Spectrum of the S-1/2, XXZ Antiferromagnet from Zero to High Longitudinal Magnetic Field

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Outline

Spin-1/2 Antiferromagnet

Heisenberg and Ising limits

Spinons and bound modes

$SrCo_2V_2O_8$ – XXZ Heisenberg-Ising chain

Free spinons $T>T_N$

bound spinons $T<T_N$

theoretical models

$SrCo_2V_2O_8$ – in Longitubinal Magnetic Field

B, T phase diagram

Bethe string states

Bethe Ansatz calculations

Neutron observation of Bethe strings

comparison to theory

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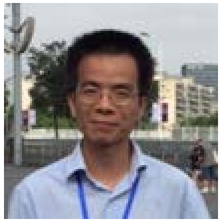

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Spin-1/2 AFM chains

$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)$$

$$H = J'\sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \Delta S_j^z S_{j+1}^z$$

$$J = J'\Delta \qquad \varepsilon = 1/\Delta$$

Spin-1/2, Heisenberg, Antiferromagnetic Chain

$$H_{AFM} = J\sum_j S_j S_{j+1} \qquad \varepsilon = 0 \quad \Delta\to\infty$$

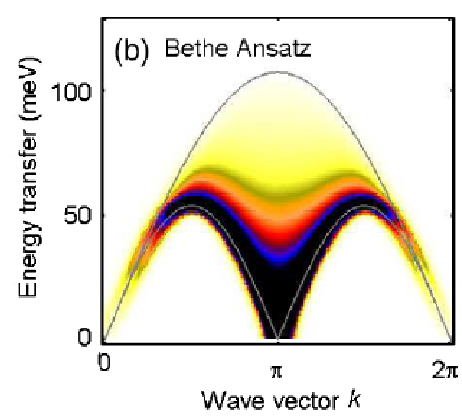
<u>Spinons</u>

- Fractional S-½ particles
- created in multipl pairs
- spinon-pair continuum

Hans Bethe, (1931)
No long-range order

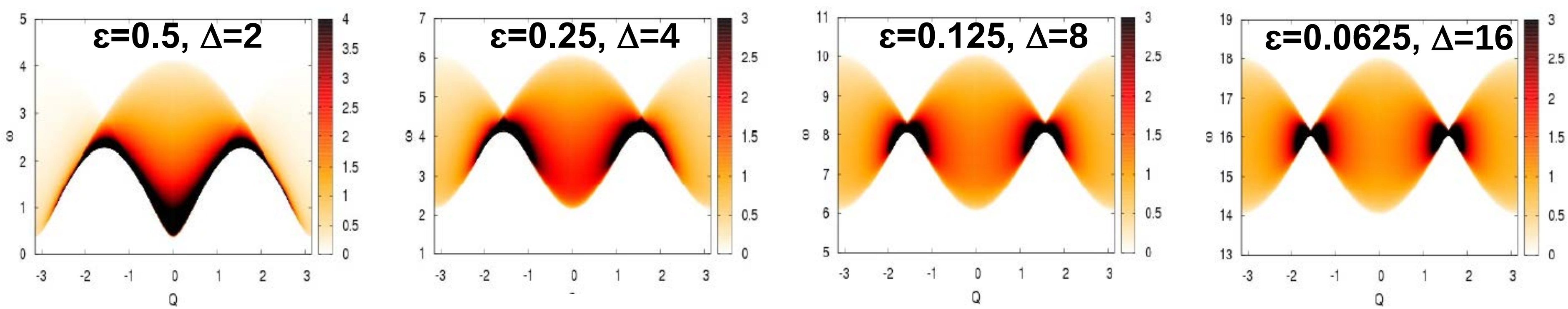
Fadeev & Taktajan (1981)
Spinon Excitations

J.-S. Caux, R. Hagemans, J. M. Maillet (2006) Spectrum



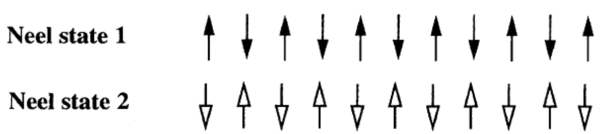
$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)$$

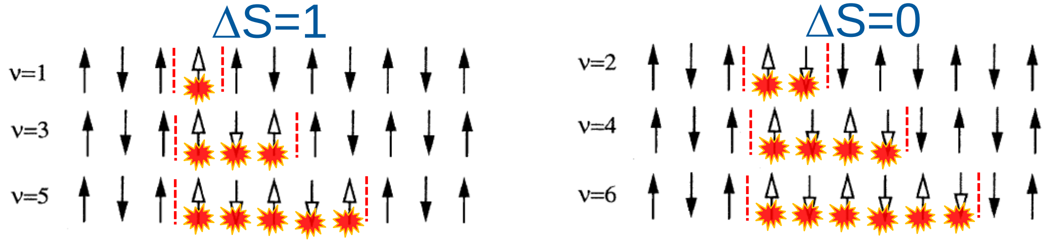
J..S. Caux J. Mossel, I. P. Castillo, (2008).
Spinon Continuum, Ising to Heisenberg 0<ε<1



doubly degenerate ground state

highly degenerate first excited states.





B. Lake; KITP, Oct 2019

Spin-1/2 Heisenberg Antiferromagnetic Chain

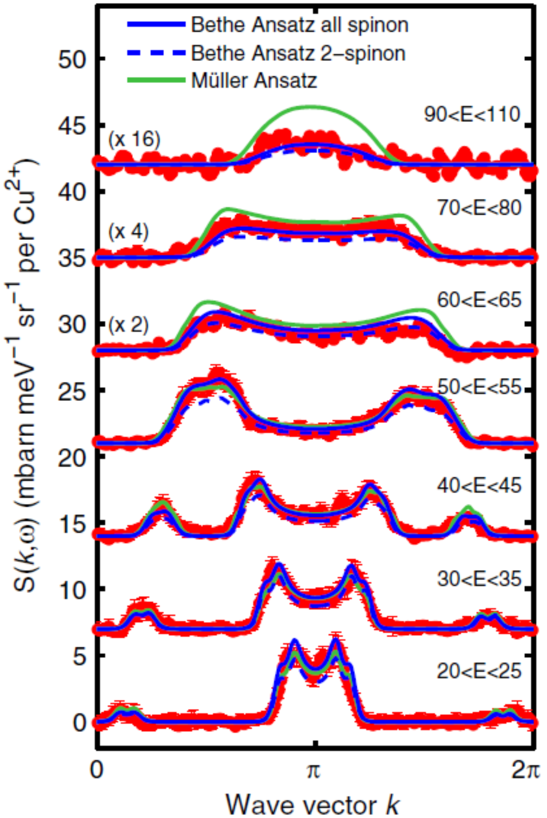
Heisenberg limit (ε = 1)

$$H = J\sum_j S_j S_{j+1}$$

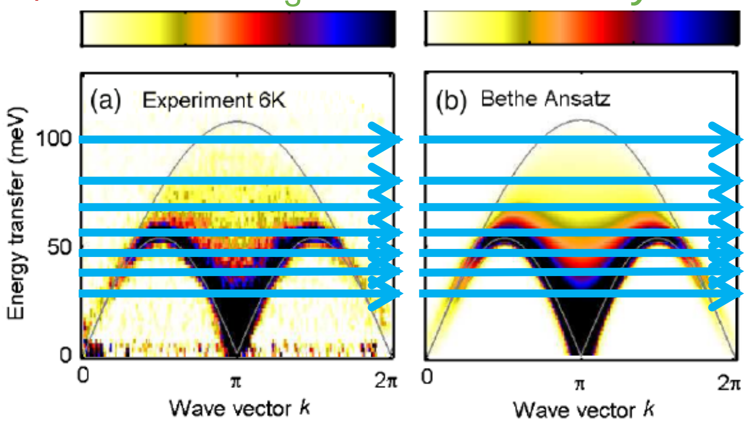
Gapless Spinon continuum

J.-S. Caux, R. Hagemans, J. M. Maillet (2006)

Comparison to theories

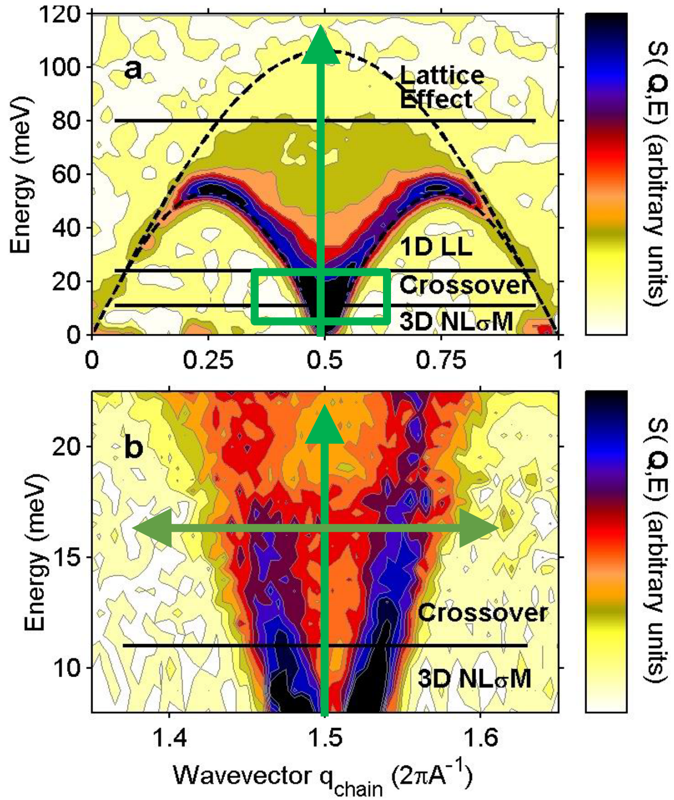


MAPS, ISIS $KCuF_3$ T=6K Theory



B. Lake et al, Phys. Rev. Lett. (2013)

Spin-1/2 Heisenberg Antiferromagnetic Chain



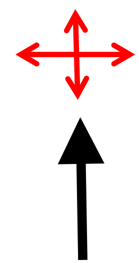
Free spinon excitations

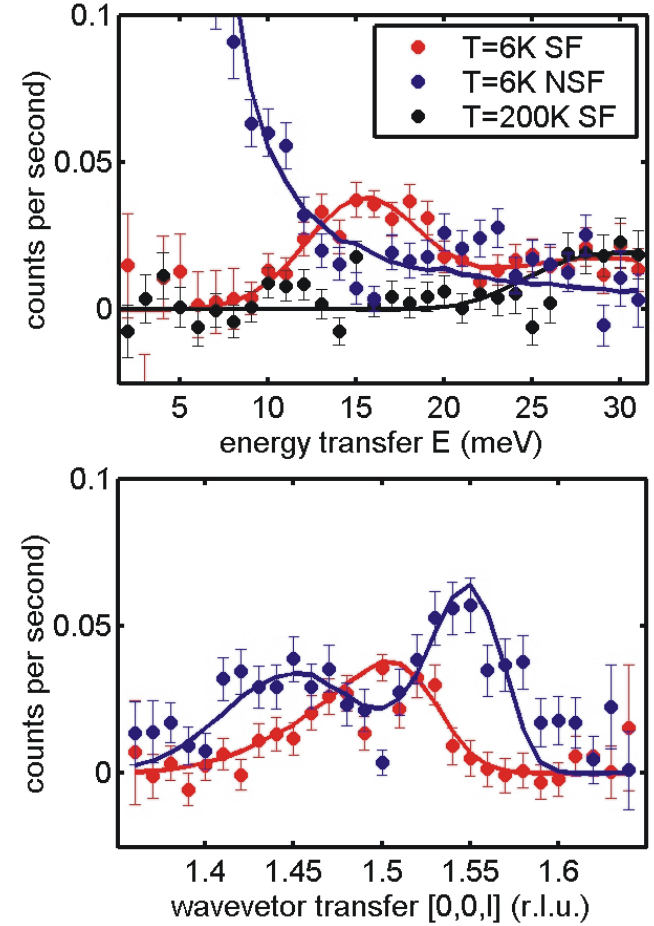
$$H = J\sum_j S_{j,r}.S_{j+1,r}$$

$$-h^z\sum_j (-1)^j S_j^z$$

T_N=39K

Polarisation analysis





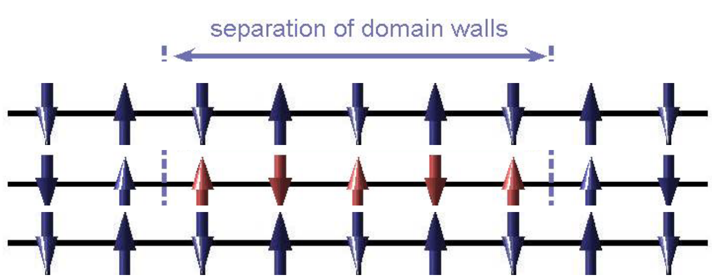
Gapless transervse S^{xx} spin-waves

Gapped longitudinal S^{zz} Mode → binding of Spinons

B. Lake, D.A. Tennant, S.E. Nagler et al Phys. Rev. Lett. (2000)

F. H. L. Essler, A.M. Tsvelik, G. Delfino, Phys. Rev. B 56, 11 001 (1997).

Spinons confined by interchain coupling



Longitudinal Mode,

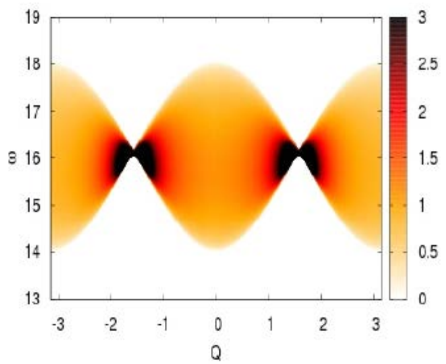
- **Observed in S^{zz}**
- **Broad, finite lifetime**

Spin-1/2 Ising Antiferromagnet Chain

$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) - h^z \sum_j (-1)^j S_j^z$$

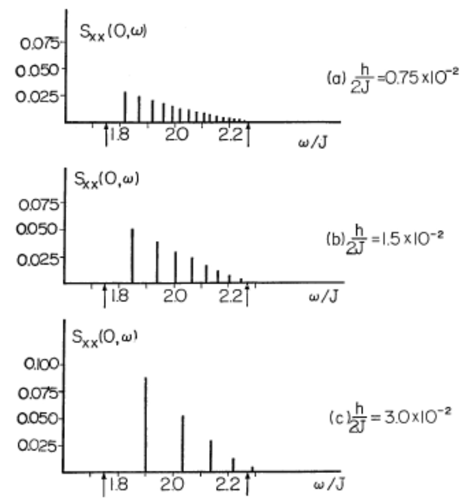
Strong Ising limit ε<<1

Free spinons/kinks

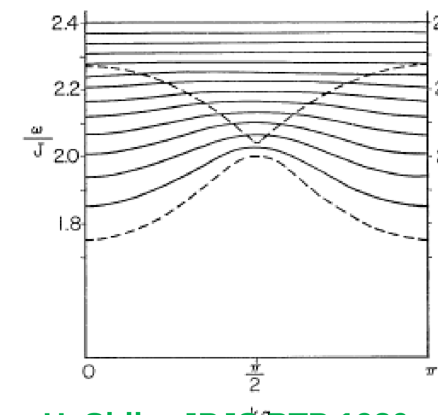


N. Ishimura, H. Shiba JPJS PTP 1980

J..S. Caux J. Mossel, I. P. Castillo, Stat Mech P08006 (2008).

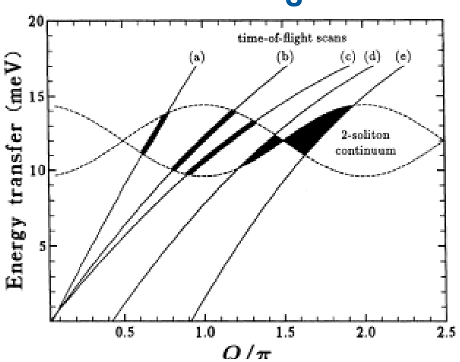


Bound spinons/kinks

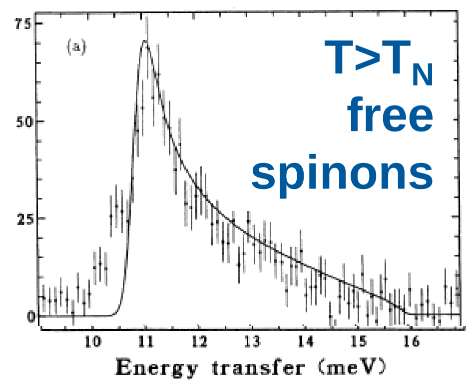


H. Shiba JPJS PTP 1980

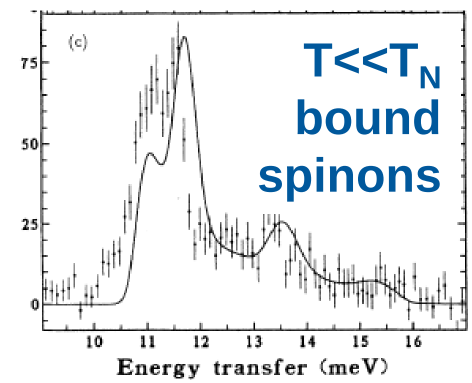
$CsCoCl_3$



J.P. Goff, D.A. Tennant, S.E. Nagler PRB 52 15992 (1995)



$T>T_N$ free spinons



$T<<T_N$ bound spinons

Transverse bound modes, S^{xx}, Sharp, long lifetime

$SrCo_2V_2O_8$
XXZ Spin-1/2 AFM chain

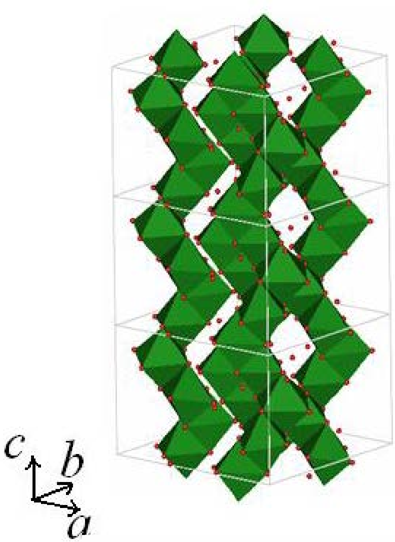
$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)$$

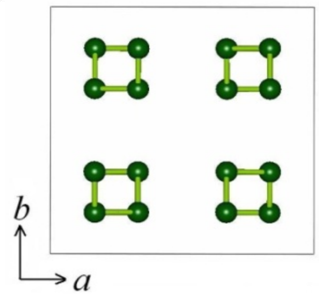
$$H = J'\sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \Delta S_j^z S_{j+1}^z$$

$$\Delta = 2 \qquad \varepsilon = 1/2$$

$SrCo_2V_2O_8$ - Quasi-1D XXZ spin-1/2 Antiferromagnetic

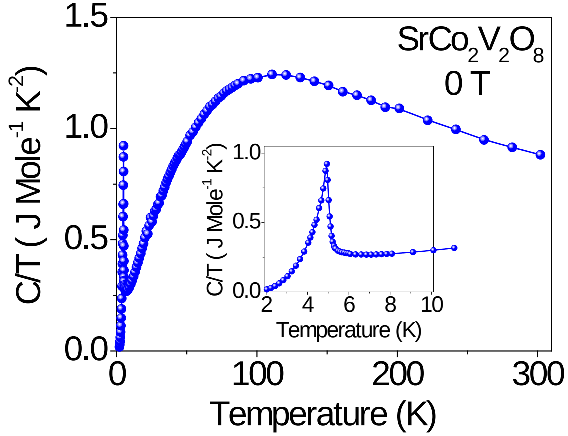
$SrCo_2V_2O_8$



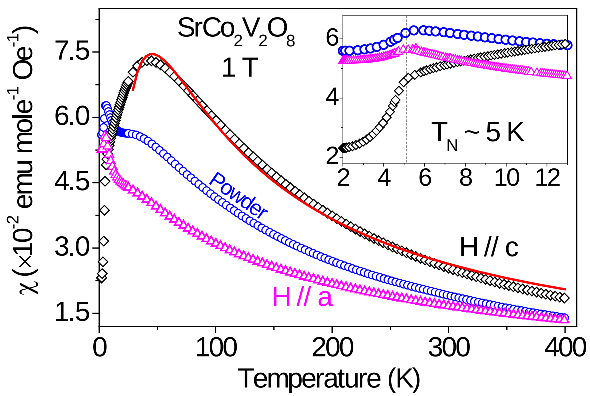


Half-integer spin-chain
Co^{2+}; $3d^7$, effective S=1/2
Kramer doublet - anisotropy

Specific heat

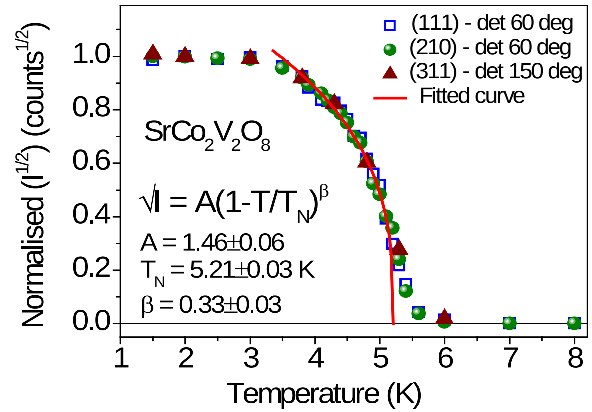


Susceptibility

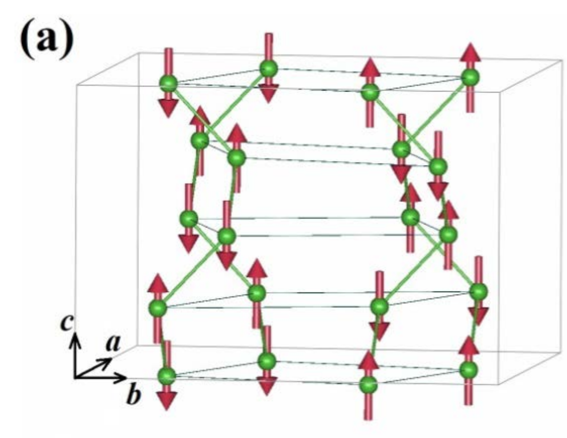


A. K. Bera, B. Lake *et. al.*,
Phys. Rev. B 89, 094402 (2014)

Neutron diffraction



M ∞ $(1-T/T_N)^\beta$ β=0.33
Ising Universality Class



Spin-1/2 screw chains along c axis.

AFM order below T_N= 5.2K
Anisotropic magnetism

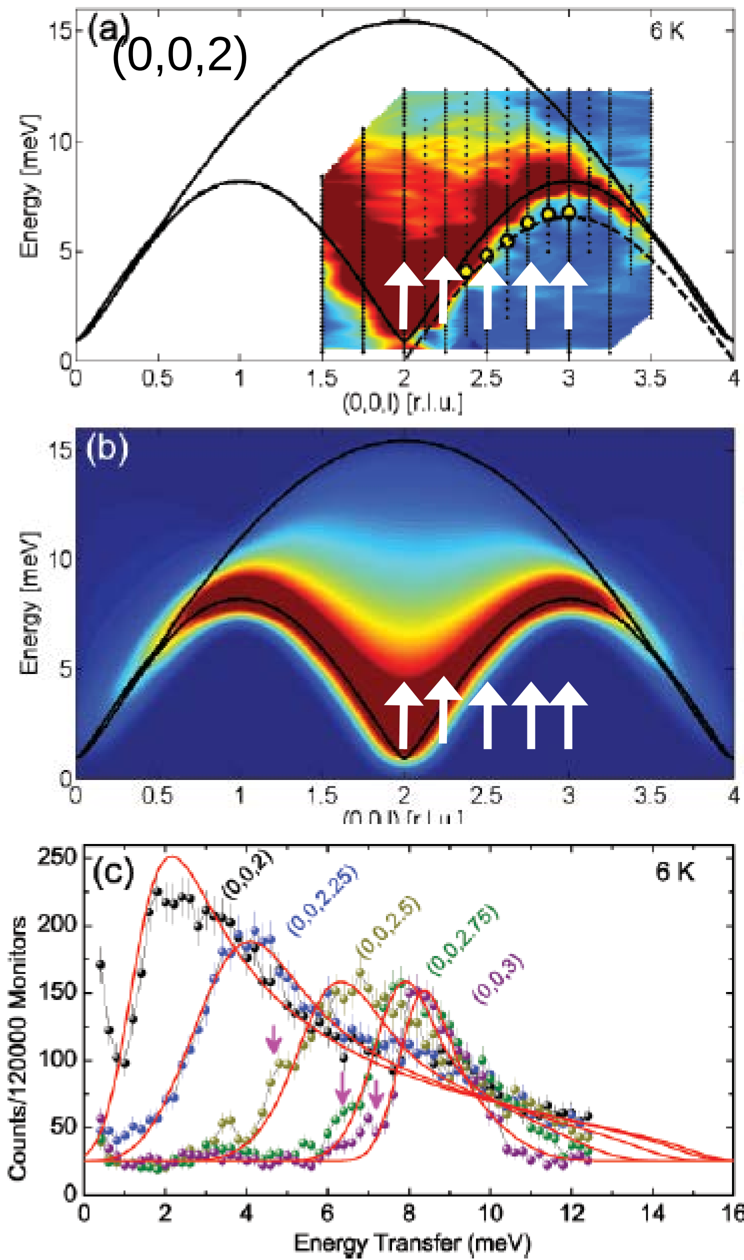
Ising universality class
Spins point along c axis

Magnetic excitations of $SrCo_2V_2O_8$ for $T>T_N$

Experiment at $T=6K > T_N=5.2$ K

- Spinon continuum
  - free spinons
- Energy gap, $\Delta \sim 1.5$ meV
  - XXZ anisotropy
- Dispersions up to 14.5 meV

A. K. Bera, *et al. Phys. Rev. B 96, 054423 (2017)*



Theory at T=0K

J..S. Caux J. Mossel, I. P. Castillo, J. Stat Mech P08006 (2008).

H. Bougourzi, M. Karbach, G. Müller, PRB 57, 11429(1998).

Fitted values

- $J=7$ meV
- $\varepsilon=0.56$

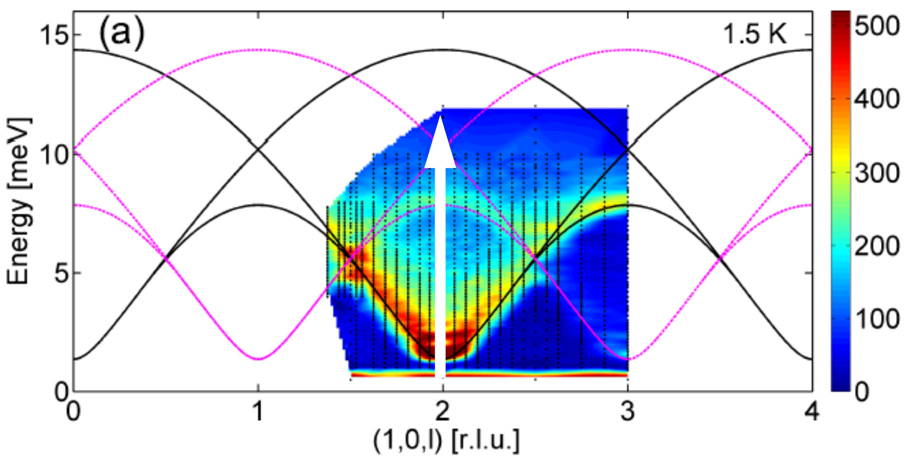
Or

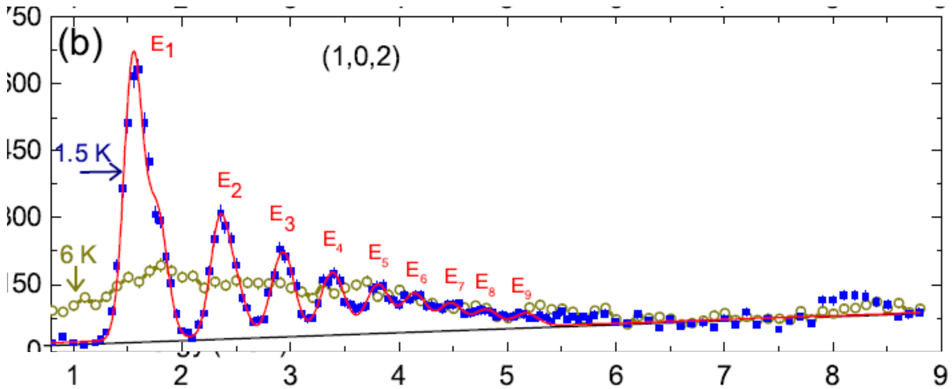
- $J=3.9$ meV
- $\Delta=1.8$

$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)$$

$$H = J'\sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \Delta S_j^z S_{j+1}^z$$

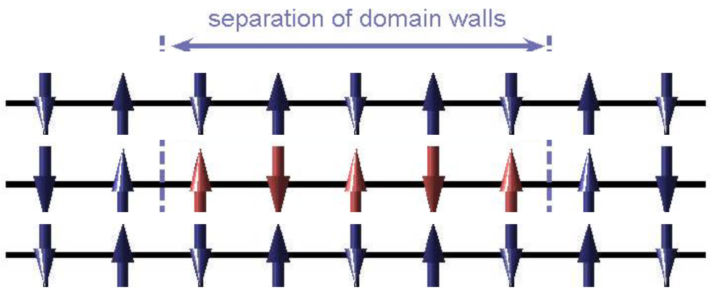
Magnetic excitations of $SrCo_2V_2O_8$ for $T<T_N$ – Spinon Confinement



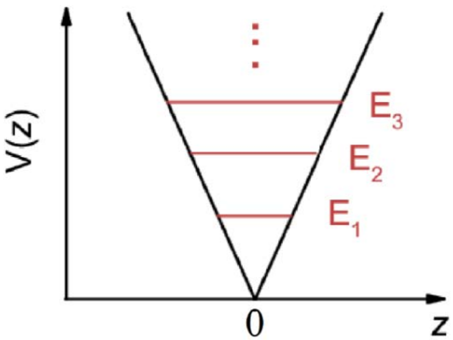


A. K. Bera, B. Lake Phys Rev B 96 054423 (2017)

- Hierarchy of discrete excited states



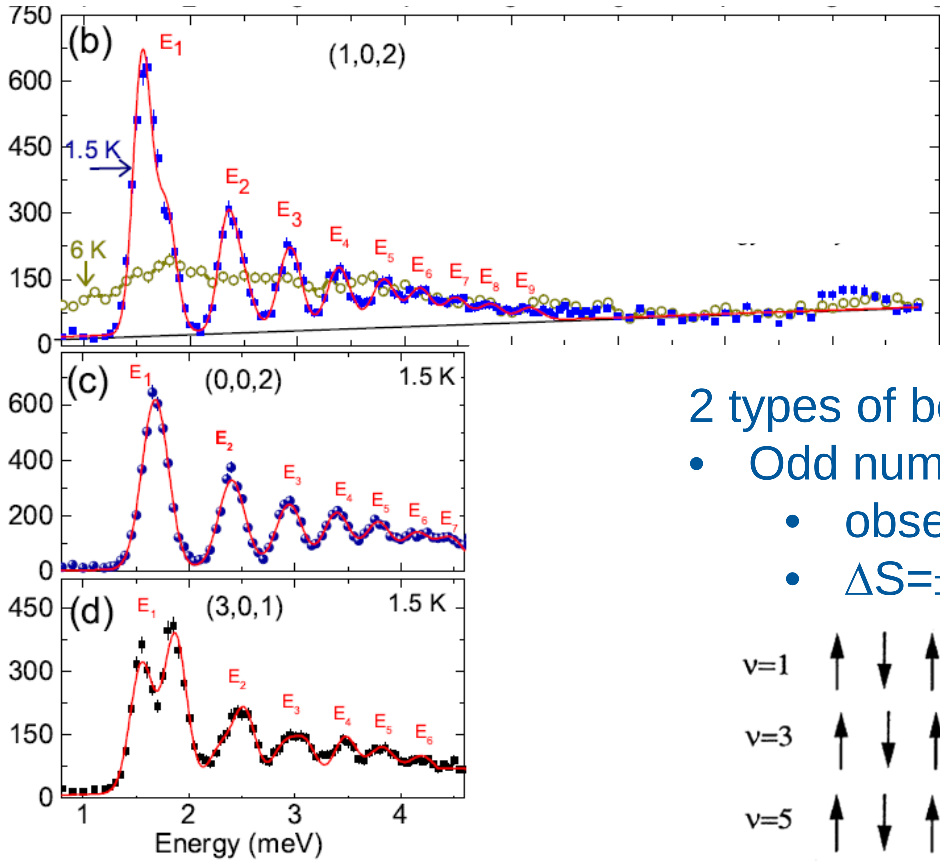
$$H_{AFM} = J \sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right)$$



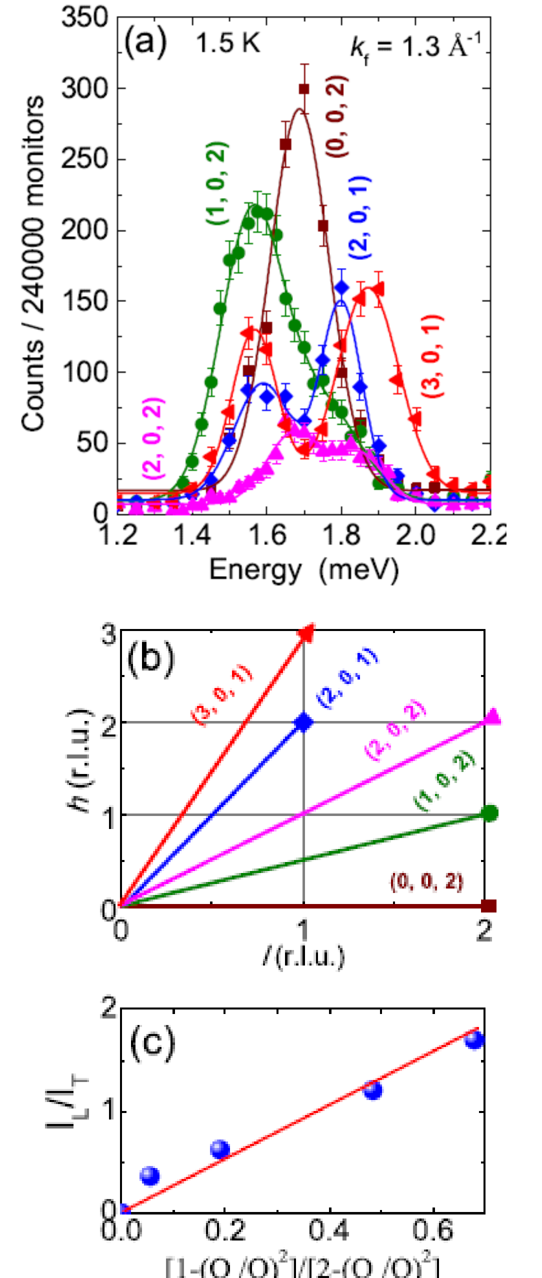
- Confinement of pairs of spinons.
- String potential due to interchain coupling.

B. Lake; KITP, Oct 2019

Magnetic excitations of $SrCo_2V_2O_8$ for $T<T_N$ – Spinon Confinement

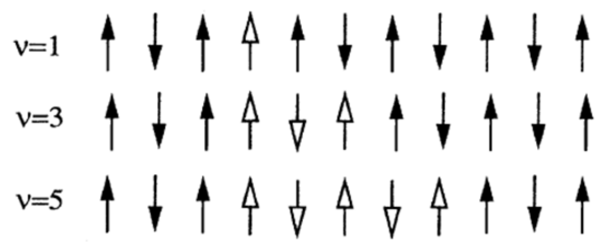


Transverse
&
Longitudinal
excitations

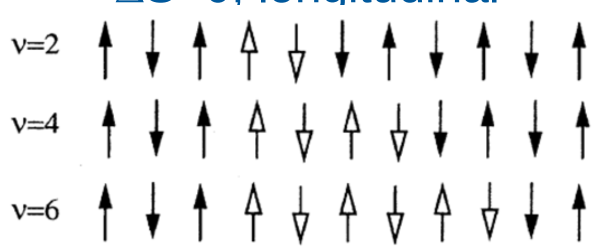


2 types of bound spinons

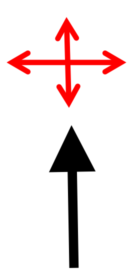
- Odd number of spin flips
  - observed in S^{xx} and S^{yy}
  - $\Delta S=\pm 1$, transverse



- Even number of spin flips
  - observed in S^{zz}
  - $\Delta S=0$, longitudinal



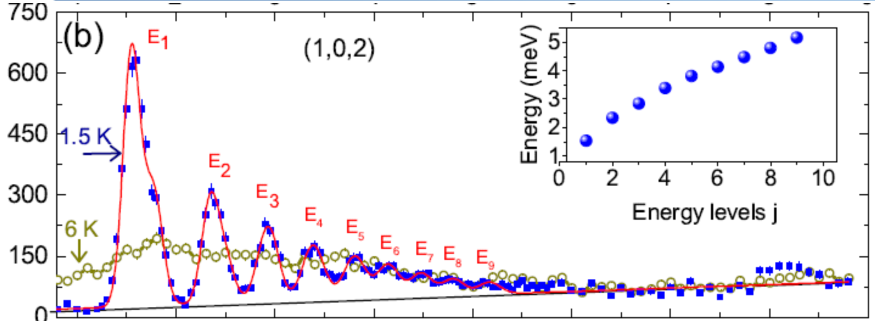
longitudinal

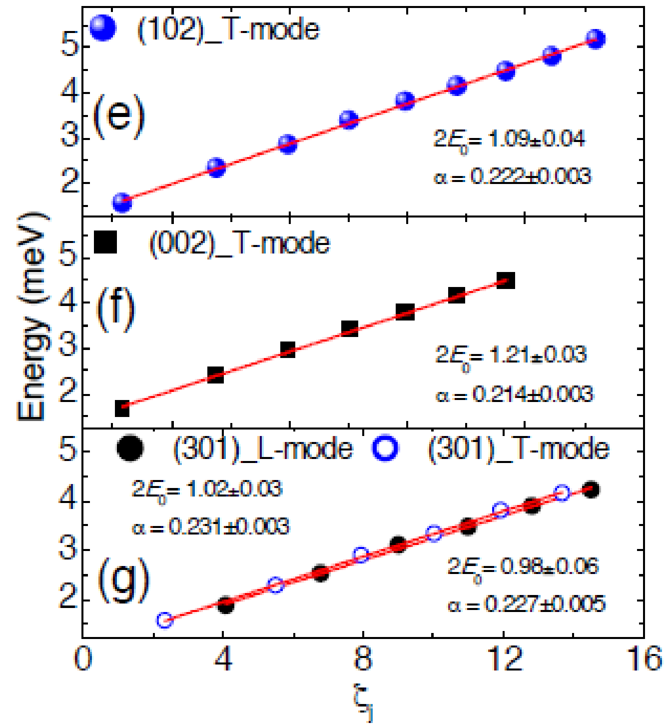


transverse

B. Lake; KITP, Oct 2019

$SrCo_2V_2O_8$ XXZ, S-1/2 1D AFM – $T>T_N$ Confined Spinons





1D Schrödinger equation with linear potential

$$-\frac{\hbar^2}{\mu}\frac{d^2\varphi}{dz^2} + \lambda|z|\varphi = (E - 2E_0)\varphi,$$

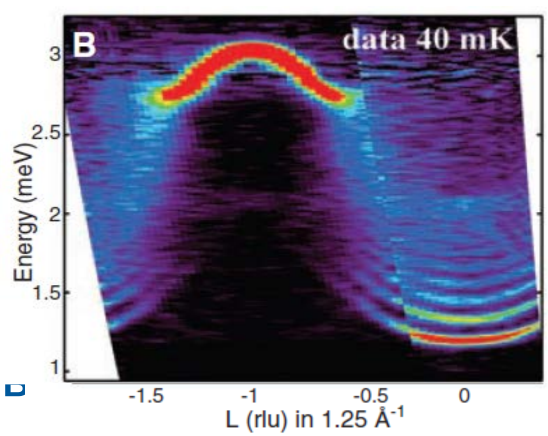
Solution: –ve zeros of the Airy function

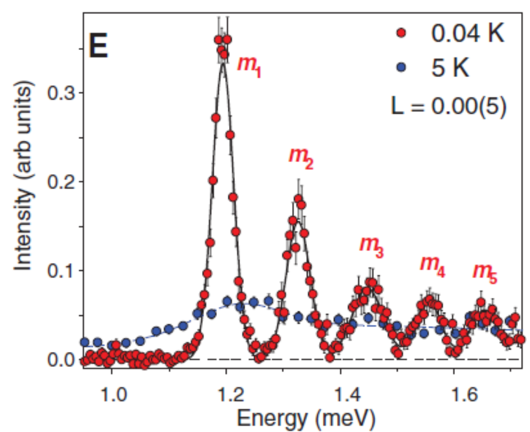
$$E_j = 2E_0 + \alpha\zeta_j \qquad j = 1, 2, 3, ...,$$

$$Ai(-\zeta_j) = 0, \quad \zeta_j = 2.338, 4.088, 5.520,$$

Similar results from $BaCo_2V_2O_8$

Spin-1/2 XXZ *Ferromagnetic* Chain – $CoNb_2O_6$





R. Coldea D.A.Tennant et al science

Bound states only observed in the *transverse* structure factor

S^{xx} & S^{yy} not S^{zz}

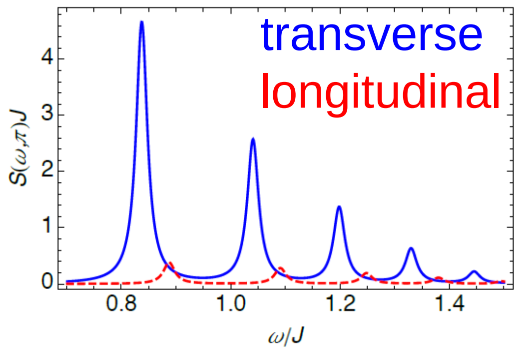
Theoretical Methods

Perturbation theory

strong Ising limit ε=0.2, h=0.05

Strong transverse, weak longitudinal

F.H.L. Essler;

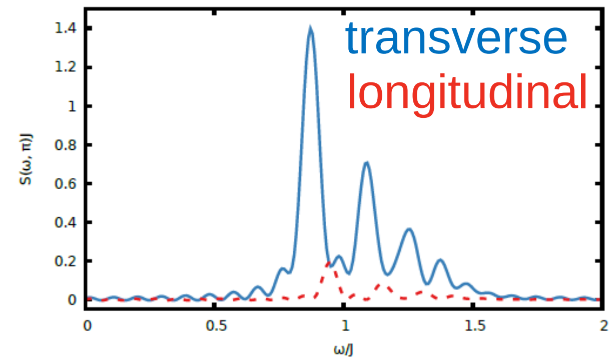


DMRG

strong Ising limit ε=0.2, h=0.05

Strong transverse, weak longitudinal

C. Hubig, U. Schollwöck

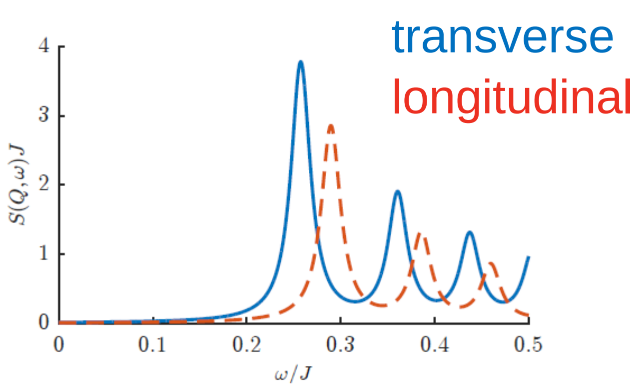


Tangent Space Matrix Product Space Method

Intermediate XXZ region, ε=0.56, h=0.006

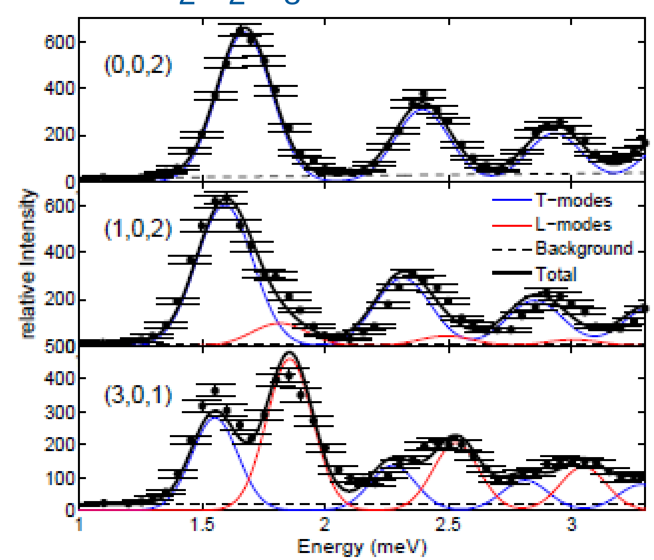
Similar strength Transverse & longitudinal

L. Vanderstraeten;



Comparison to data

$SrCo_2V_2O_8$ ε=0.56, h=0.006



B.

$SrCo_2V_2O_8$
in a Longitudinal Magnetic Field

$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) - g\,\mu_B \sum_i S_i^z B$$

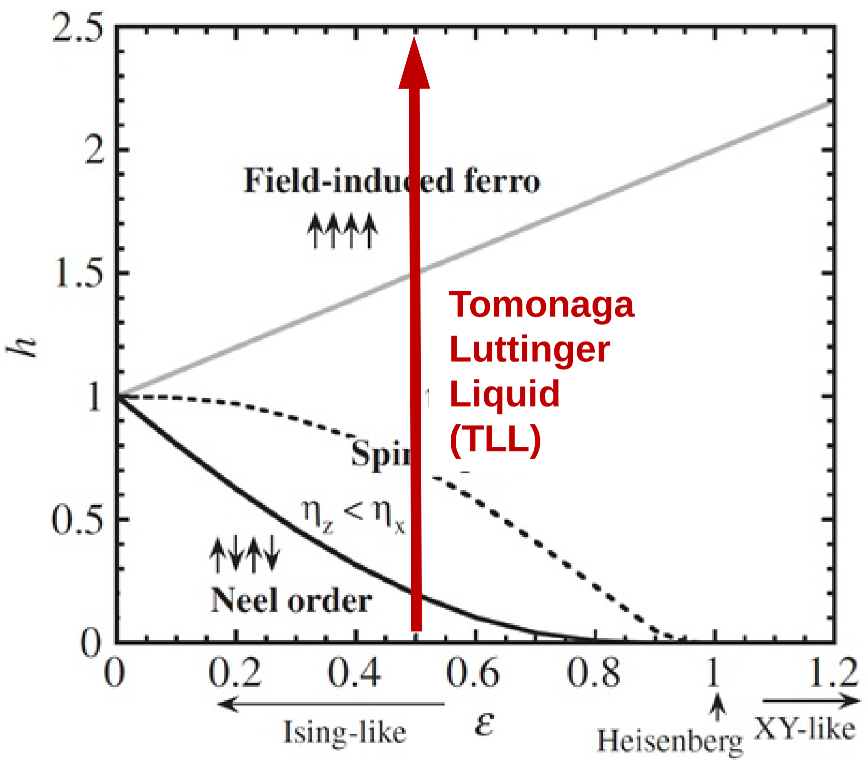
$$H = J'\sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \Delta S_j^z S_{j+1}^z - g\,\mu_B \sum_i S_i^z B$$

$$\Delta = 2 \qquad \varepsilon = 1/2$$

Spin-1/2 XXZ AFM Chain in a Longitudinal Magnetic Field

$$H = J\sum_j S_j^z S_{j+1}^z + \varepsilon\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) - g\,\mu_B \sum_i S_i^z B$$

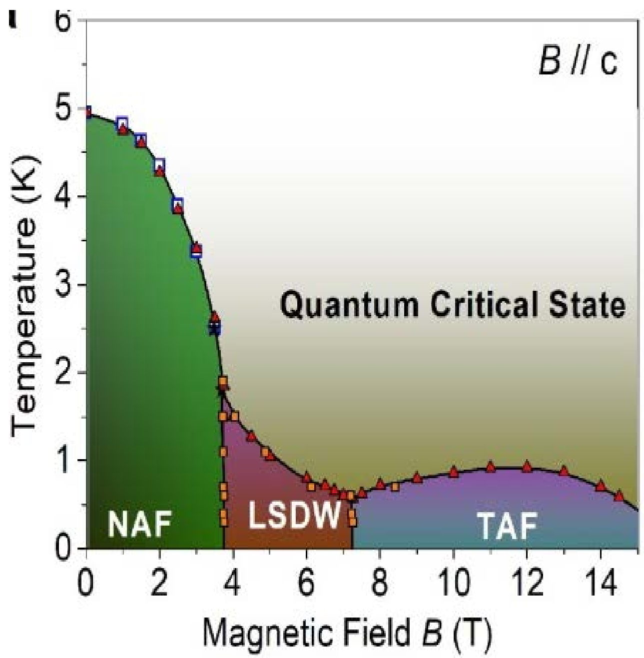
$$H = J'\sum_j \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + \Delta S_j^z S_{j+1}^z - g\,\mu_B \sum_i S_i^z B$$

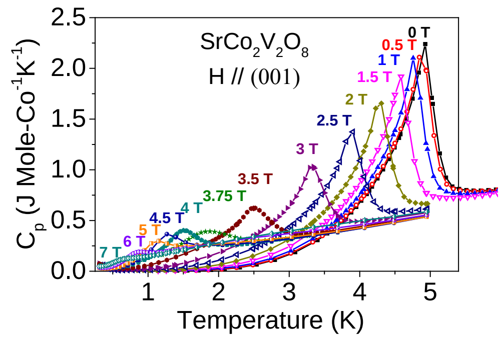


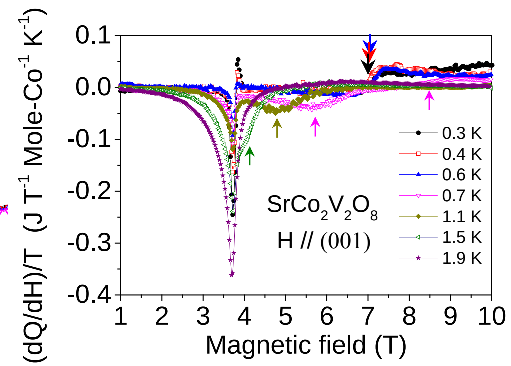
Ising-like (ε < 1; Δ > 1):

- Field induced quantum critical behavior
- Incommensurate longitudinal spin component
- Staggered transverse component

Phase diagram for $SrCo_2V_2O_8$ in a Longitudinal Field







2 Field-induced phase transitions.

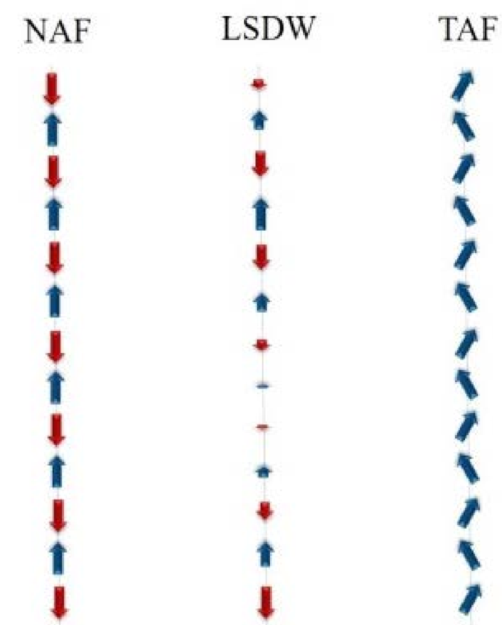
B_{c1} = 3.7 T: B_{c2} = 7.2 T:

NAF: $B < B_{c1}$

LSDW: $B_{c1} < B < B_{c2}$

TAF: $B_{c2} < B < B_s$

Long-range magnetic order is strongly suppressed above B_{c1}

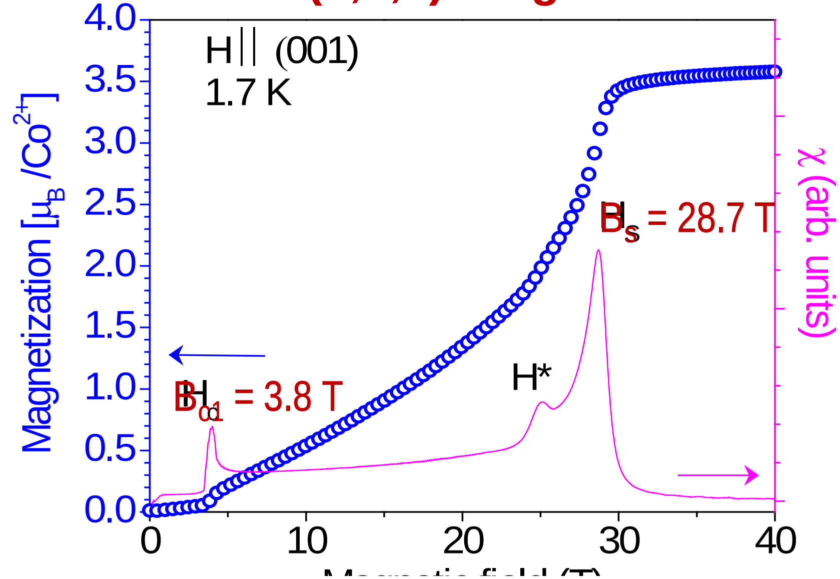


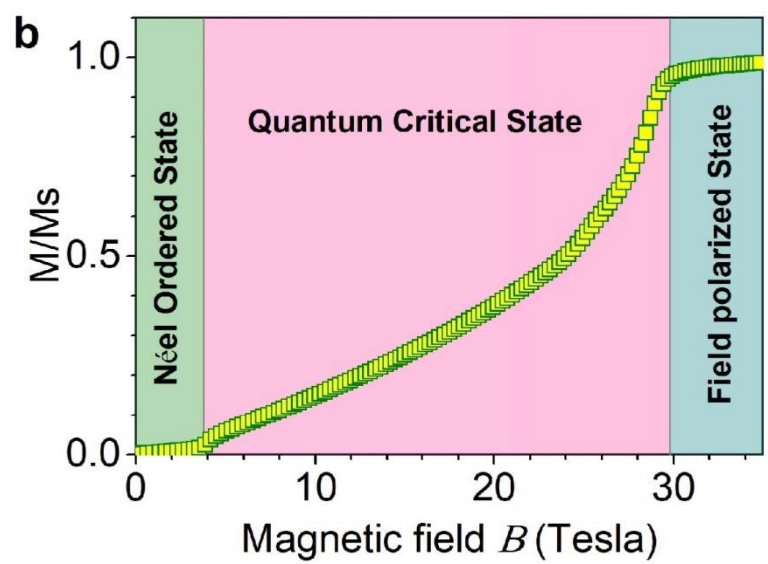
Phase diagram for $SrCo_2V_2O_8$ in a Longitudinal Field

Longitudinal field

- Field induced QPT at *B*=3.8T to quantum critical Tomonaga Luttinger Liquid.
- Non-linear magnetization indicates strong quantum fluctuations
- Saturation at Bs=28.7 T

H//(0,0,1) longitudinal





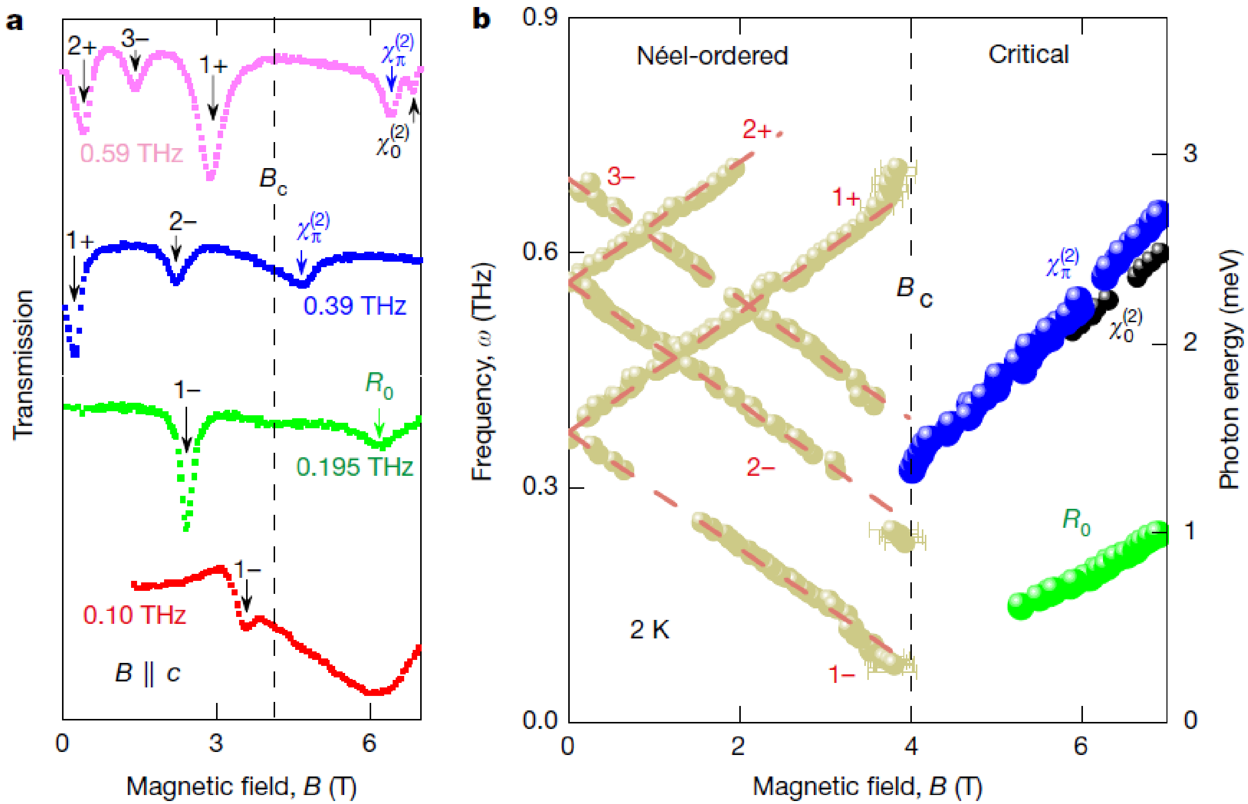
Excitations of $SrCo_2V_2O_8$ in a small longitudinal field

Terahertz Optical Spectroscopy

Field-dependent spectrum at Q = 0, π/2, π; 3 π/2

Transverse excitations only

Zhe Wang, Jianda Wu, Wang Yang et al
Nature 554 221 (2019)



B < B_{c1} Zeeman splitting of the the bound spinons

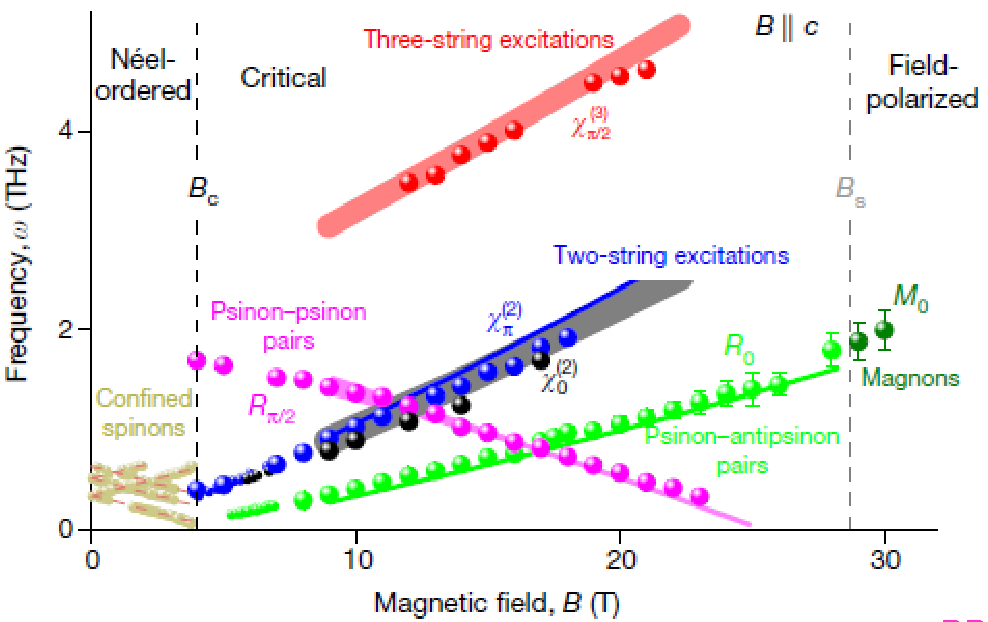
B = B_{c1} Lowest E excitation goes into the ground state

B > B_{c1} Complete change in the spectrum

Excitations of $SrCo_2V_2O_8$ in a high longitudinal field

Terahertz Optical Spectroscopy for B > Bc1

Field-dependent spectrum at Q = 0, π/2, π
Transverse excitations only



New excitations observed for B > B_{c1} identified by comparison to Bethe Ansatz

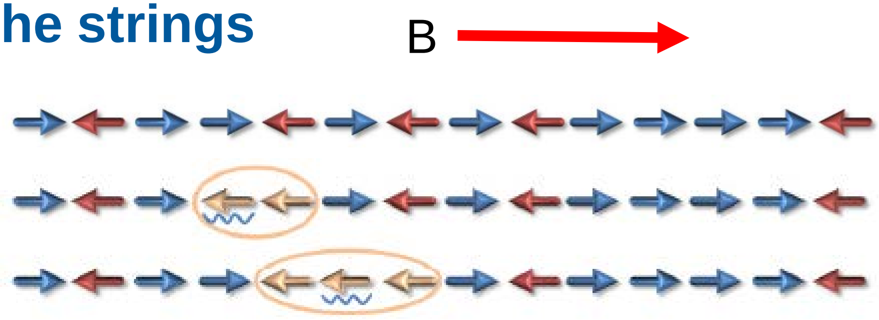
Zhe Wang, Jianda Wu, Wang Yang et al
Nature 554 221 (2019)

R^{PP} psinon-psinon pair
R^{PAP} psinon-antipsinon pair
$\chi^{(2)}$ 2-string Bethe
$\chi^{(3)}$ 3-string Bethe
n-string = addition of n bound magnons (spins pointing against the field)

First observation of Bethe strings

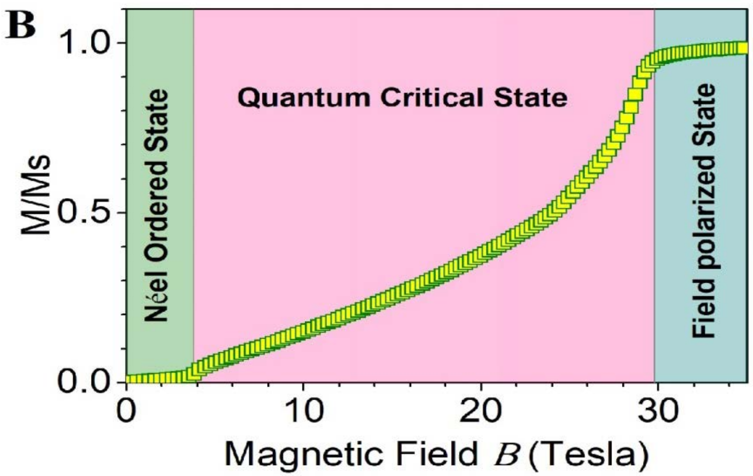
Bethe Strings

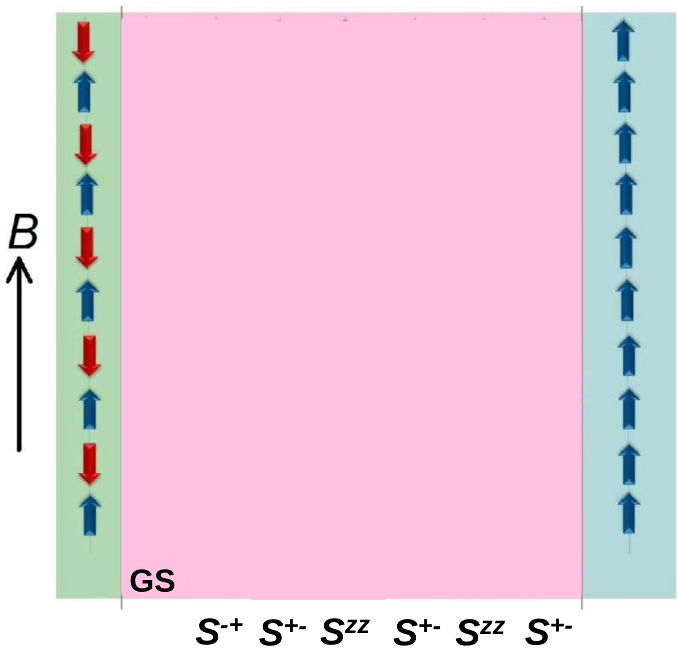
History of Bethe strings



- A sequence of flipped spins or magnons bound together within the strongly correlated background of single spin flips
- 2-string state first predicted for Heisenberg chain in zero field by Hans Bethe in 1931
- Multi-string states later predicted by several theorists stabilized by anisotropy
- Not observed due to their weak signal dominated by the spinon spectrum.
- Observeable for XXZ chain in a longitudinal magnetic field which separates them from the other excitations

Theory for S-1/2 1D XXZ AFM in longitudinal Field

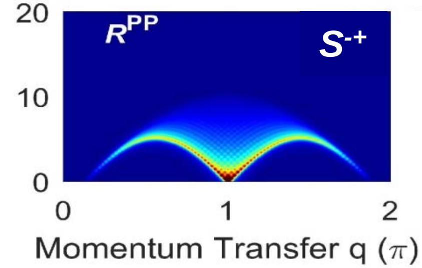




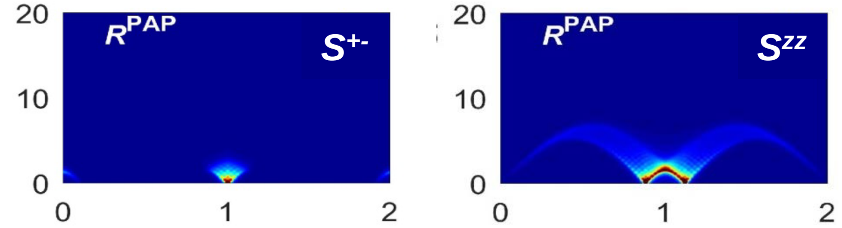
Bethe Ansatz
Jianda. Wu,
Wang Yang

- J=3.9 meV
- Δ=1.8
- 2m=0.12

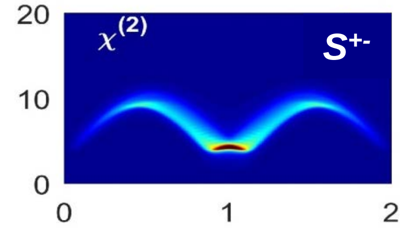
Psinon-psinon pair



Psinon-antipsinon pair



2-magnon Bethe String

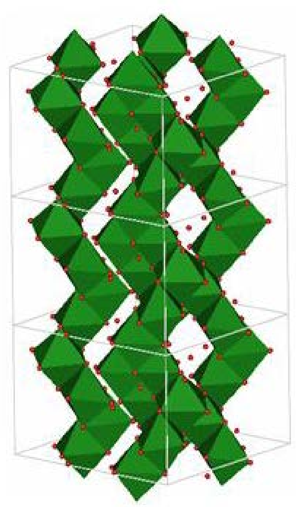


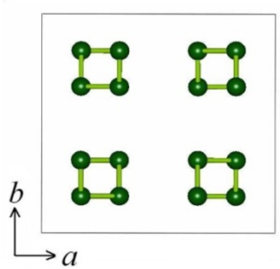
3-magnon Bethe String

B

Dispersions of Psinon, Anti-Psinon & Bethe Strings

$SrCo_2V_2O_8$

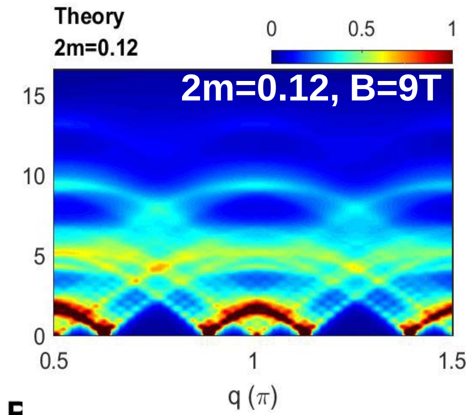




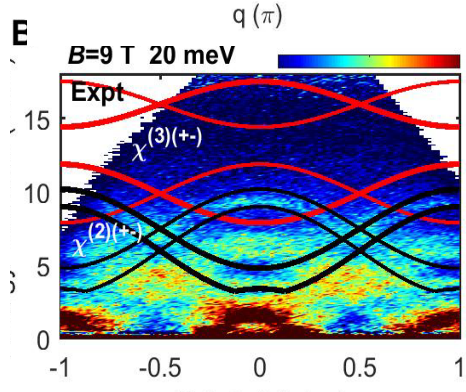
4-fold screw chain

$\Rightarrow$

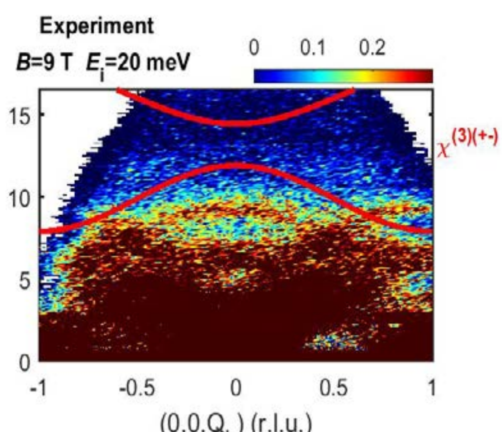
Zone folding



Theory

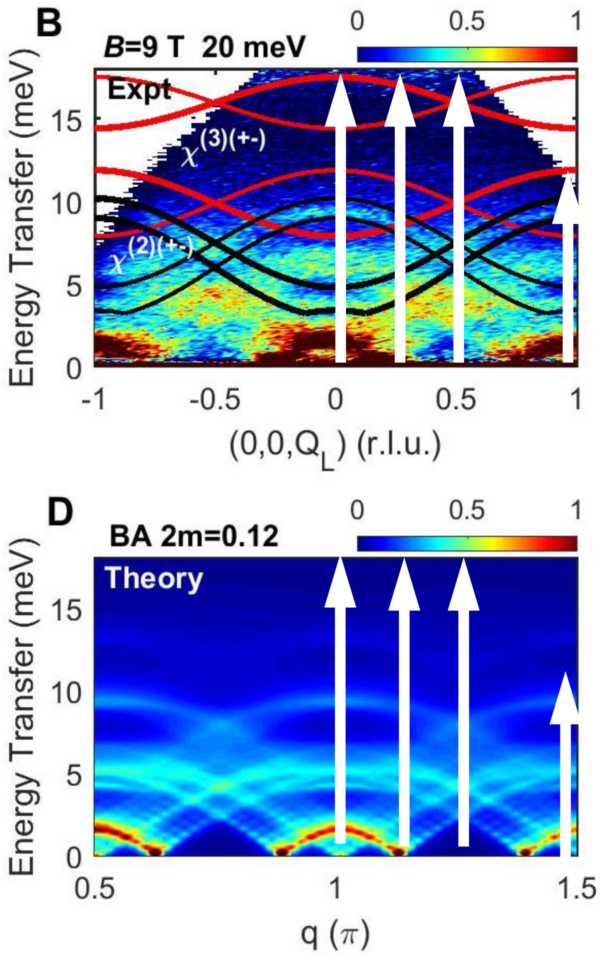


Experiment

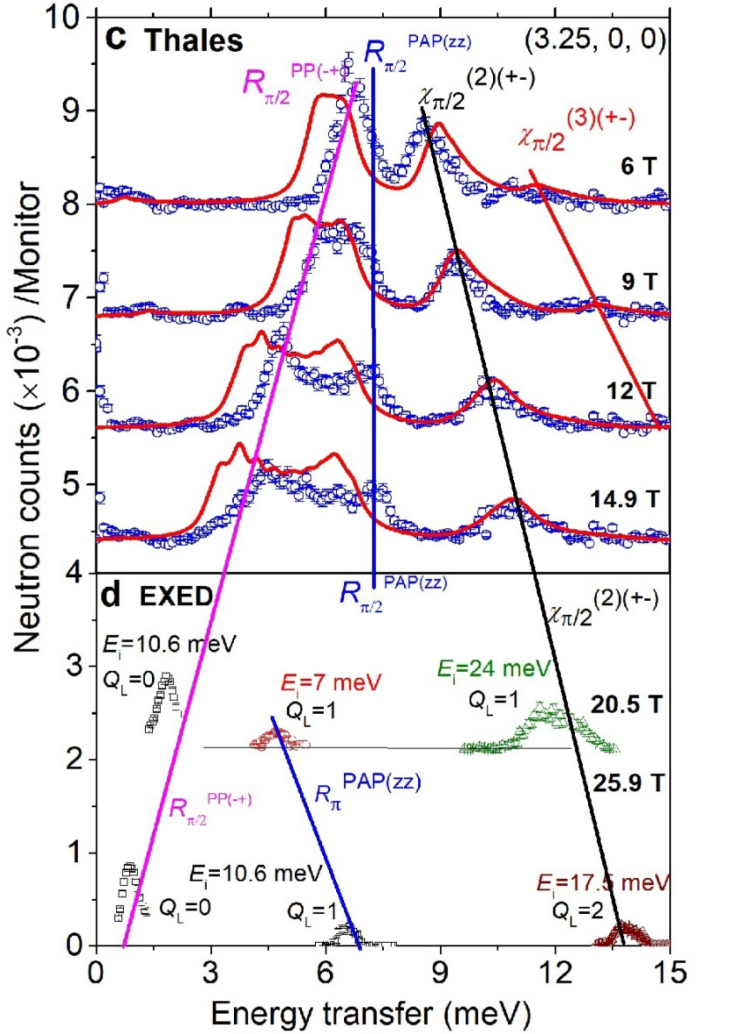


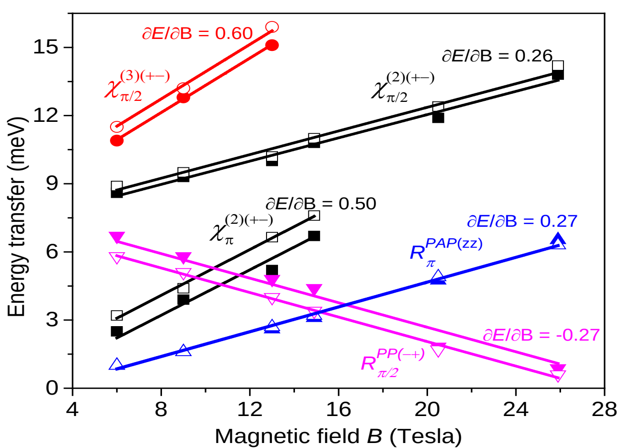
Dispersions of Psinon, Anti-Psinon & Bethe Strings

Detailed comparison to Bethe Ansatz



Field-Dependence of Psinon, Anti-Psinon & Bethe Strings





Good agreement between experiment and theory for the field dependence and intensity

B. Lake; K

Summary

Spin-1/2 Antiferromagnet

Heisenberg and Ising limits
Spinons and bound modes

$SrCo_2V_2O_8$ – XXZ Heisenberg-Ising chain

Free spinons $T>T_N$
bound spinons $T<T_N$
theoretical comparison

$SrCo_2V_2O_8$ – in Longitubinal Magnetic Field

B, T phase diagram
Bethe string states -terahertz
Bethe Ansatz calculations
Neutron observation of Bethe strings
Agreement for dispersion, field, intensities,