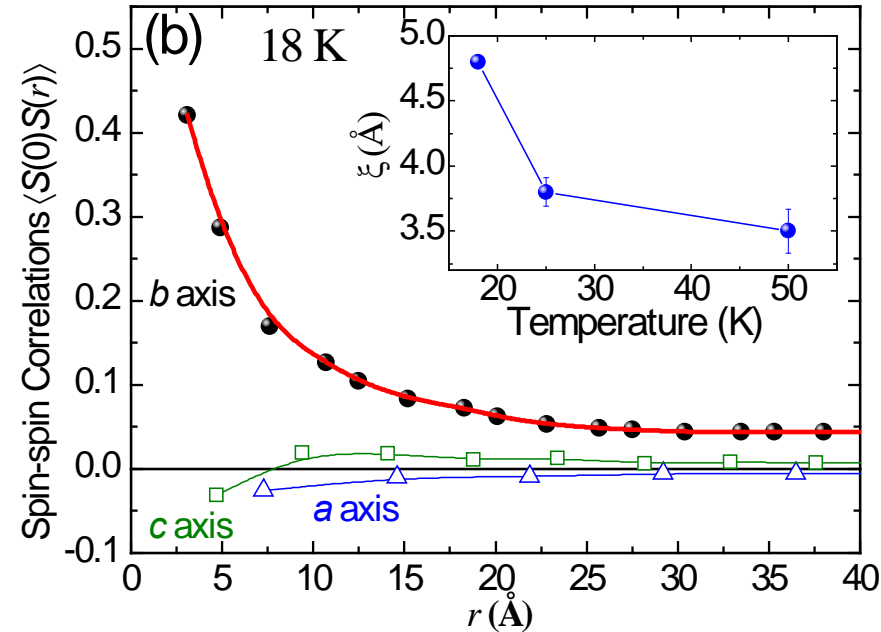
Super cell $8 \times 8 \times 8$ containing
3072 spins

Reverse Monte Carlo (RMC) analysis

Super cell $8 \times 8 \times 8$ containing 3072 spins



Realization of a 3D magnetic
system with $S = 1$ trimer chains



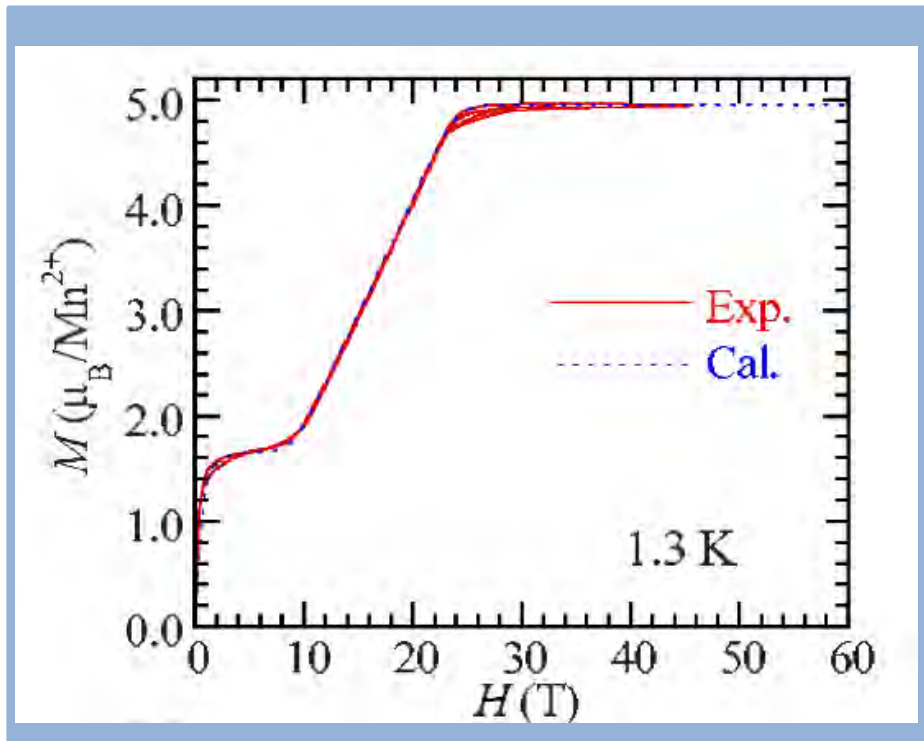
1D short-range FM
correlations along b-axis

A. K. Bera, S. M. Yusuf, *et al.*
Phys. Rev. B 95, 094424 (2017)

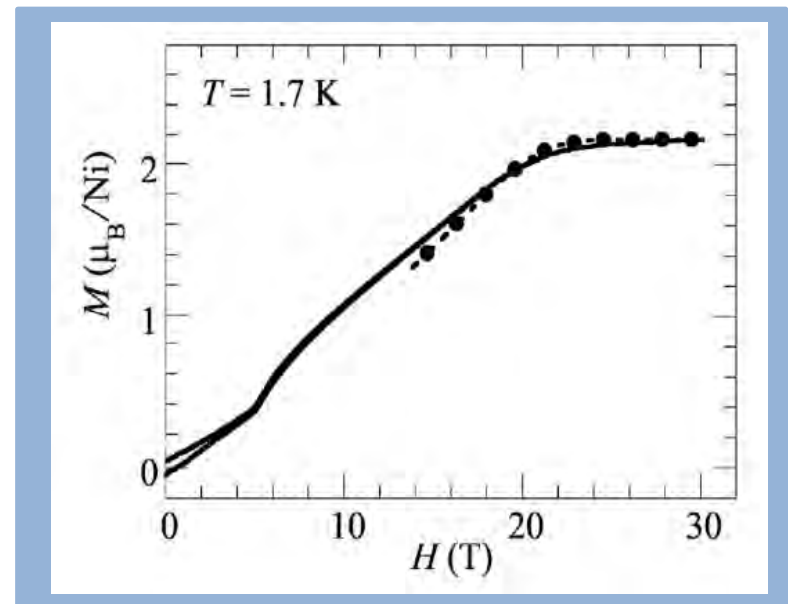
Trimer chain compounds $AM_3P_4O_{14}$

($A = \text{Ca, Ba, Sr}$, and $M = \text{Co, Mn, Ni}$)

Plateau state $\text{Mn} (S=5/2)$



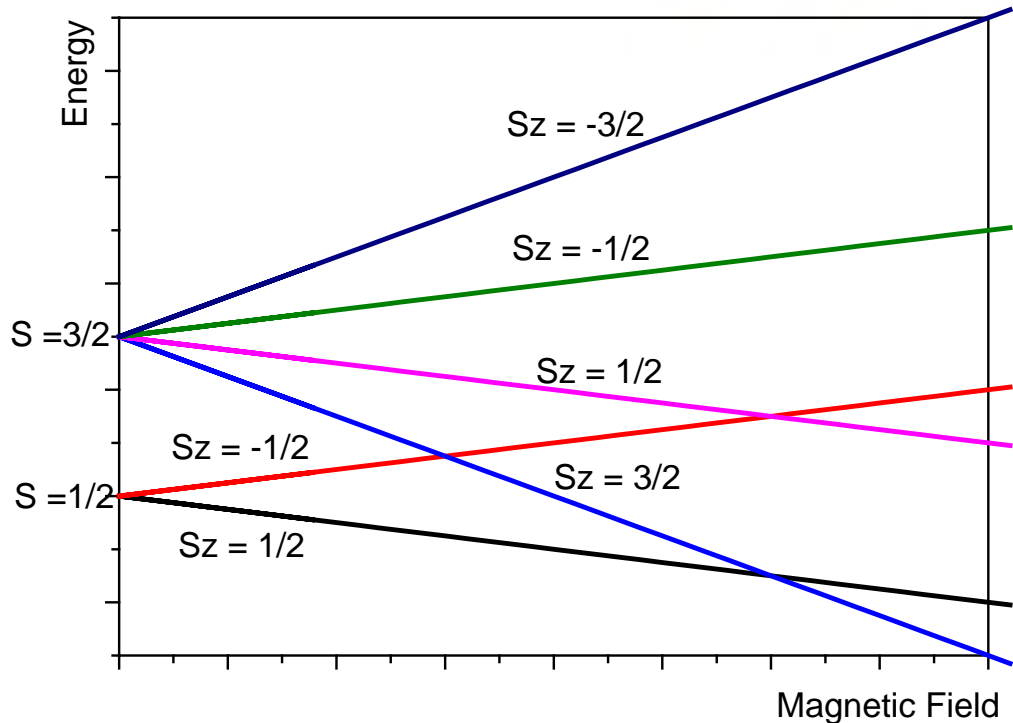
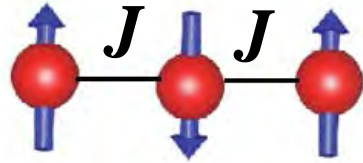
No Plateau state $\text{Ni} (S=1)$



The 1/3- magnetization Plateau

A. K. Bera, S. M. Yusuf *et al.* Phys. Rev. B 97, 224413 (2018)

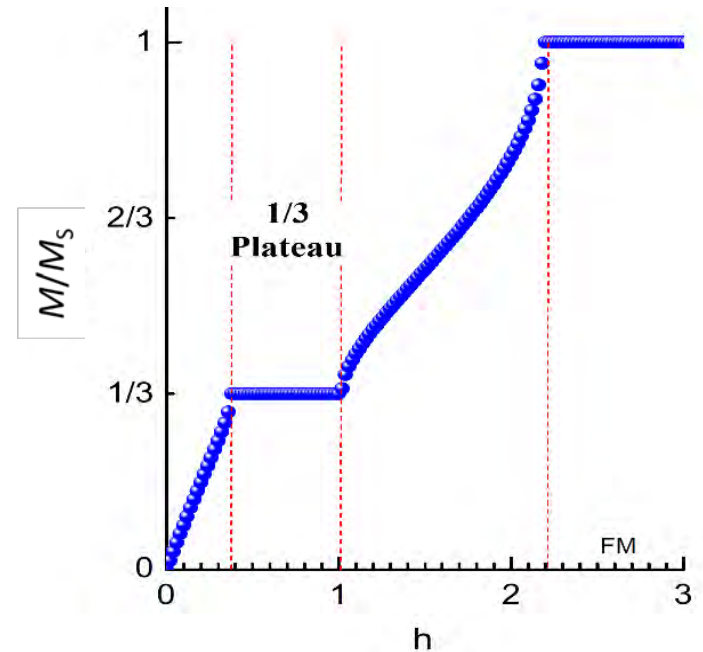
Spin = $\frac{1}{2}$ Trimer



Appears when the magnetization of the ground state $S_z = \frac{1}{2}$ saturates.

Width of the Plateau state: from the saturation of the $S_z = 1/2$ state to the crossover of $S_z = 1/2$ to $S_z = 3/2$ state.

Magnetization plateau



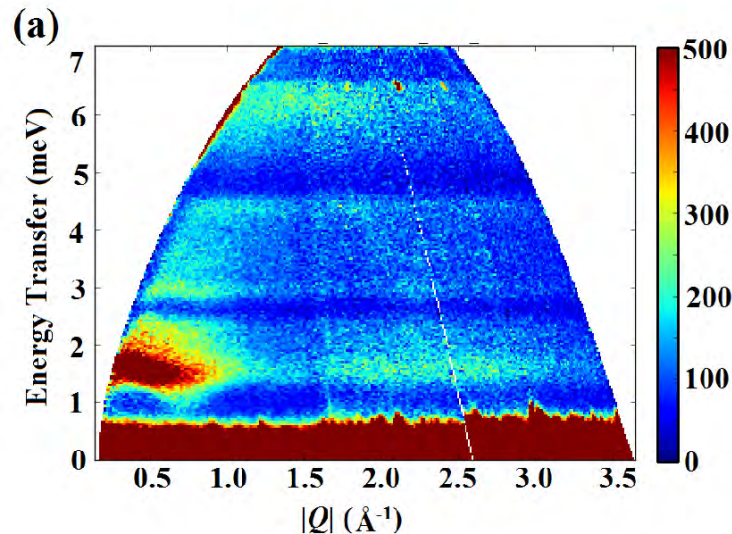
Excited state :

$$S = 3/2, S^z = \pm 3/2, \pm 1/2$$

Ground state :

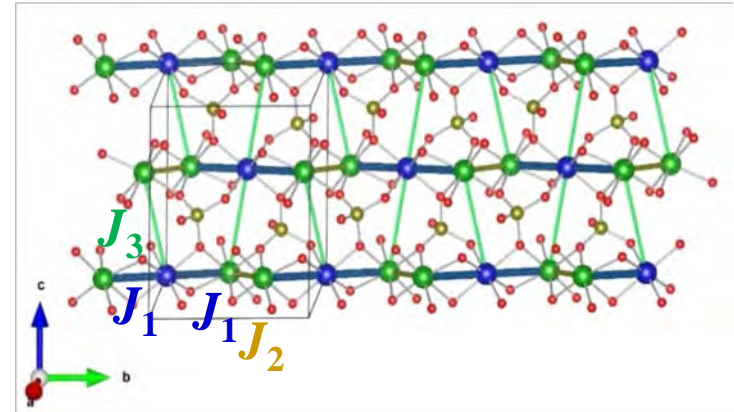
$$S = 1/2, S^z = \pm 1/2$$

1D trimer spin-chain Compound $\text{CaNi}_3\text{P}_4\text{O}_{14}$



Exchange Interactions

Inelastic neutron scattering



□ Strong interchain interactions

$$H = J_1 \sum_i (\vec{S}_i \cdot \vec{S}_{i+1}) + J_2 \sum_i (\vec{S}_i \cdot \vec{S}_{i+1}) \quad \text{Intra chain}$$

$$+ J_3 \sum_{ij} (\vec{S}_i \cdot \vec{S}_j) \quad \text{Inter chain}$$

$$+ \sum_i D(S_i^z)^2 \quad \text{anisotropy}$$

| Exchange interaction (meV) | Neutron scattering |
|-------------------------------|-------------------------------|
| J_1 | -1.30 ± 0.05 (ferro) |
| J_2 | -1.05 ± 0.05 (ferro) |
| J_3 | 0.9 ± 0.1 (anti-ferro) |
| D | -0.25 ± 0.02 |

A. K. Bera, S. M. Yusuf *et al.* Phys. Rev. B 97, 224413 (2018)

Main Contributors

A. K. Bera

C. Ritter

Thank you