Symmetry, topology, and magnets: Neutrons with a twist

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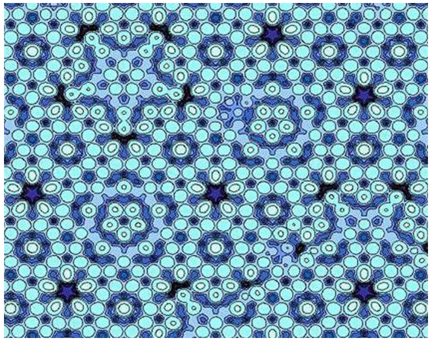
Symmetry is familiar but topology is also important

Topology is a global property

Remarkable properties can emerge

Hidden order

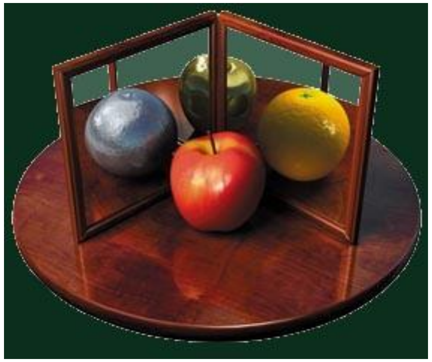


Quasicrystals

Topological states in nature

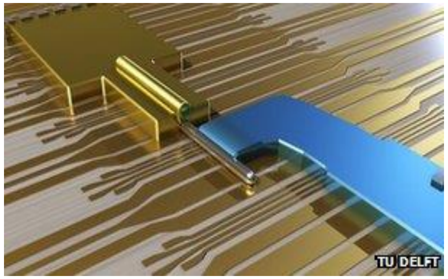
Vortex is a familiar topological state

Symmetry in particle physics



Supersymmetry implies relationships between the fundamental building blocks

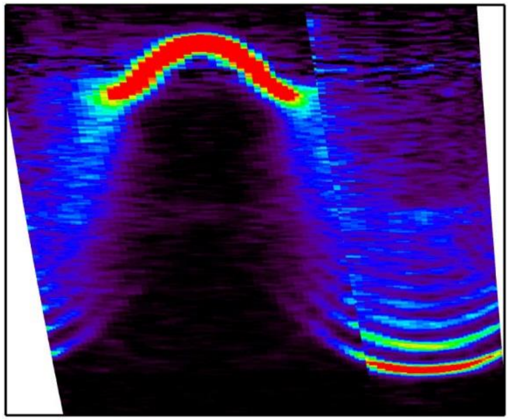
Applying topological quantum states



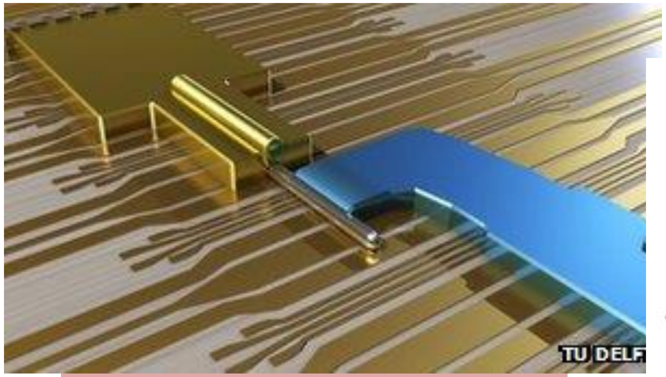
Topological quantum computer

Oak Ridge National Laboratory

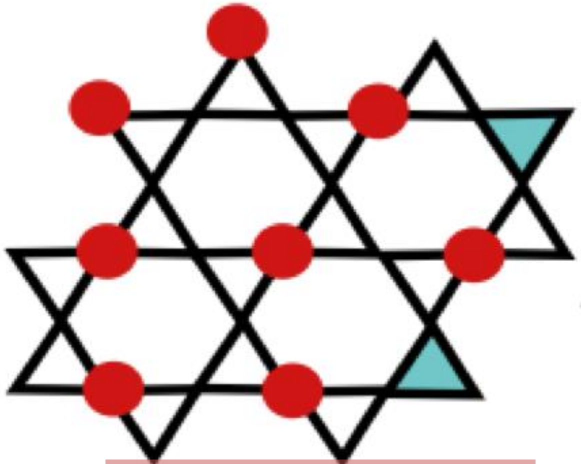
Unexpected symmetries and topologies govern the remarkable properties in quantum materials



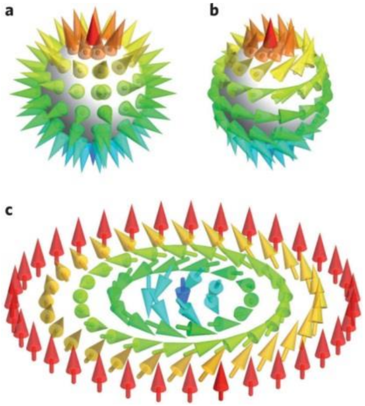
Quantum Matter



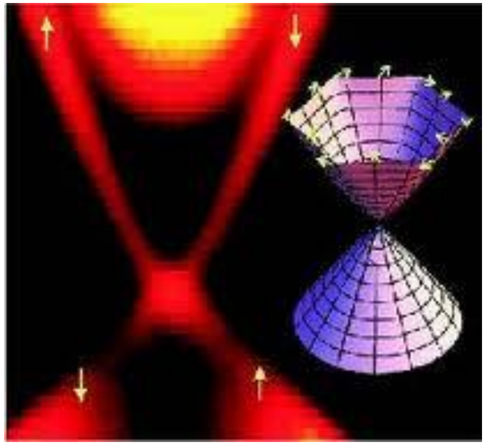
Topological quantum computing



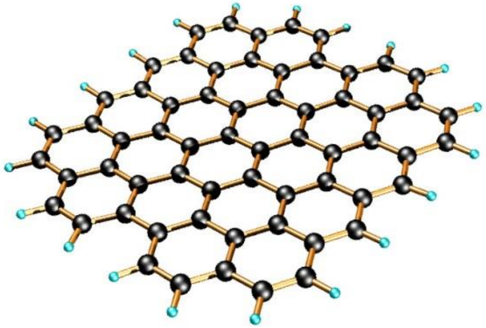
Fractional states



Knots and skyrmions

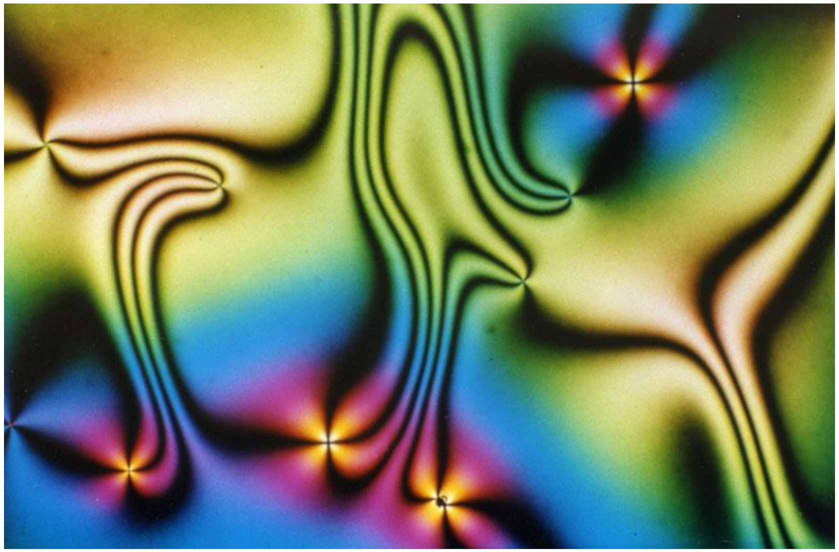


Topological insulators and iridates

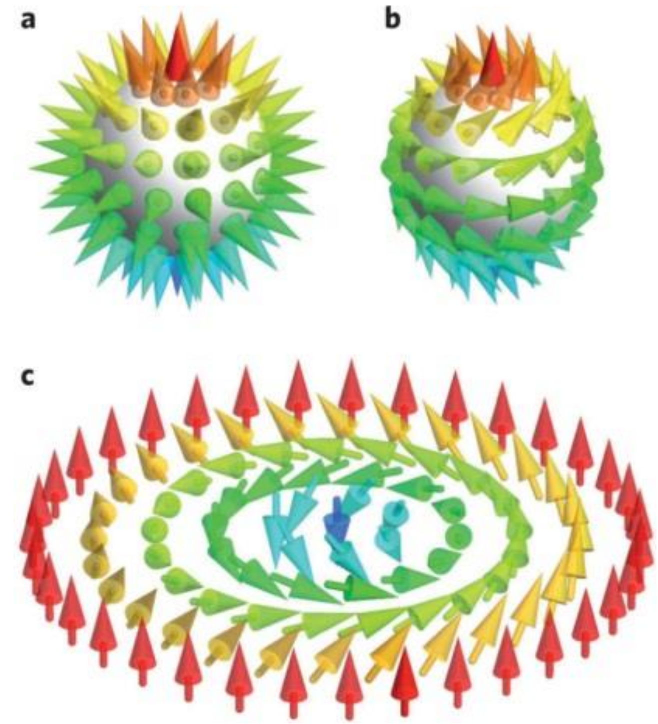


Low dimensional systems

Stable particles can carry energy or information, these are knots or twists

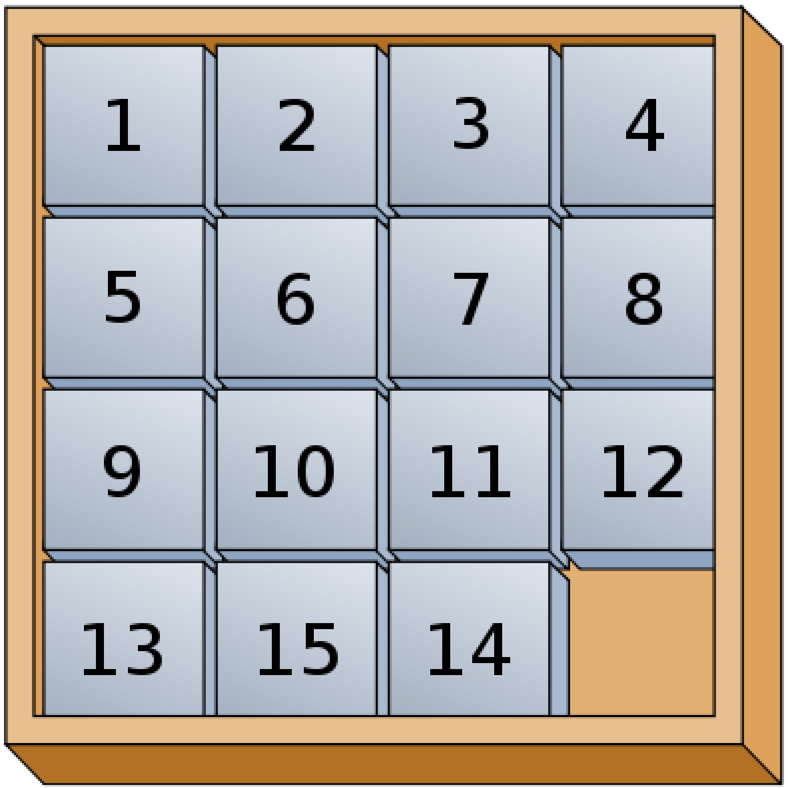


Defects in local ordering of liquid crystals that
can‘t be simply unknotted



Anisotropies
stabilise textures and defects in magnets

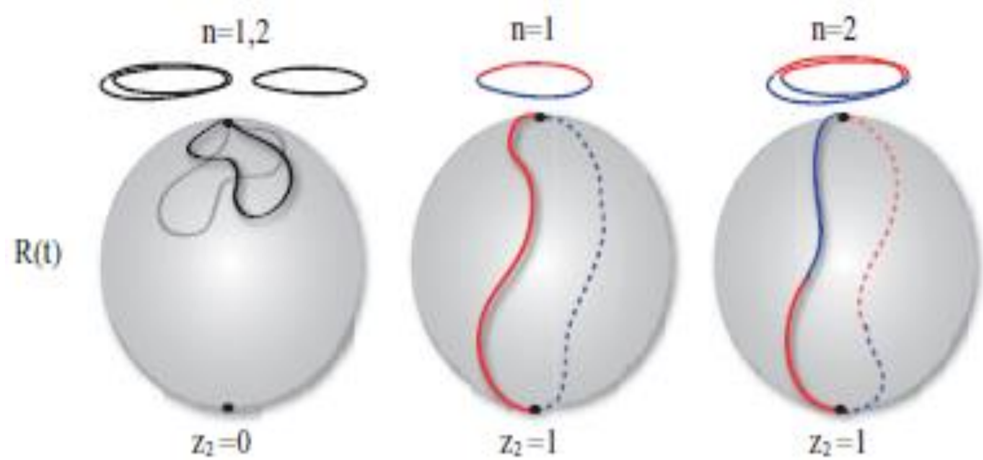
We are searching for new stable particles that can carry energy, information, etc…



•Puzzle 15 is split into sectors

These can carry fractional quantum numbers

- Anderson's RVB state
- Fractional quantum Hall effect



•Berry's phases

This talk covers some pretty exotic behavior in some very simple physical systems

1D Transverse Ising Model

- kinks as defects

Quantum critical resonances

- emergent E8 symmetry

General behavior of quantum wires

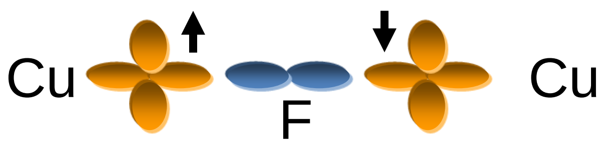
How to get defects in higer dimensions :

- spin ice
- monopoles in 3D

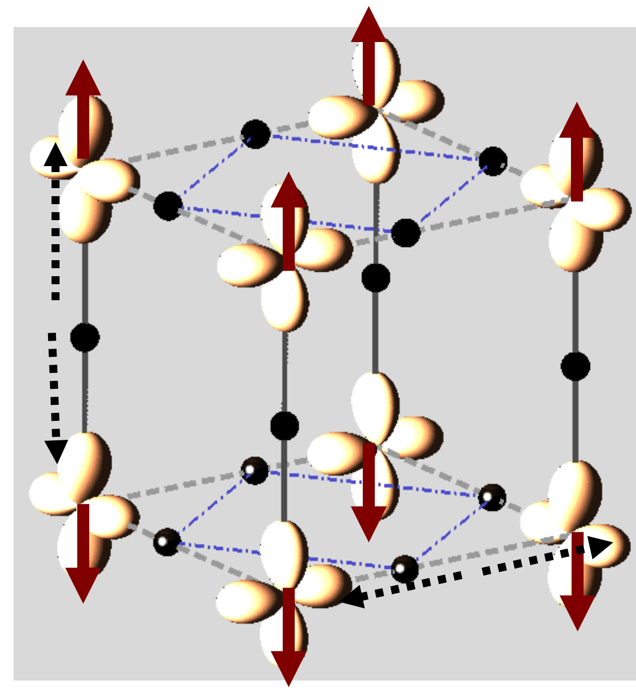
Opportunities to look at well defined quantum systems are rare : Magnets are pristine systems for basic research

Magnetic insulators

antiferromagnetic
Superexchange through diamagnetic space



Magnetism originates on the unpaired electrons in solids

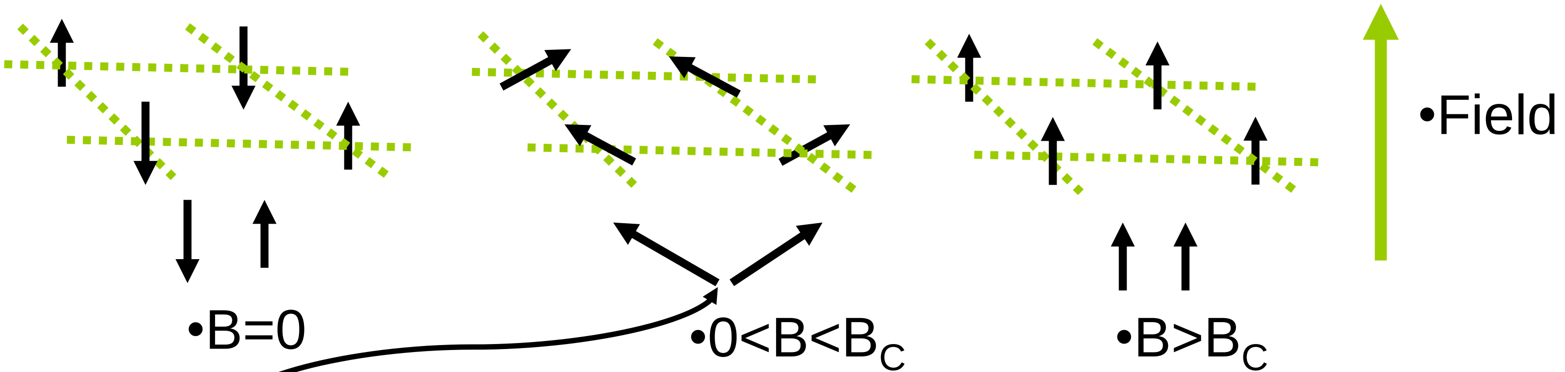


Magnetism originates on the unpaired electrons in solids

$$H=\sum_{<ij>}[J_{ij}^{z}S_i^{z}S_i^{z}+J_{ij}^{xy}\left(S_i^{x}S_j^{x}+S_i^{y}S_i^{y}\right)]+g\mu_B B\sum_i S_i^{z}$$

Magnets are simulators for many quantum systems

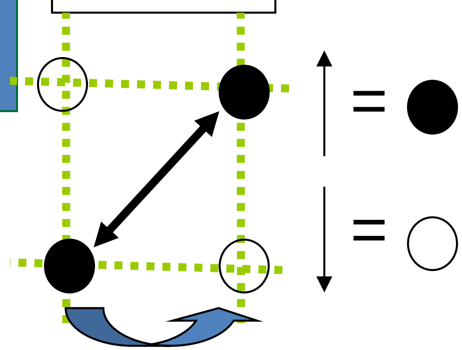
Magnetic insulators : e.g. spin-1/2 2D antiferromagnet maps onto interacting quantum gas on a lattice



spin flop phase has ODLRO

$$< a_i^+ a_j > \propto < S_i^x S_j^x > + < S_i^y S_j^y >$$

$$V_{ij} = J_{ij}^z$$



$$t_{ij} = J_{ij}^z / 2$$

chemical potential

$$\eta = -g\mu_B B + J_{ij}^z$$

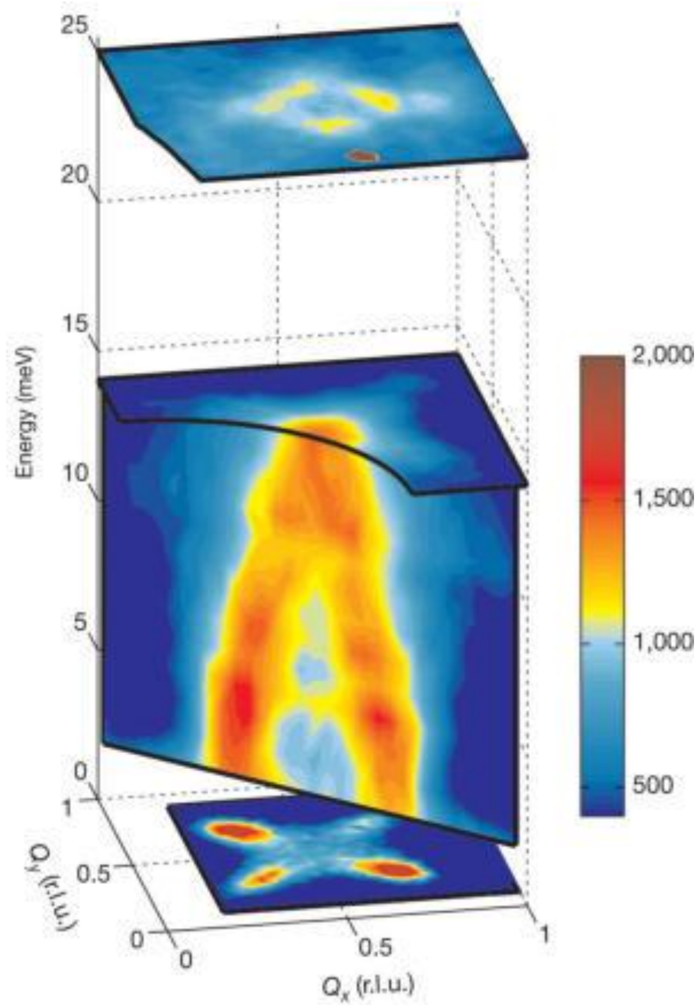
Particle density NS-<M>

$$S_i^z = 1/2 - a_i^+ a_i$$

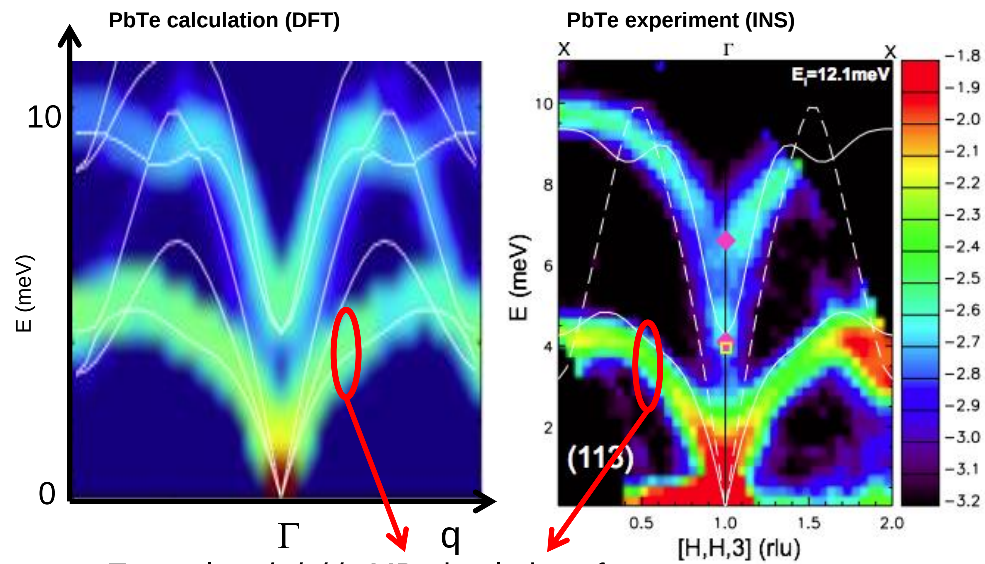
$$S_i^x = \frac{a_i^+ + a_i}{2}; S_i^y = \frac{i(a_i^+ + a_i)}{2}$$

$$S_i^+ = a_i^-; S_i^- = a_i^+$$

Neutrons are the most powerful probe of the energy levels and wavefunctions



Unconventional superconductor



•Example: *ab-initio* MD simulations for ferroelectrics/thermoelectrics. Focus on *width* of dispersions

Thermoelectric devices

A world leading neutron science center at ORNL

High Flux Isotope Reactor:

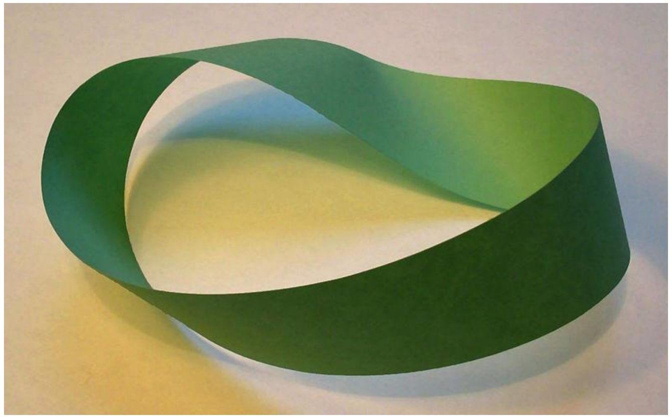
Intense steady-state neutron flux
and a high-brightness cold neutron source

Spallation Neutron Source:

World's most powerful
accelerator-based neutron source

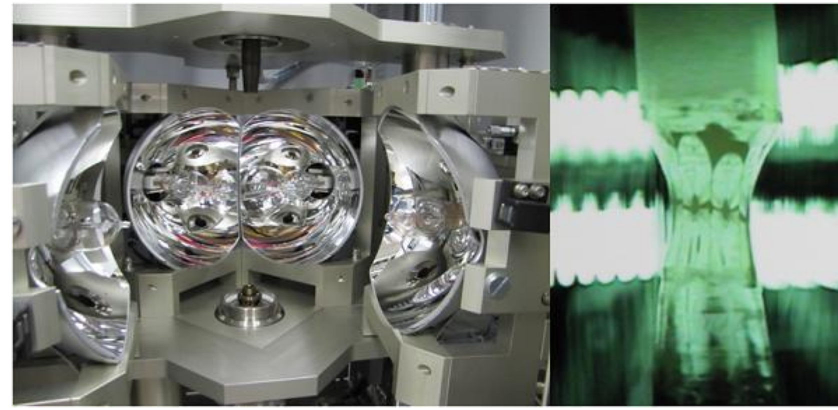
•U.S. Department of Energy investments have provided forefront capabilities

Kinks and quantum symmetries in 1D



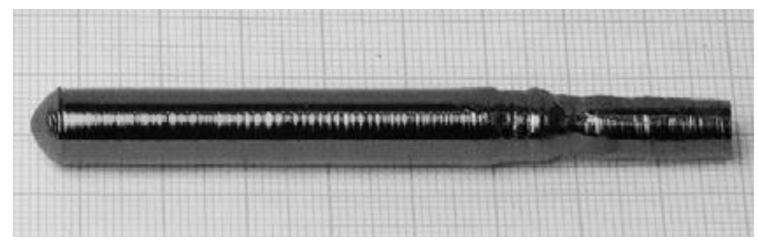
„Magnetic wires“ arise naturally in certain crystal structures

- Very high purity single crystals
- Ferromagnetic Ising chain



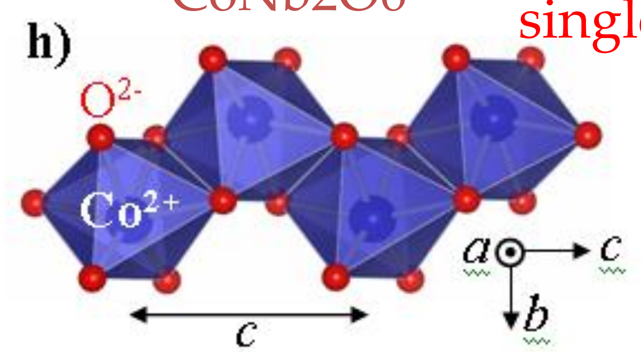
Grow crystals using light ovens

Thermodynamic and transport measurements



An 8cm long high purity single crystal of CoNb2O6

CoNb2O6



• Field along *b*

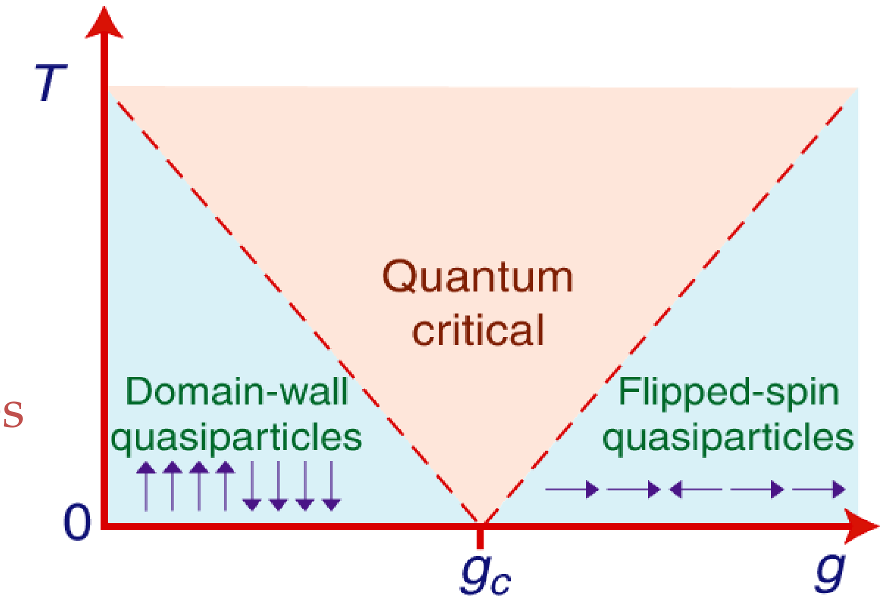
Theory of our wire is the famous Ising model in transverse field

$$H = J\sum_i S_i^z S_{i+1}^z + hS_i^x = J\sum S_i^z S_{i+1}^z + \frac{h}{2}\left(S_i^+ + S_i^-\right)$$

$$\cdots\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\cdots$$

$$\cdots\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\cdots$$

- Field h<hc
- Two ground states



- Excitations are pairs of kinks

$$\cdots\uparrow\uparrow\uparrow\uparrow\boxed{\downarrow}\uparrow\uparrow\uparrow\cdots$$

$$\cdots\uparrow\uparrow\uparrow\boxed{\downarrow\downarrow}\uparrow\uparrow\uparrow\cdots$$

$$\cdots\uparrow\uparrow\boxed{\downarrow\downarrow\downarrow}\uparrow\uparrow\uparrow\cdots$$

- Field h>hc
- One ground state

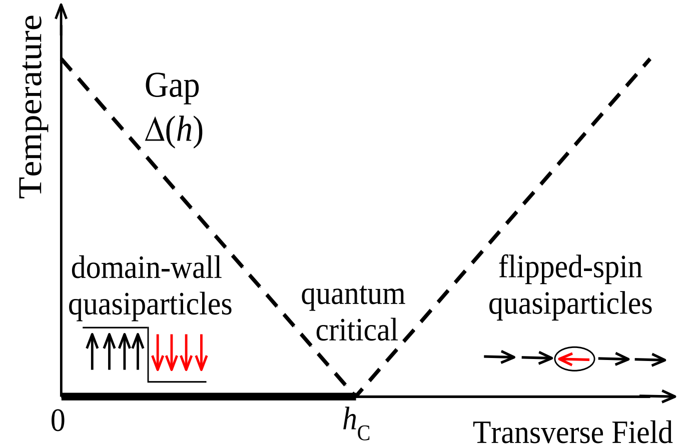
$$\cdots\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\cdots$$

- Excitation is spin flip

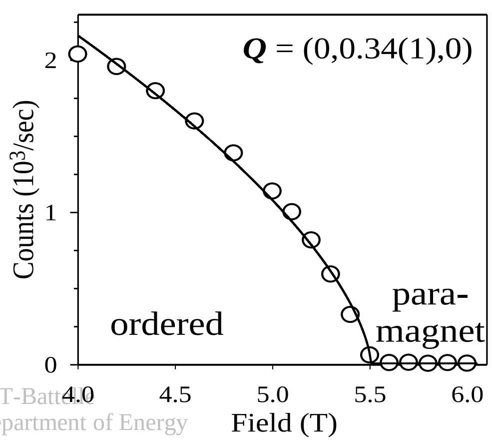
$$\cdots\rightarrow\rightarrow\rightarrow\rightarrow\leftarrow\rightarrow\rightarrow\rightarrow\cdots$$

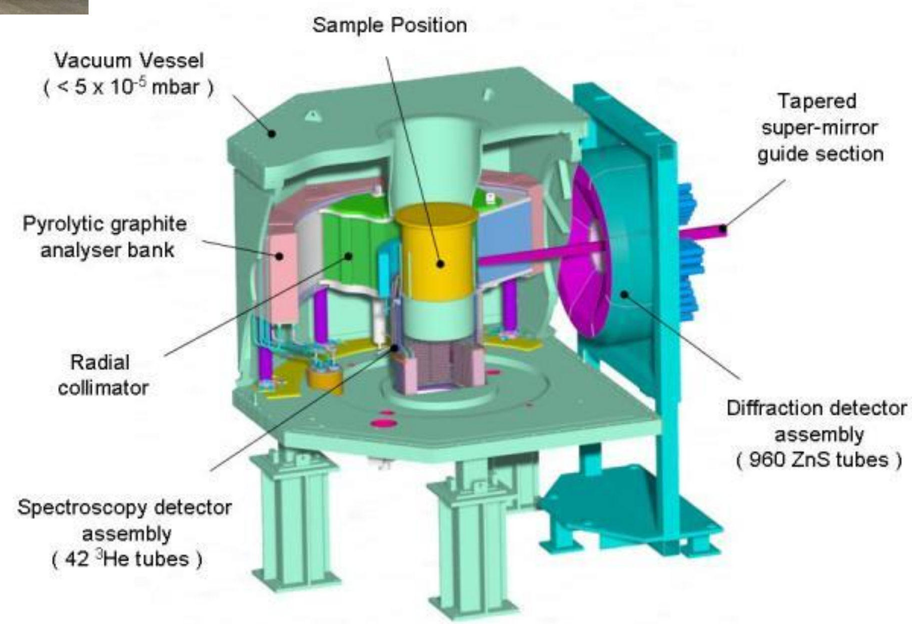
- "Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent E-8 Symmetry",
- Science 327, 177-180 (2010).

We can fully control the experimental system with magnetic field and temperature



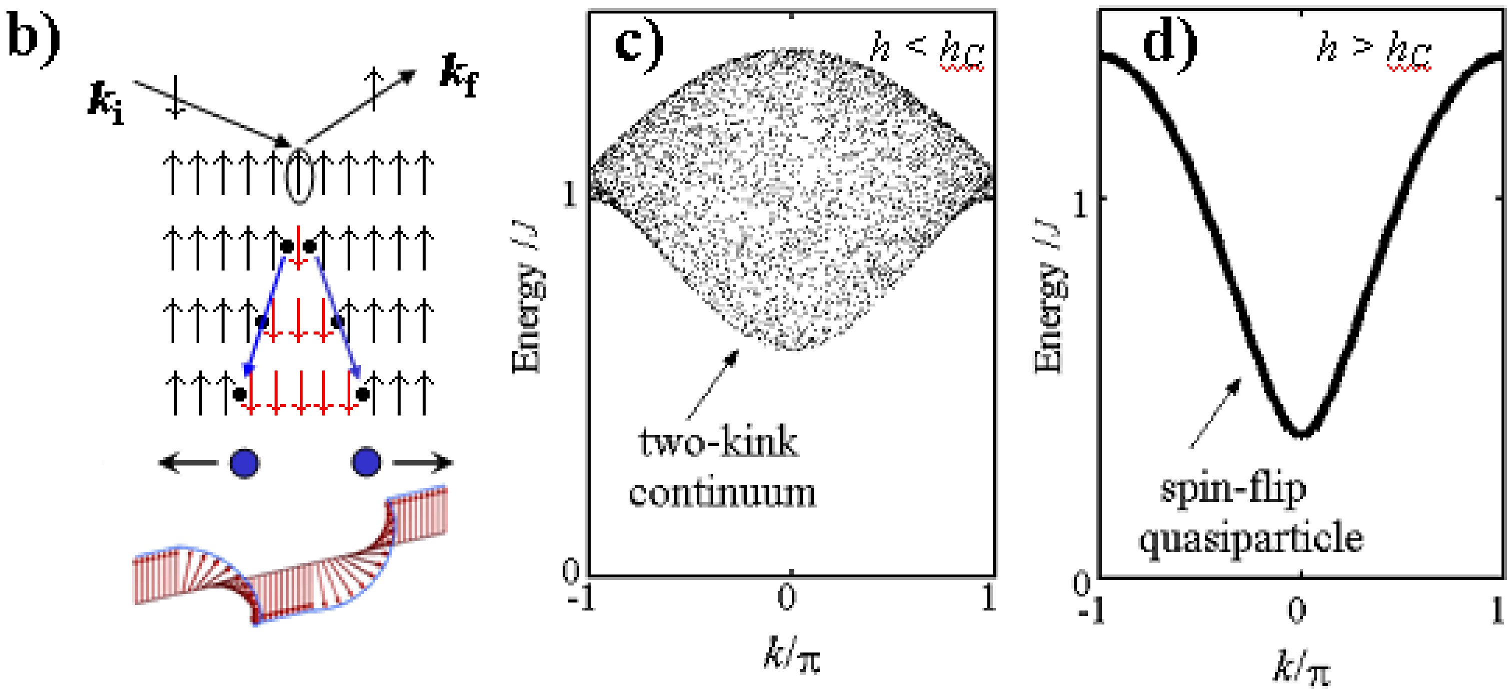
- Attain and control quantum states
- High fields & millikelvin tempera
  - Order parameter



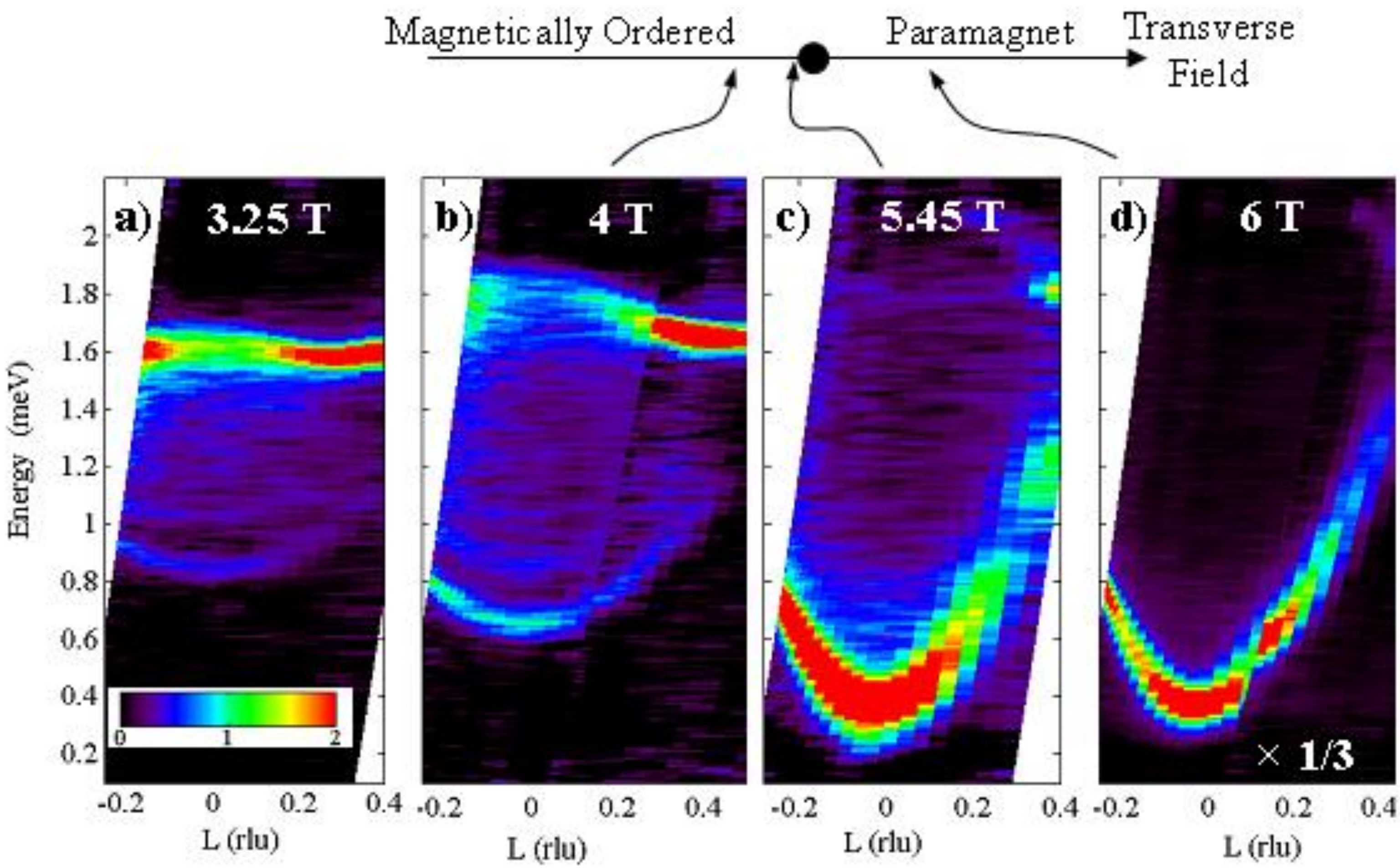


How neutrons measure states of our system

•Neutrons carry magnetic moment
•Scatter inelastically from quasiparticles

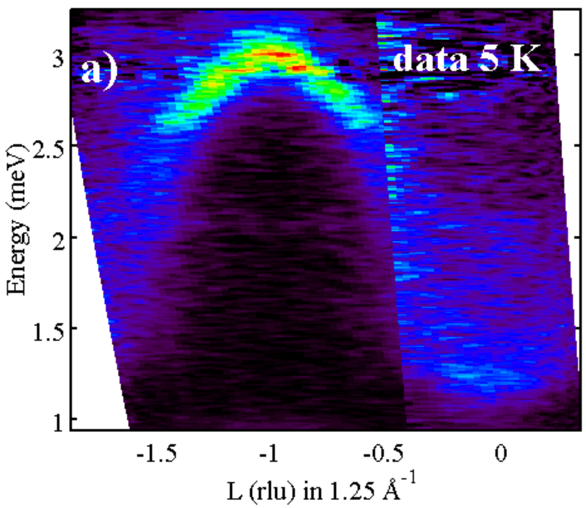


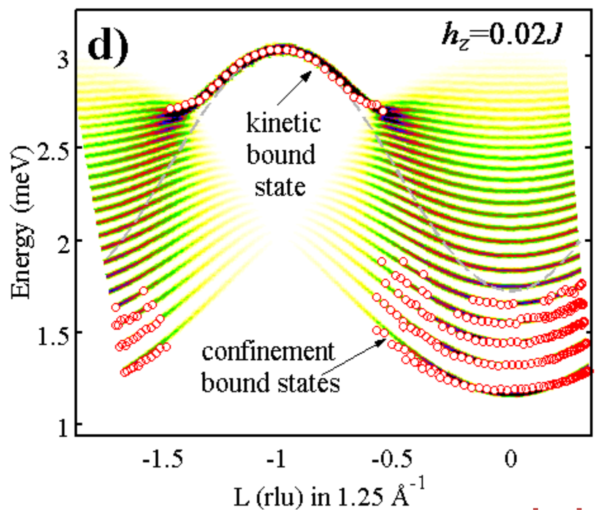
Sweeping field shows the dynamics change when we go through the quantum phase transition at 5.5 Tesla



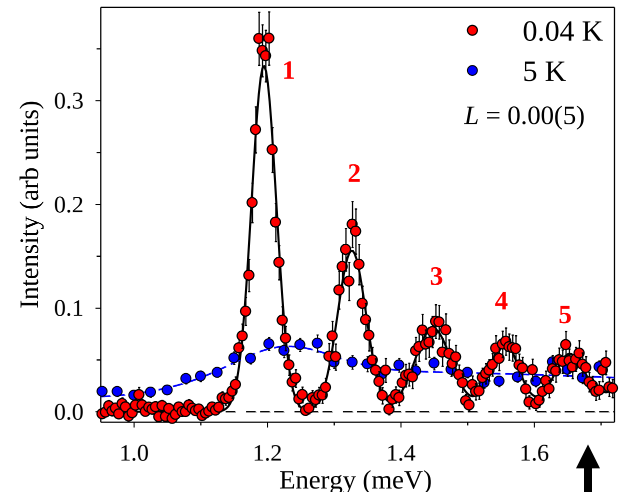
•"Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent E-8 Symmetry",
•Science 327, 177-180 (2010).

Away from the quantum phase transition we can look at some interesting quantum effects of particles in a confining well

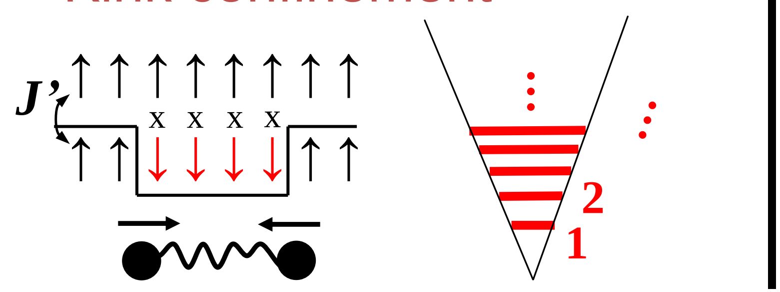




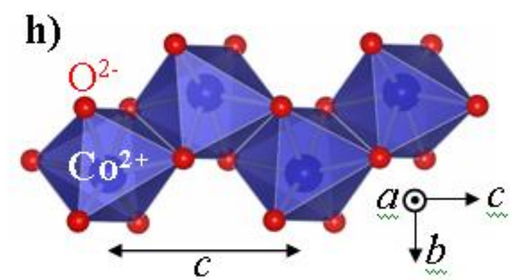
Roots of Airy Function



•Kink confinement



$$H = -J' \sum_n S_n^z S_{n+1}^z - h^x \sum_n S_n^x - h^z \sum_n S_n^z$$
$$-J_p \sum_n \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) + J_B \sum_n S_n^z S_{n+2}^z.$$

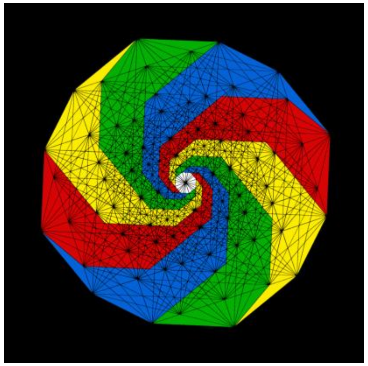


•McCoy and Wu (1978) solved the Schrödinger eqn for small confinement potential

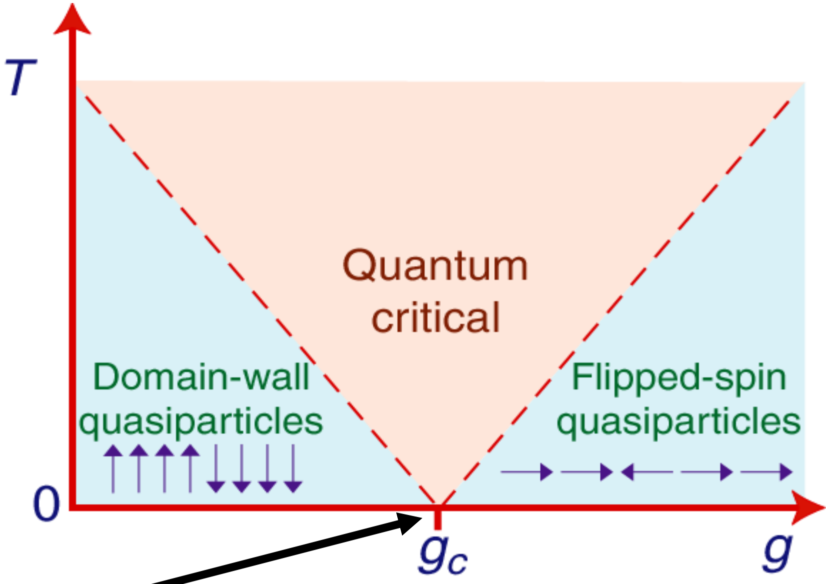
•SB Rutkevich, J. Stat. Mech. (2010) P07015

Near the quantum critical point new physics starts to emerge

- Emergent symmetry



Lie groups deal with continuous symmetry e.g. rotations



Form quantum fractal states

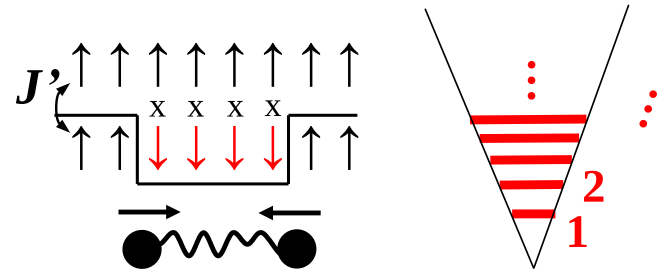
- Hidden E8 symmetry
- Emerges at Quantum Critical Point
- Symmetry -> conservation laws
- 8 modes predicted in excitation spectrum
- Mutual bound states of each other
- Supersymmetry – no hierarchy

What is the signature of E8 symmetry?

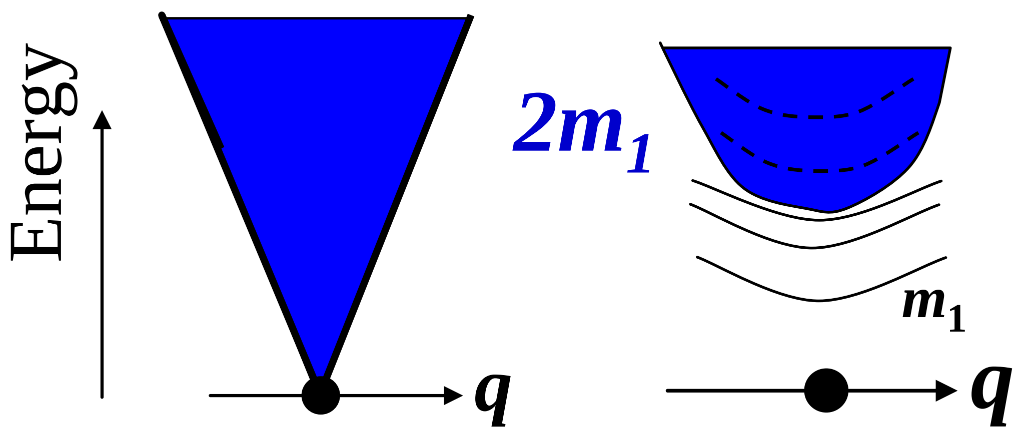
E8

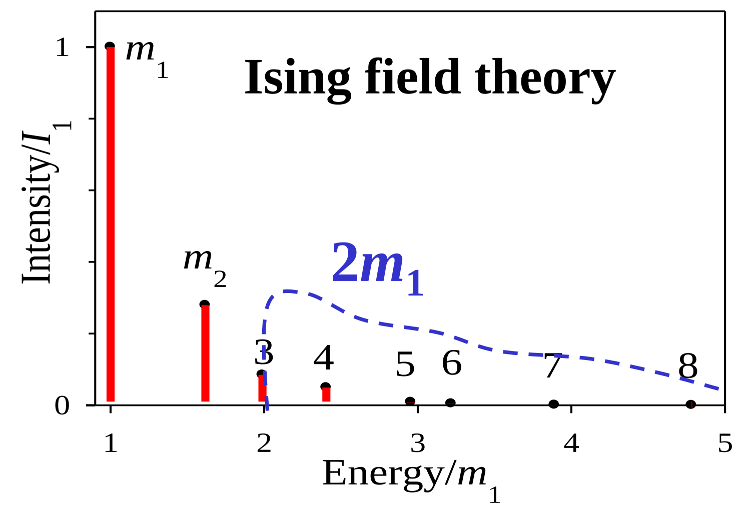
- Ultimate symmetry
- Never observed before
- Representations have just been solved

•Kink confinement



•Ising resonances



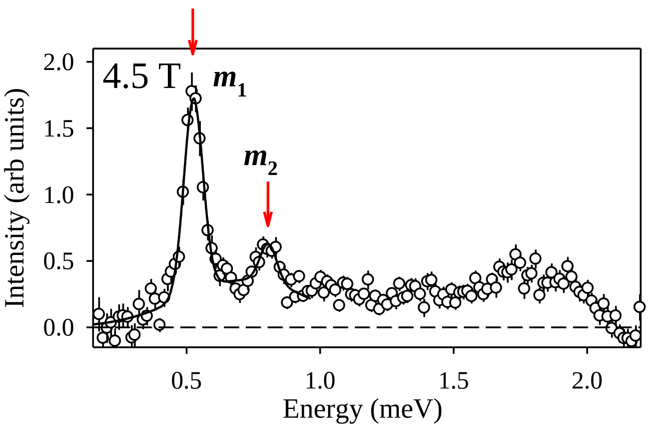


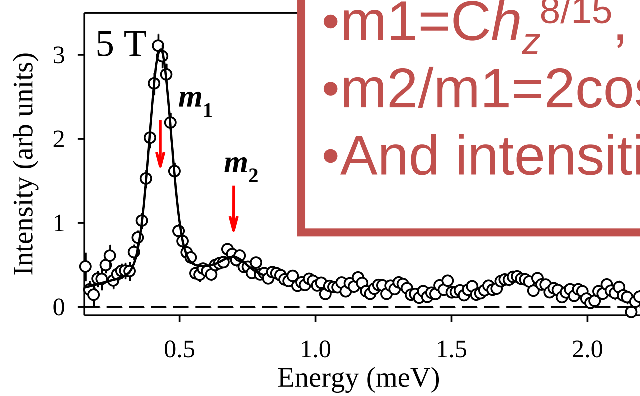
•A.B. Zamolodchikov. *Int. J. Mod. Phys.* A4, 4235 (1989).

•G. Mussardo

Intensities and energies follow the E8 predictions

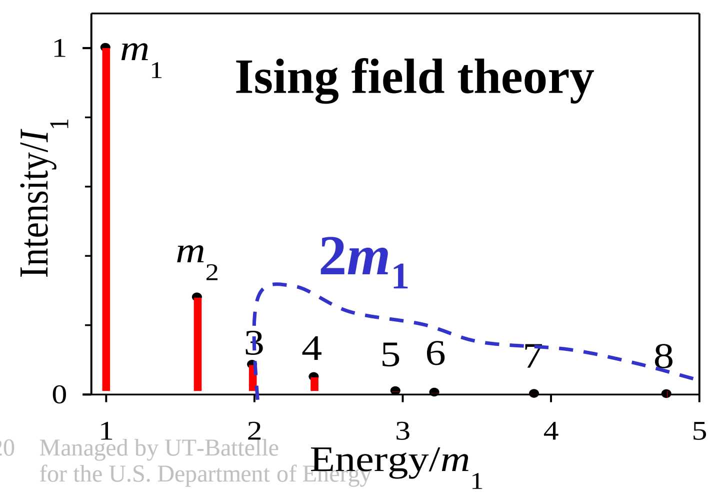
- Modes are observable

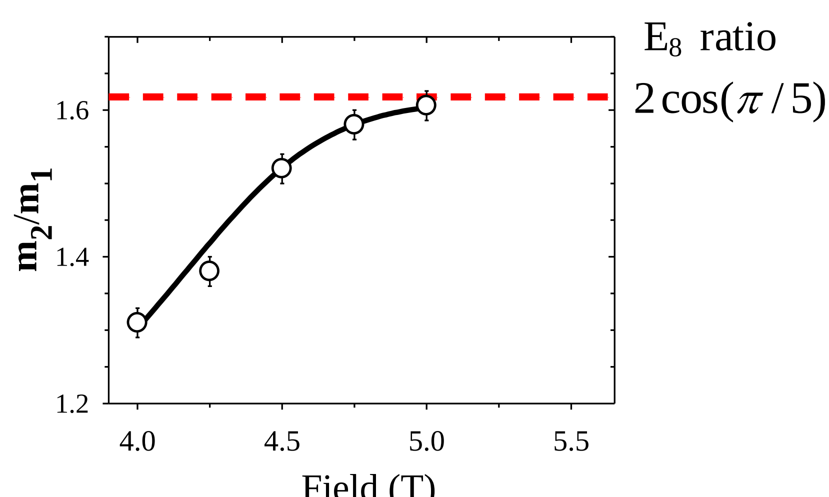




- E8 exceptional Lie group give the energy gaps (masses)
- $m1=Ch_z^{8/15}$, C≈4.4
- $m2/m1=2\cos(\pi/5)$
- And intensities

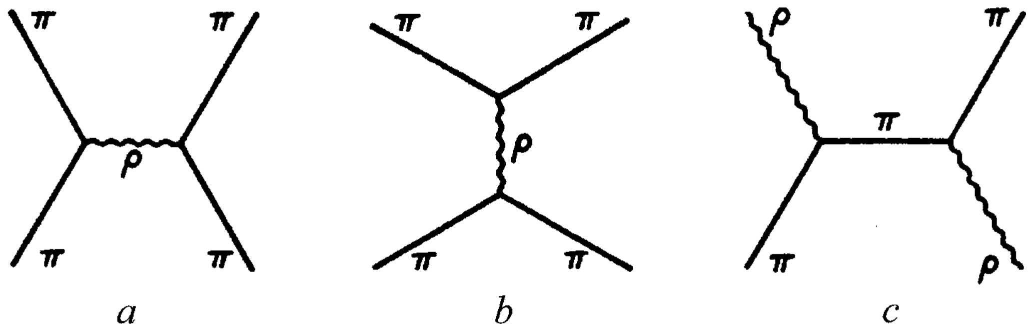
- Golden Ratio





Some of this is familiar from supersymmetry...

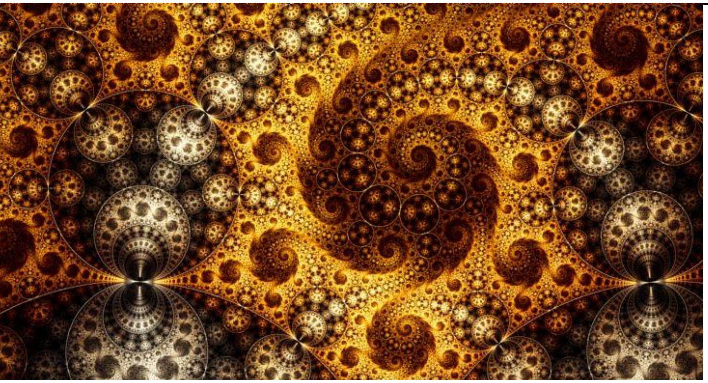
- Exact mass ratios can come about
- Particles are all bound states of each other

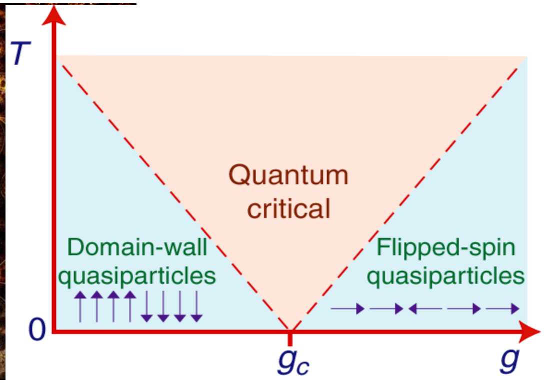


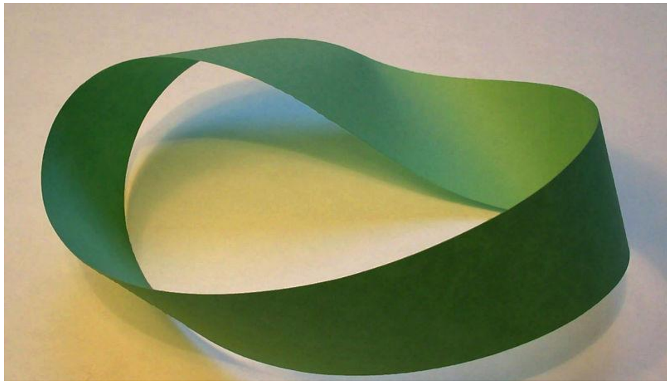
In strongly correlated matter bound states, intermediate states, and quasiparticles become resonances on an equal footing

u	c	t	γ
d	s	b	g
ν_e	ν_μ	ν_τ	Z^0
e	μ	τ	$W^\pm$

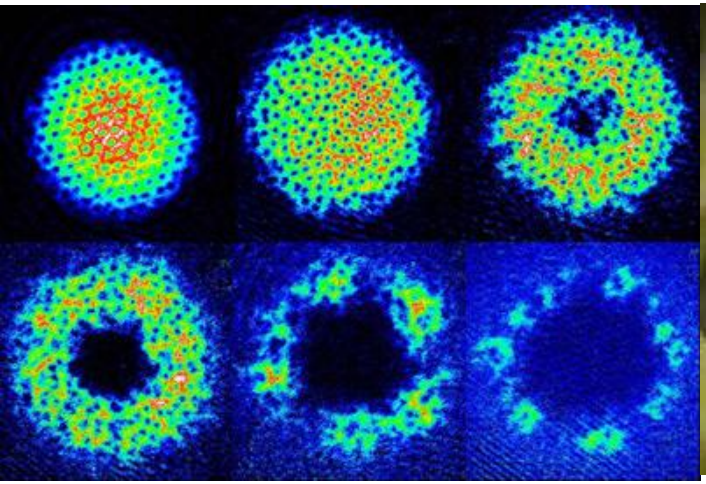
Particles in the standard model

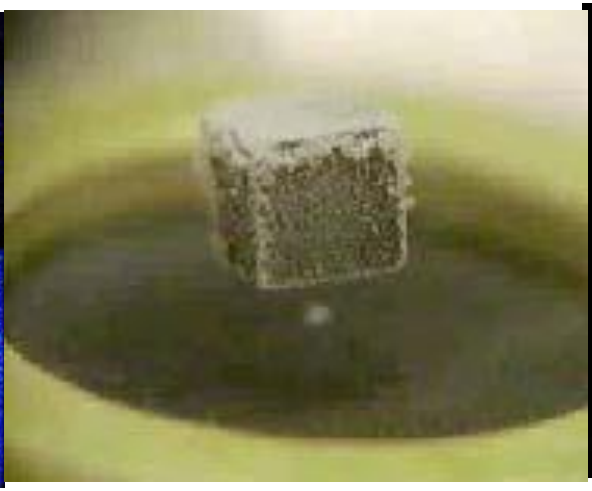


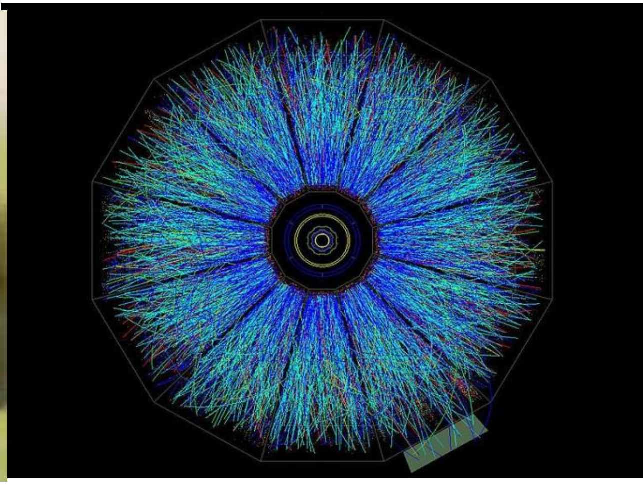




Just the start of a series of Quantum Critical Points...







- Ultracold atoms
- High T_C superconductor
- Gold nuclear collisions produce quark gluon plasmas @RHIC

Quantum critical points matter because they address the most highly entangled quantum systems

Scaling at phase transitions

- α,β,γ,δ,ν critical exponents
- Universality classes: symmetry and dimensionality of system
- Scaling laws e.g. $\gamma = \nu(2-\eta)$

$C \sim |T - T_C|^{-\alpha}$ Heat capacity

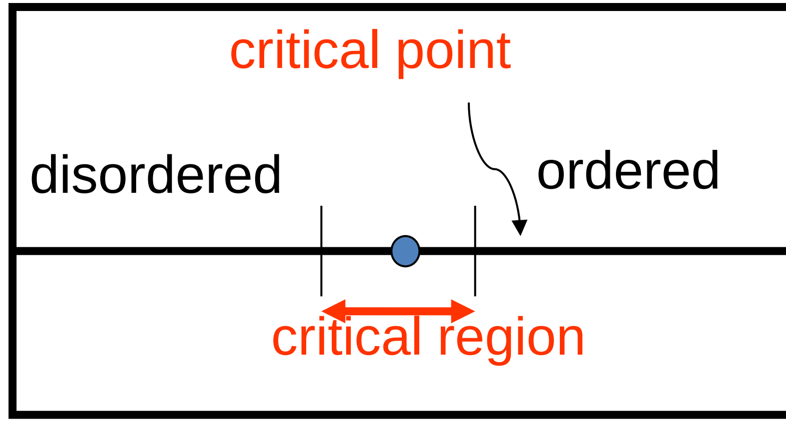
$M_0 \sim (T_C - T)^{\beta} \quad (T < T_C)$ Order parameter

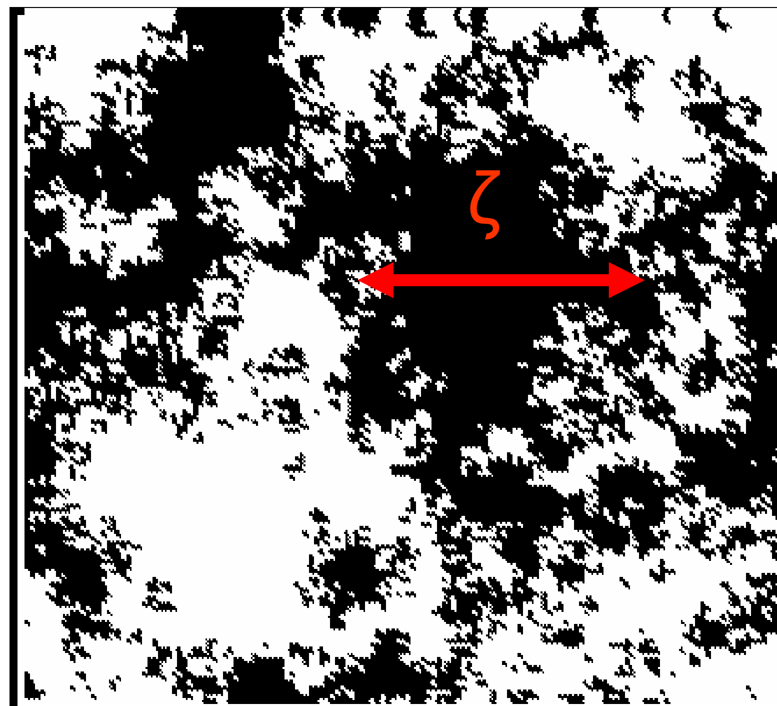
$\chi \sim |T - T_C|^{-\gamma}$ Susceptibility

$B \sim M^{\delta}$ Critical field

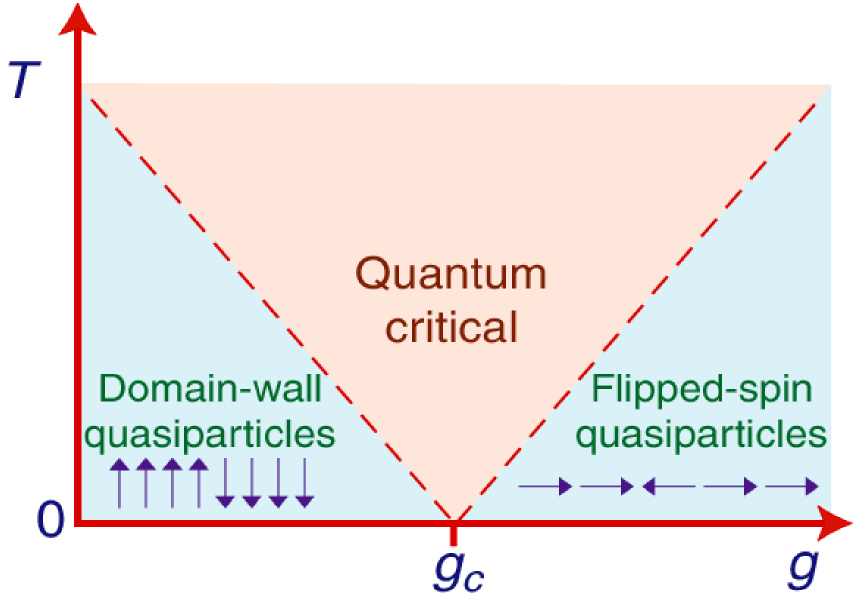
$\zeta \sim |T - T_C|^{\nu}$ Correlation length

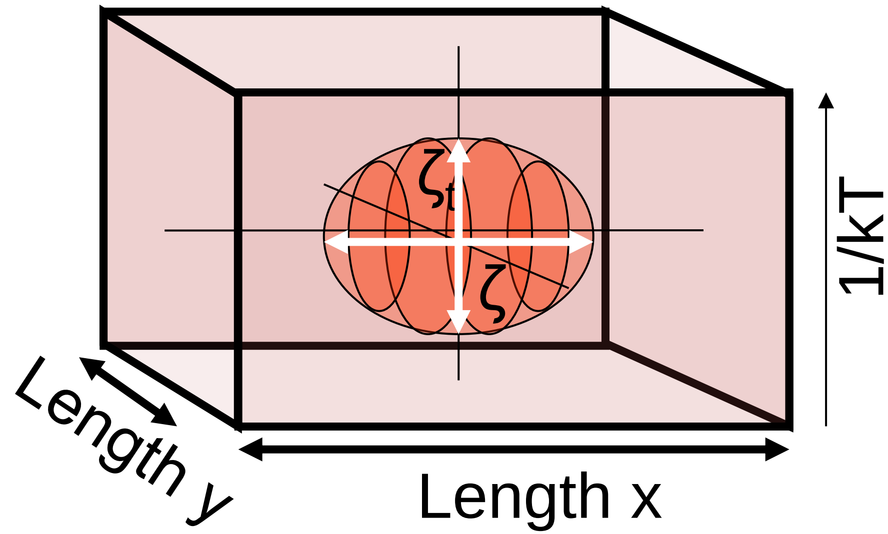
Near criticality, in the „critical region“, ζ is the only scale.



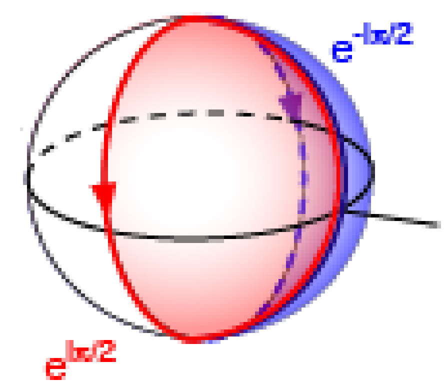


The structure of Quantum Critical Volumes





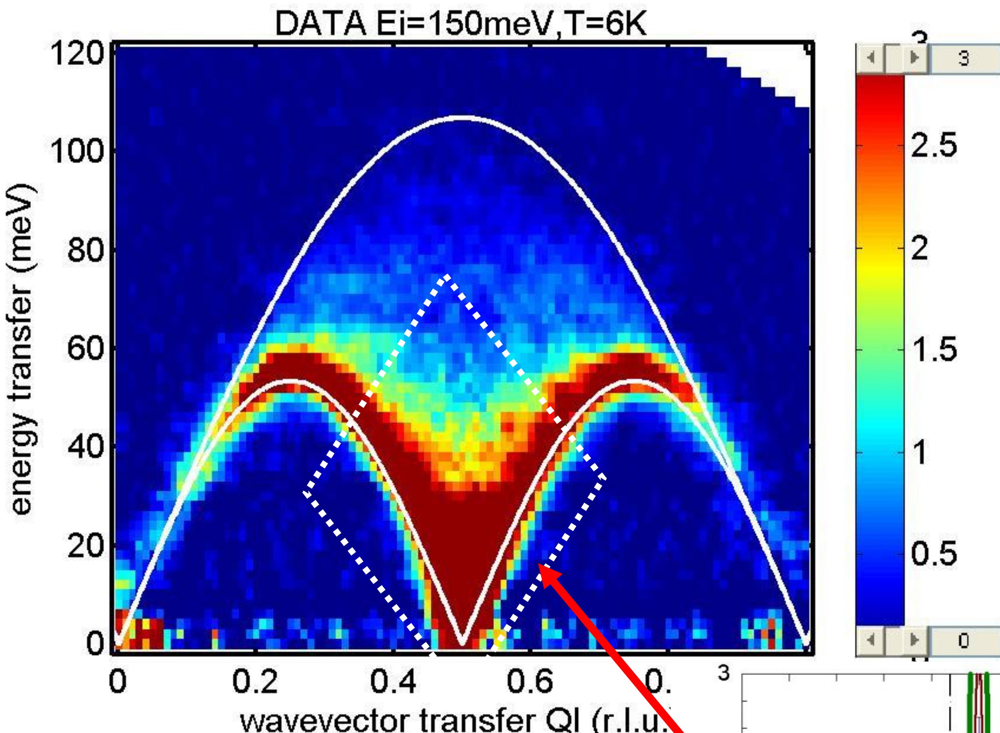
- Quantum – extra effective „time“ dimension (d+1)
- e.g.1D Quantum Ising model -> 2D Ising model



Berry phase

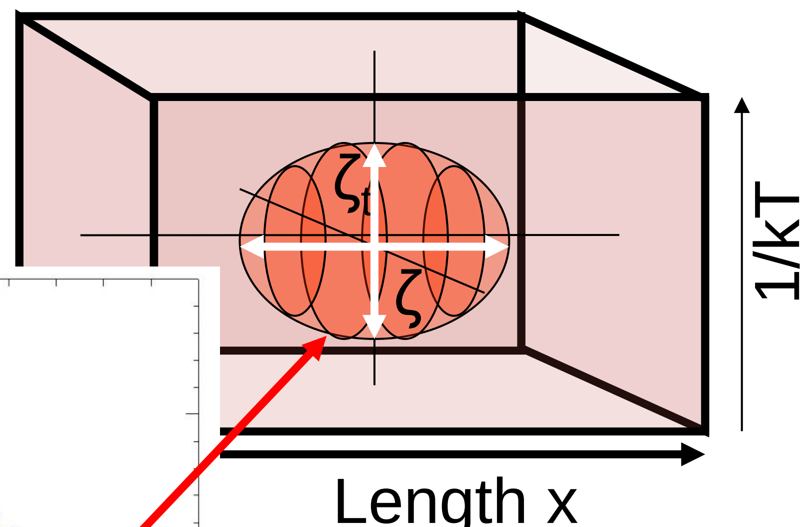
Probing directly the Quantum Critical Volume in space and time

Material KCuF3 realizes a spin ½ Heisenberg chain

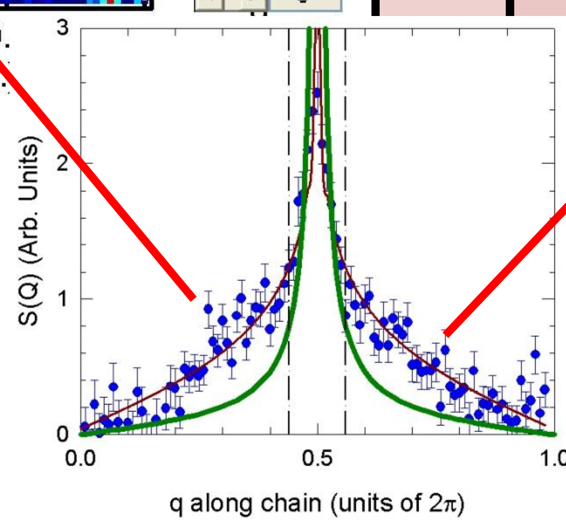


$$H = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Critical – power law behaviour

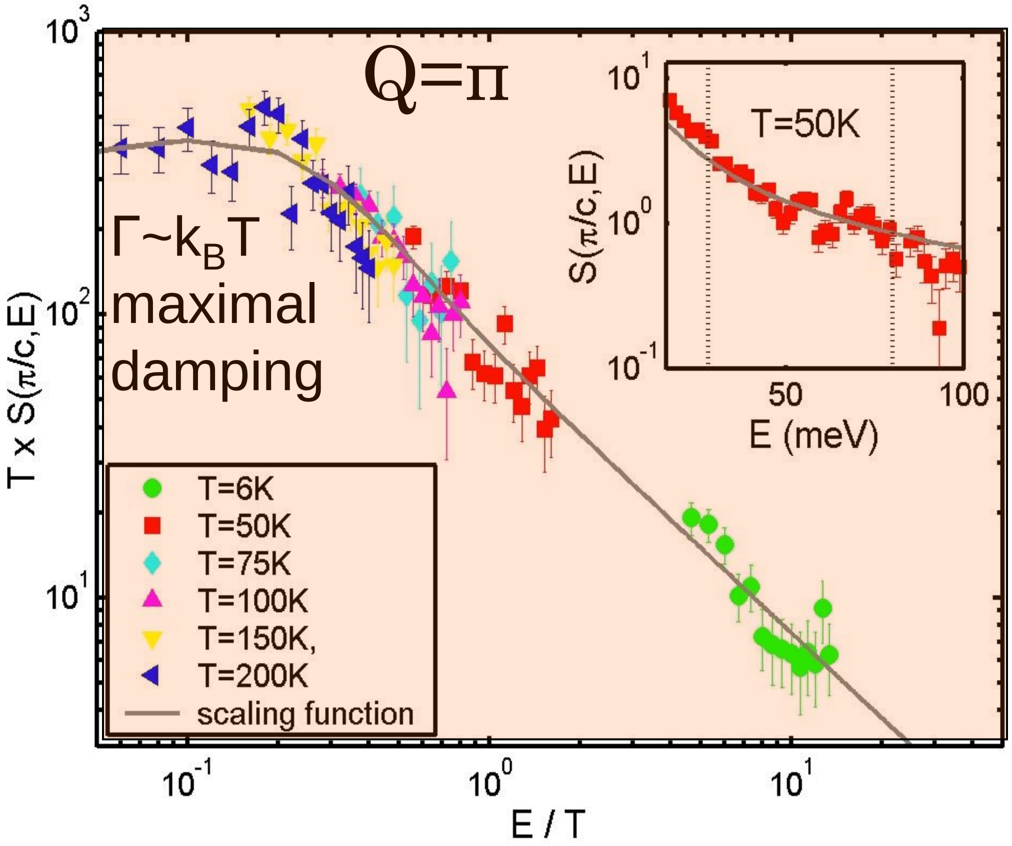


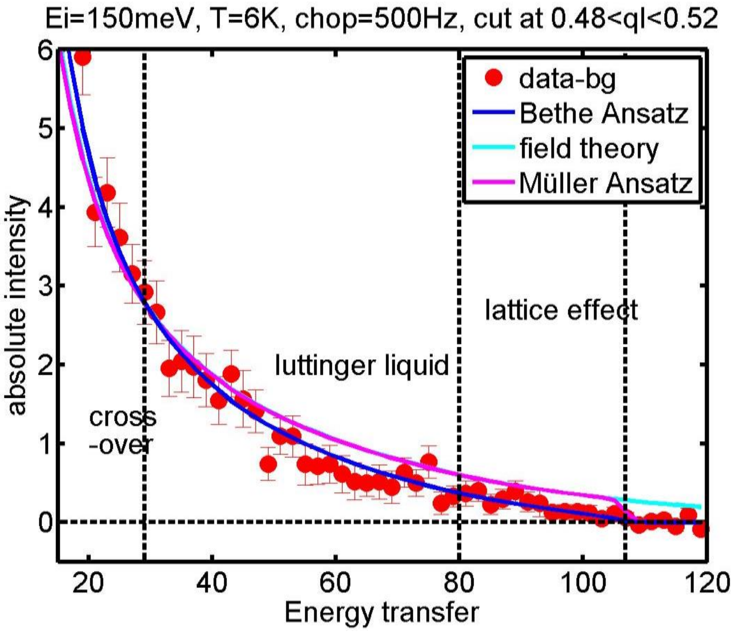
B. Lake, A. Tennant,
S. Nagler, C. Frost,
Nature Materials. 4, 329 (2005)



Universal theories for Luttinger liquid and Energy/Temperature scaling confirmed

Nature Materials. 4, 329 (2005)





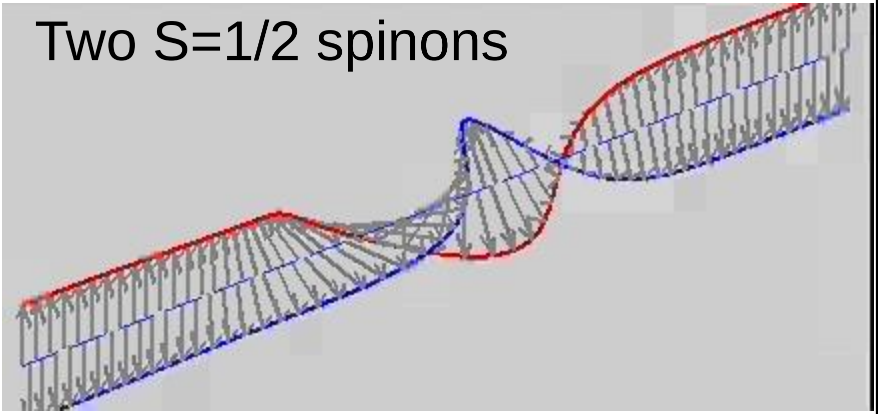
The excitations are twists with fractional quantum numbers

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

-Haldane - semiclassical mapping (1983)

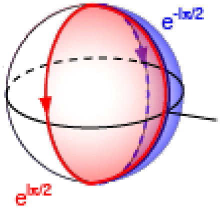
-Quantum critical Luttinger liquid

-Spinons - fractional statistics



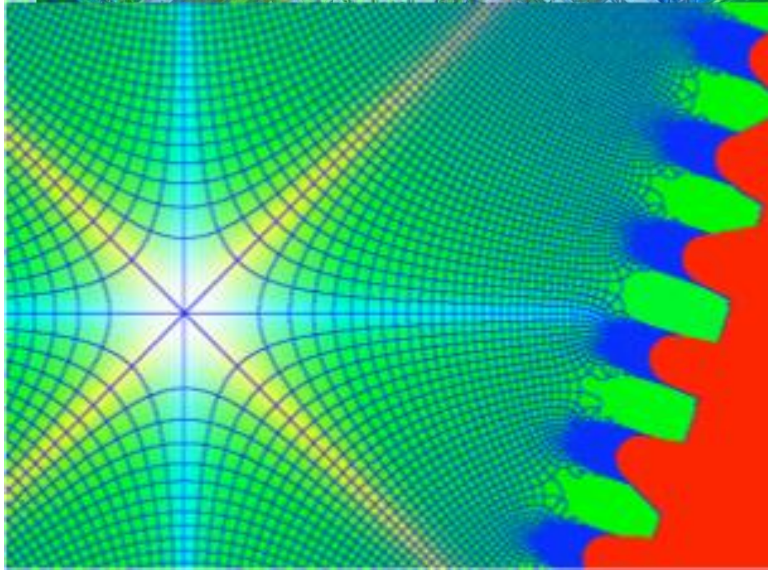
Semiclassical kinematics of two spinons F.D.M. Haldane PRL 50, 1153 (1983).

Spinons are stabilised by a Berry‘s phase and are special to S=1/2, 3/2,…



$$\hat{H} = J_{\parallel} \sum_r \vec{S}_{r,l} \cdot \vec{S}_{r+1,l} + J_{\perp} \sum_{l,\delta} \vec{S}_{r,l} \cdot \vec{S}_{r,l+\delta}$$

The possible quantum critical states in wires form a set according to conformal field theory

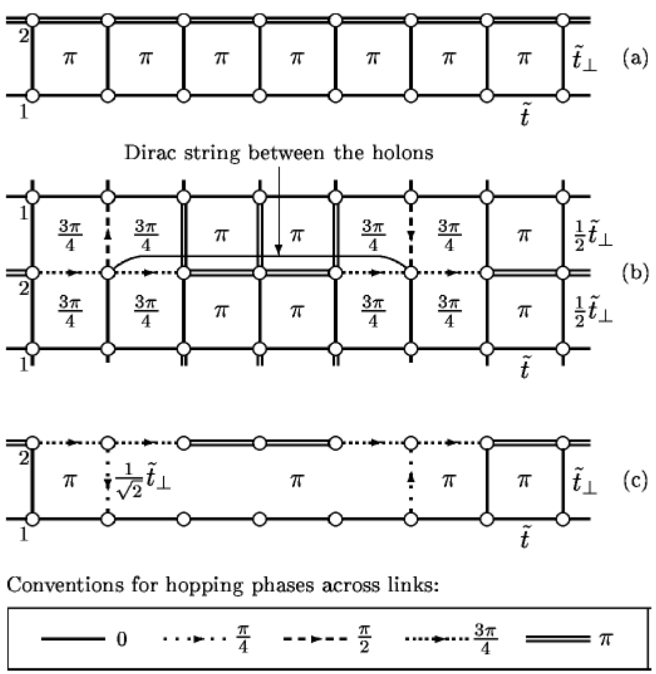


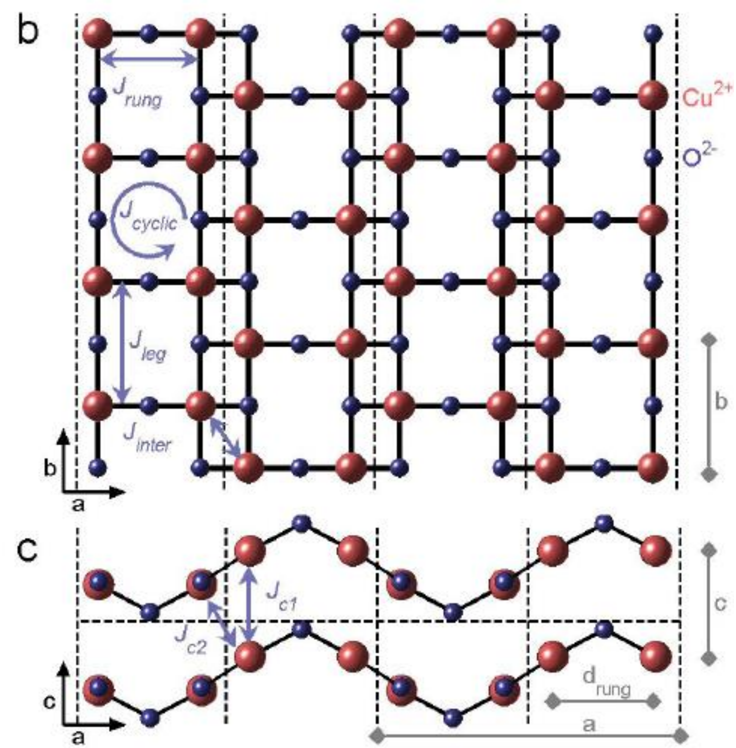
- 1D quantum systems
- Conformal field theory
- Central charges classify the states
- C=1/2, 1, 3/2, ….

Central charge	Quantum State	Type of kink	Where to see it…
1/2	Transverse Ising model	Domain wall	Anisotropic spin chains
1	Luttinger liquid	Semion	S=1/2 Heisenberg chain Carbon nanotubes v=1/2 FQHE edge states
3/2	SU(2)2 Wess-Zumino-Novikov-Witten	Exotic	Ladder with cyclic exchange Babujian-Takhtajan model (biquadratic spin exchange)

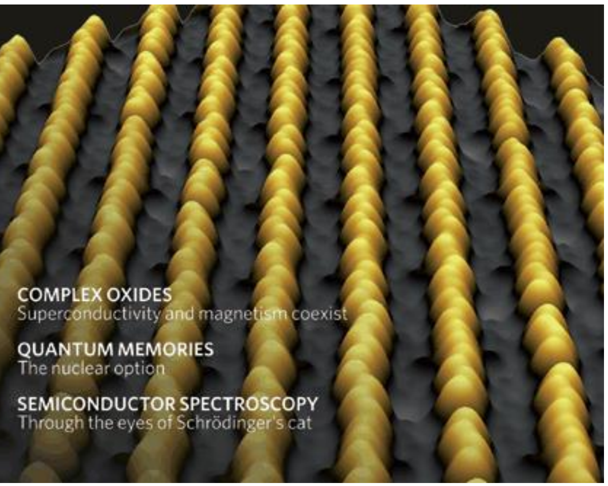
Wess Zumino Novikov Witten state is seen in spin ladders

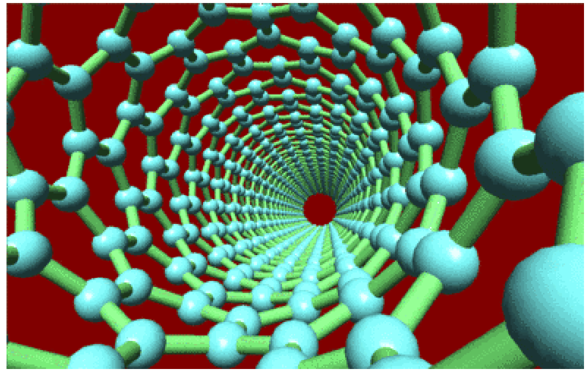
Lake, B, Tsvelik, AM, Notbohm, S, Tennant, DA, Perring, TG, Reehuis, M, Sekar, C, Krabbes, G, Buchner, B “Confinement of fractional quantum number particles in a condensed-matter system”, Nature Physics 6, 50-55 (2010).

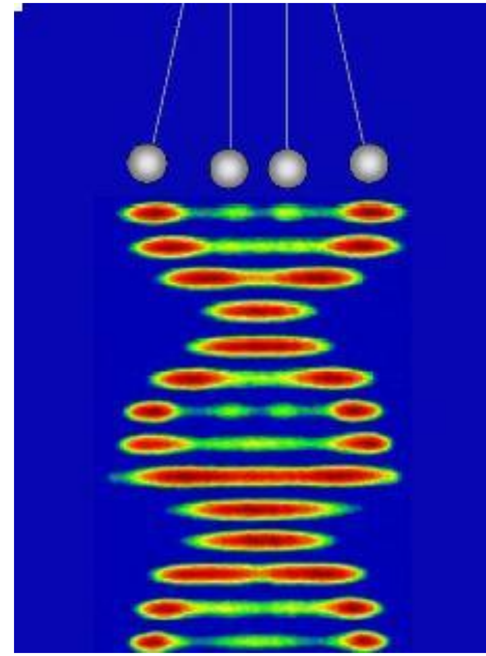




Quantum wires should be very important in the future

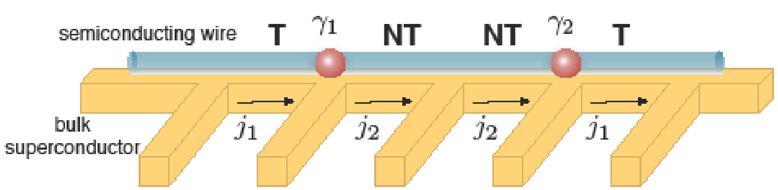


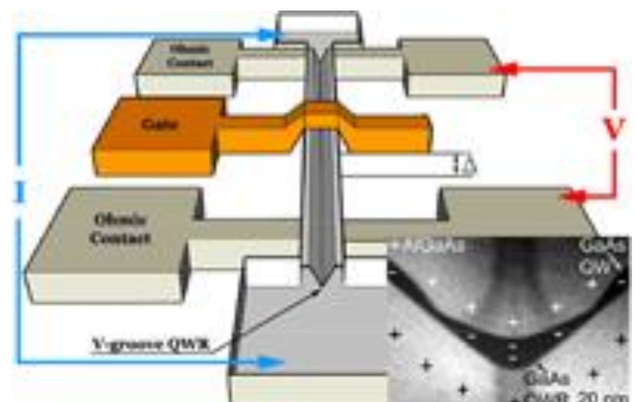




Giant thermal conductivity

Superconductivity

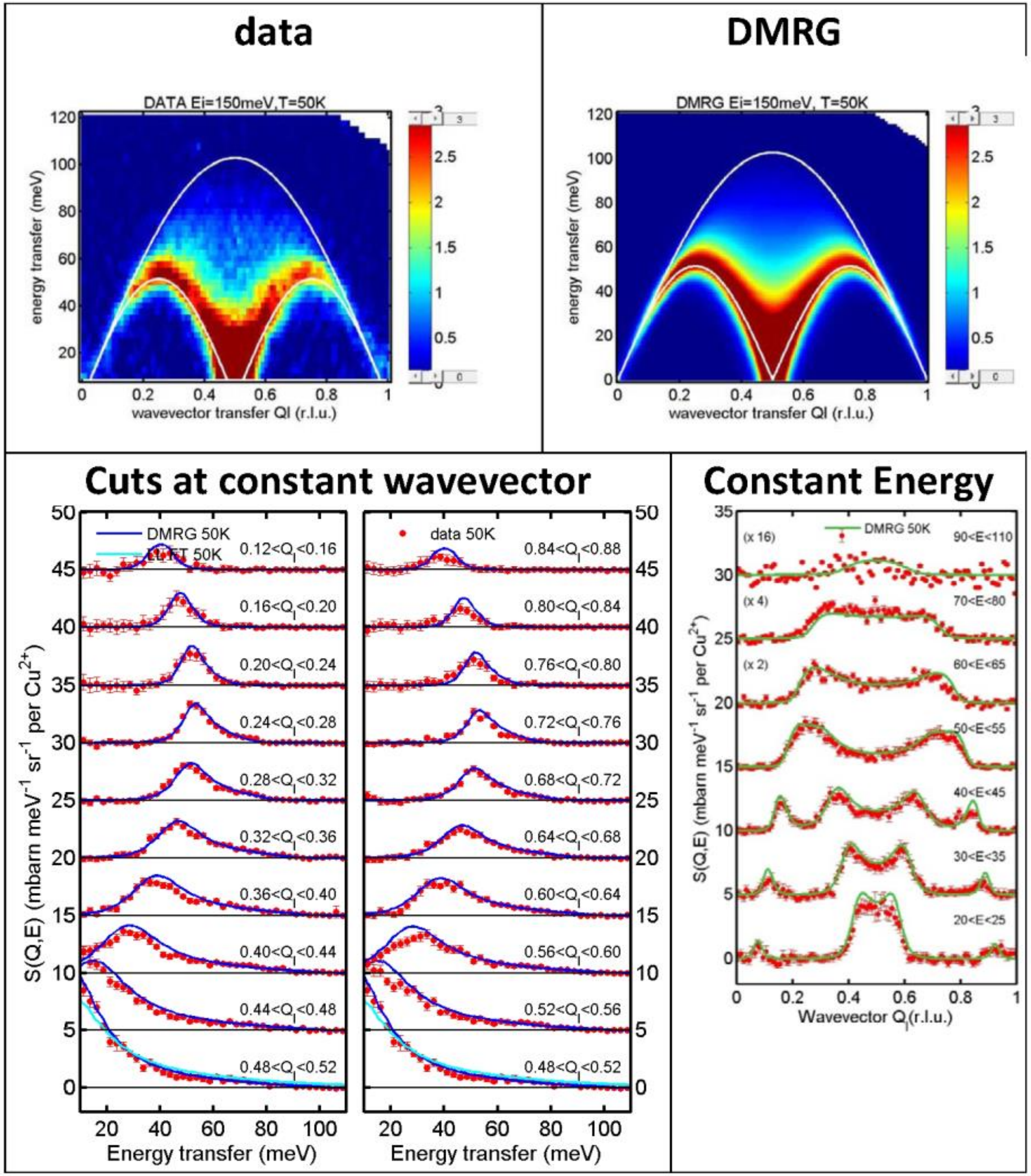




www.sciencemag.org SCIENCE VOL 336 25 MAY 2012

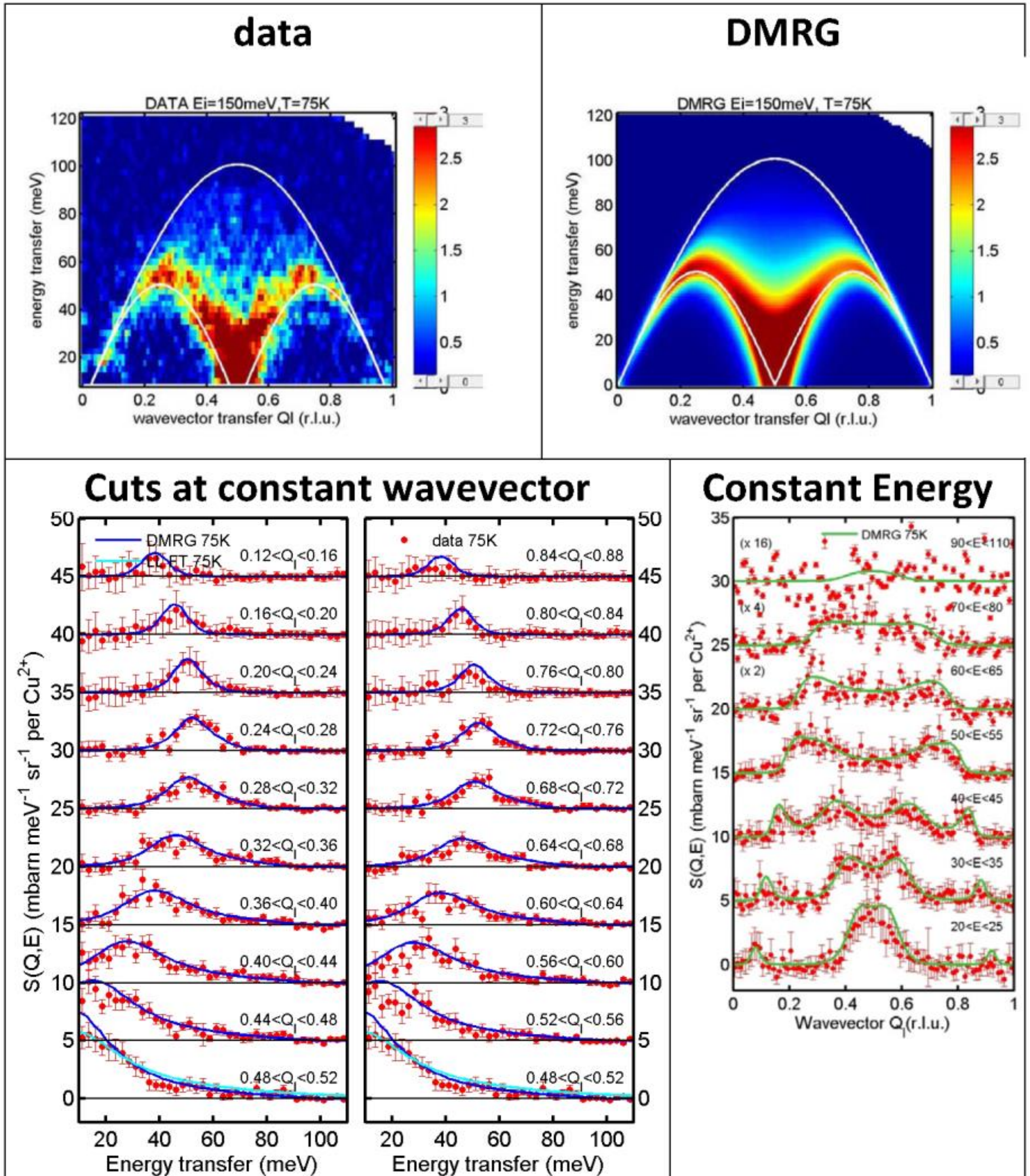
T=50K; J=32.74meV

Tensor network theory calculates properties



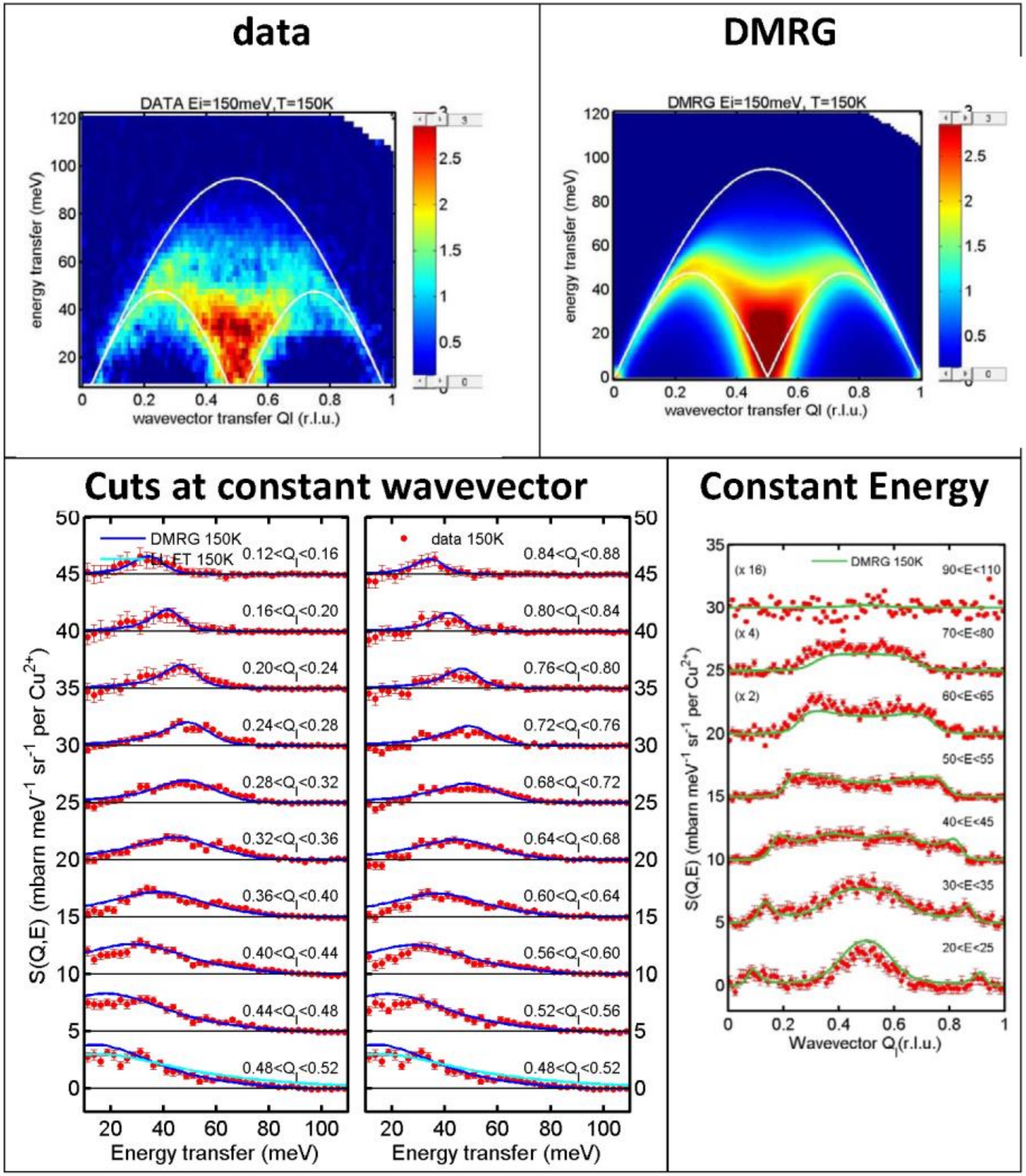
T=75K; J=32.08meV

Tensor network theory calculates properties



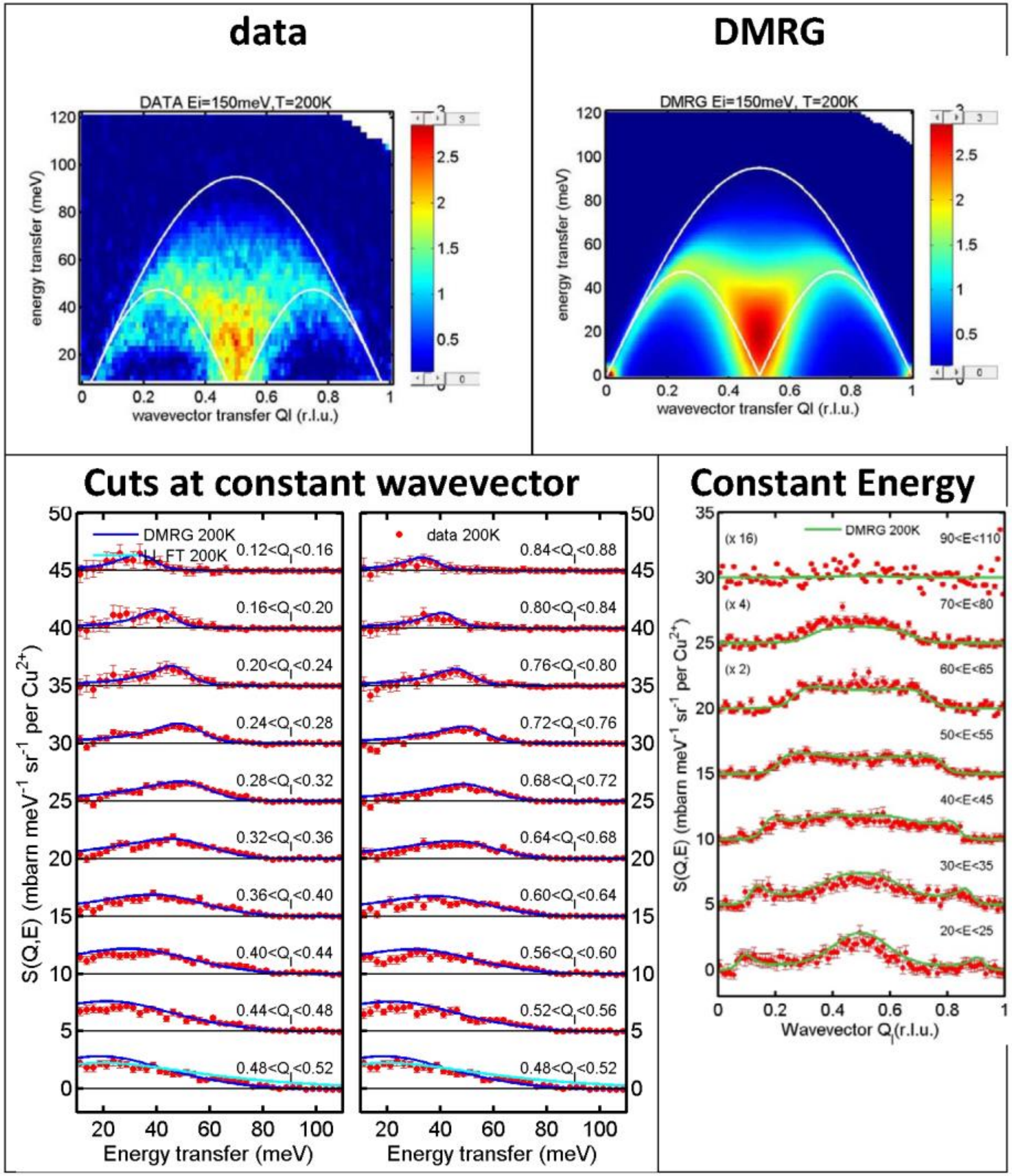
Tensor network theory calculates properties

T=150K; J=30.24meV



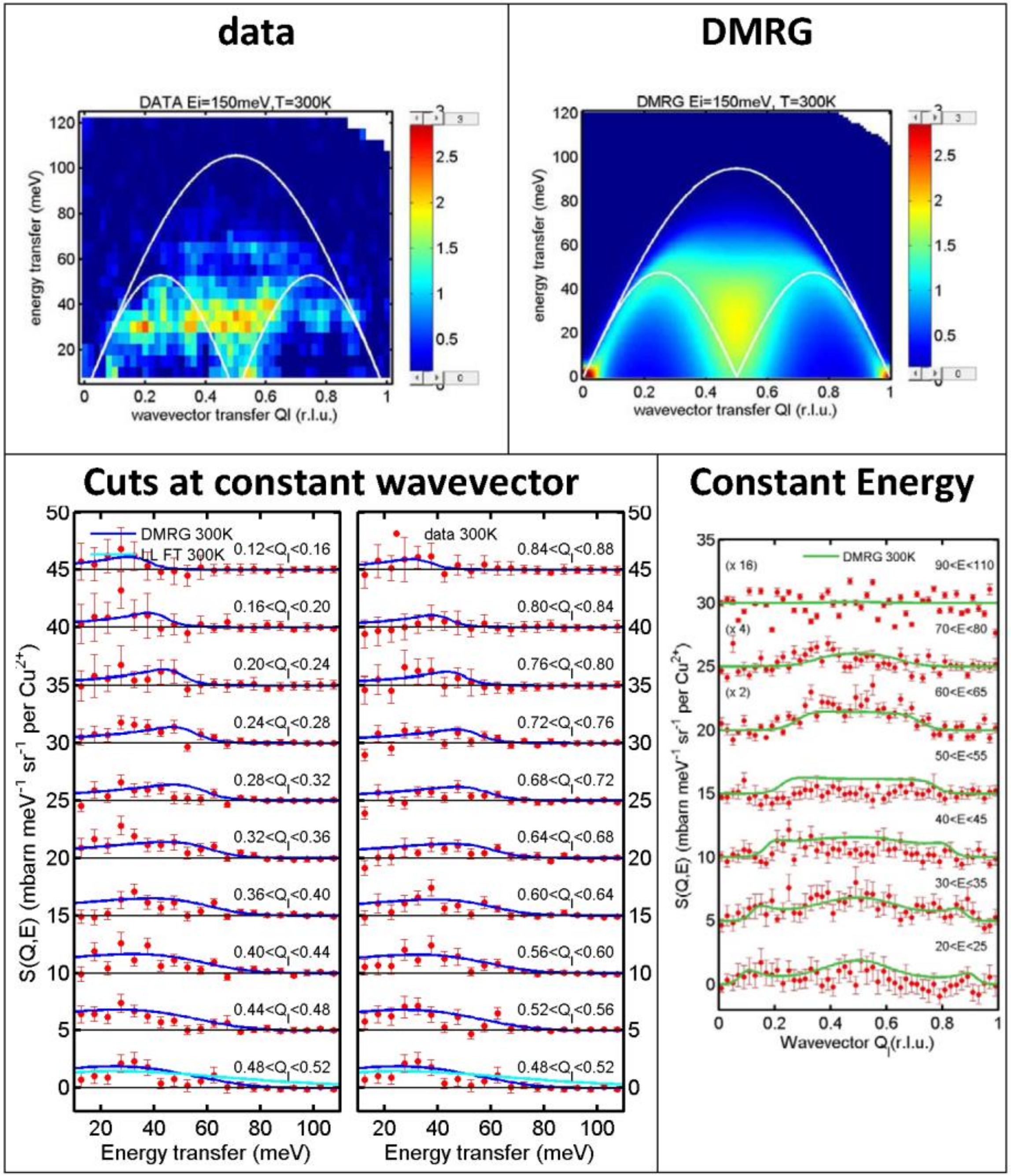
T=200K; J=30.24meV

Tensor network theory calculates properties



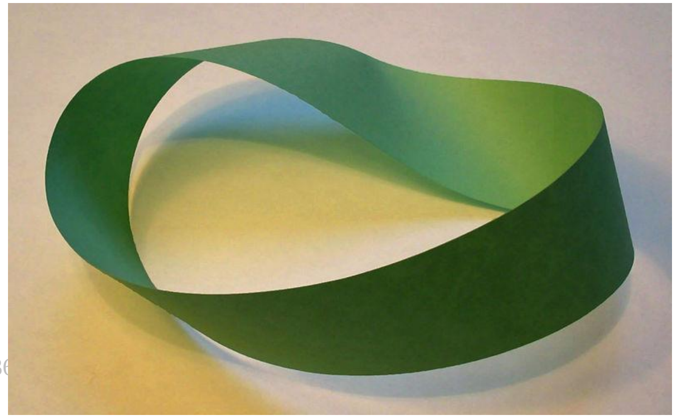
T=300K; J~30.24meV

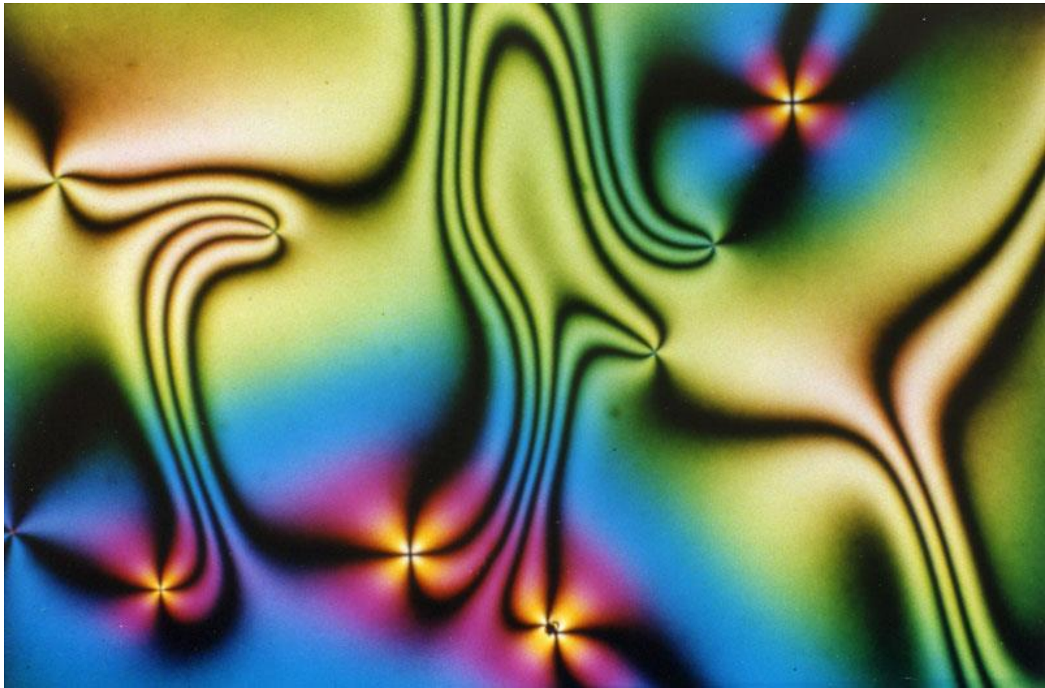
Tensor network theory calculates properties



How to get fractional states in 3D : Deconfinement of magnetic monopoles

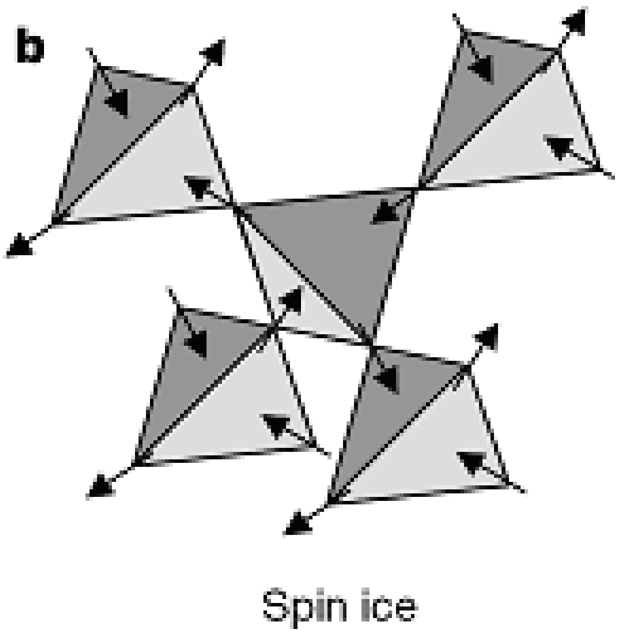
•Morris, DJP, Tennant, DA, Grigera, SA, Klemke, B, Castelnovo, C, Moessner, R, Czternasty, C, Meissner, M, Rule, KC, Hoffmann, JU, Kiefer, K, Gerischer, S, Slobinsky, D, Perry, RS “Dirac Strings and Magnetic Monopoles in the Spin Ice Dy2Ti2O7”, Science 326, 411-414 (2009).



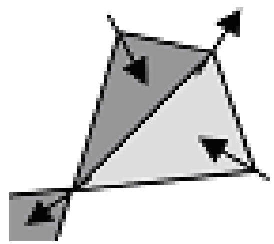


Trick to get deconfined defects in 3D comes from ice

Spin Ice



- Effective spin-1/2 pyrochlore $Dy_2Ti_2O_7$.
- Ice rules apply below 1.2K
- 2-in-2-out
- Rules not strong enough to impose long range order
- Macroscopic ground state degeneracy
- Pauling ice entropy

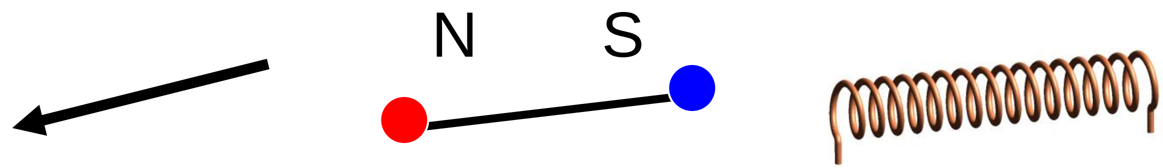


$$S \approx \frac{N}{2} k \ln \frac{3}{2}$$

Bramwell, S.T. and Gingras, M.J.P. “Spin ice state in frustrated magnetic pyrochlore materials” Science **294**, 1495-1501 (2001)

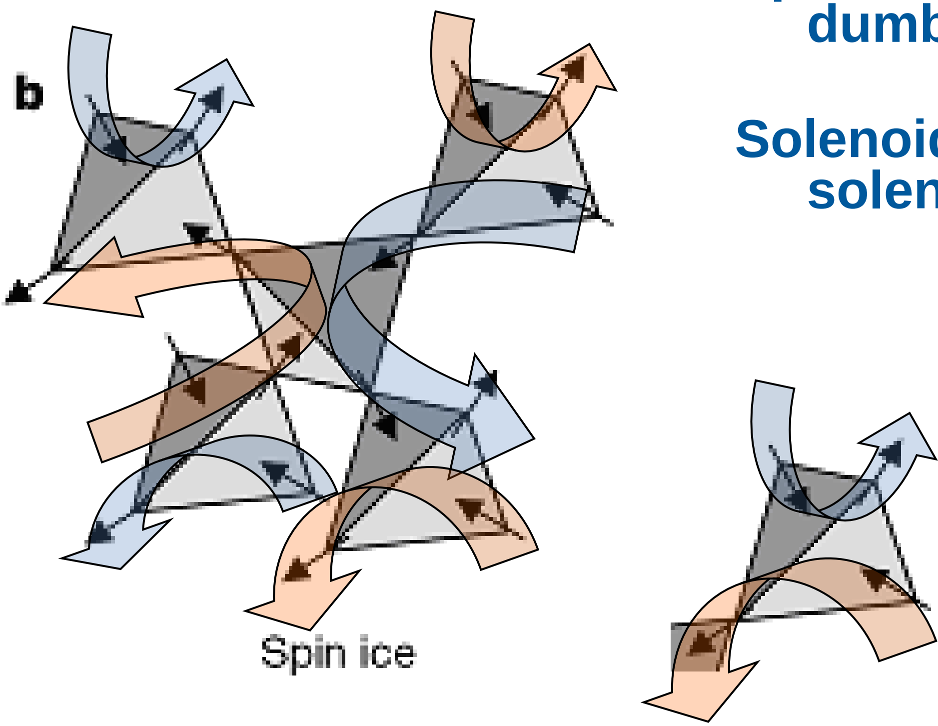
The magnetic state in spin ice is a new state called a Gauge Liquid

Spin Ice



Spin can either be thought of as a vector, a dumbbell, or a solenoid.

Solenoid picture leads to spins within solenoidal tubes – "spaghetti".



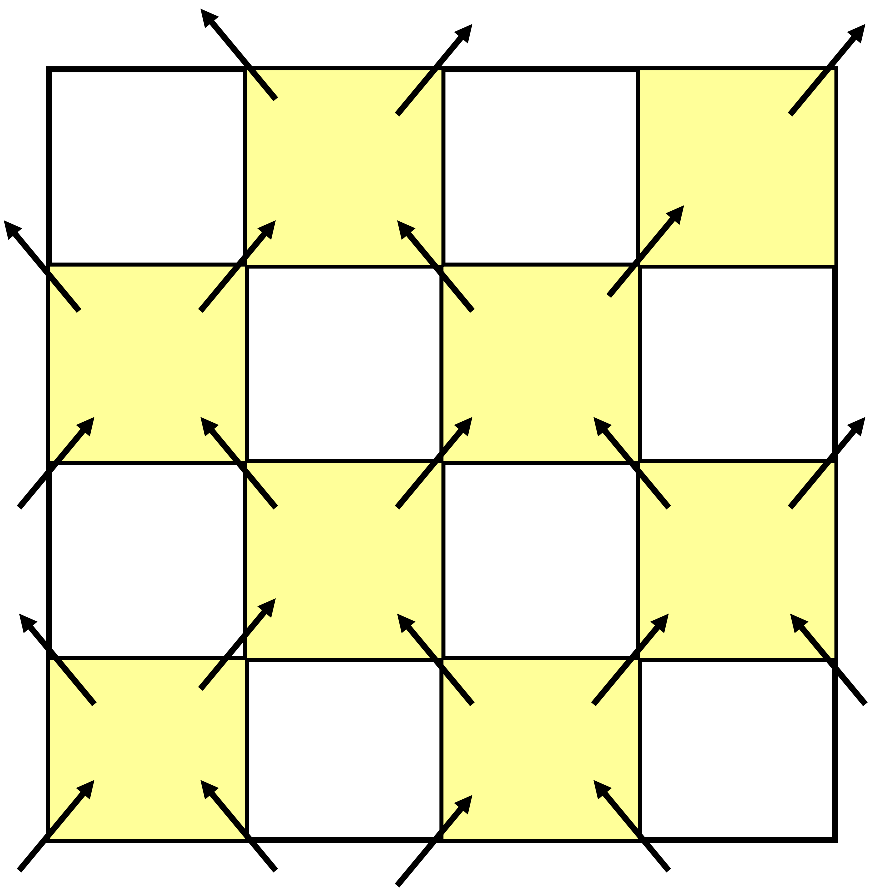
$$S \approx \frac{N}{2} k \ln \frac{3}{2}$$

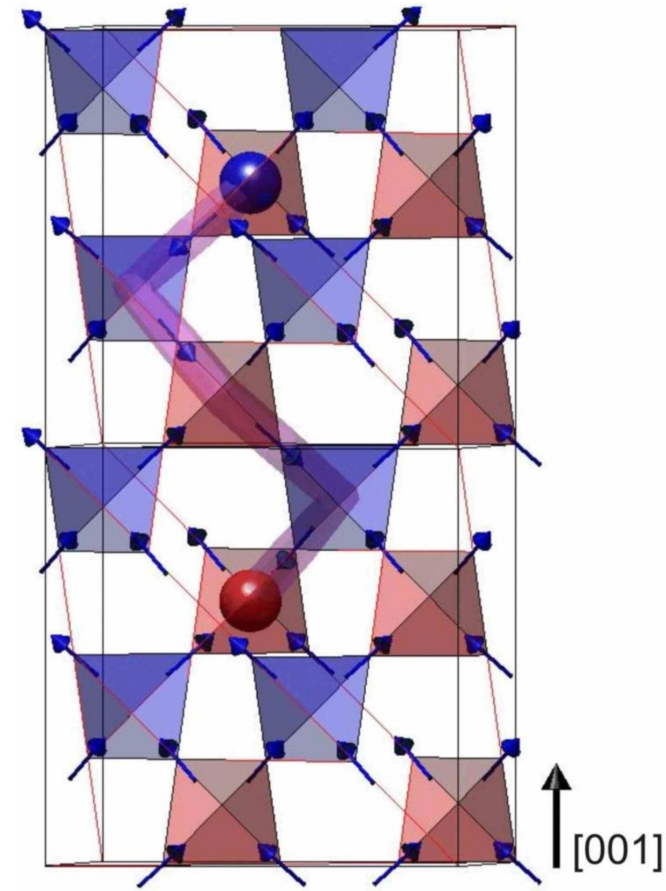
3: Choices for string to exit

2: Shared with neighbouring tetrahedra

Blue spagetti's path determines red's

Pauling, L. "The Structure and Entropy of Ice and of Other Crystals with some Randomness of Atomic Arrangement" J. Am. Chem. Soc. **57**, 2680-2684 (1935).

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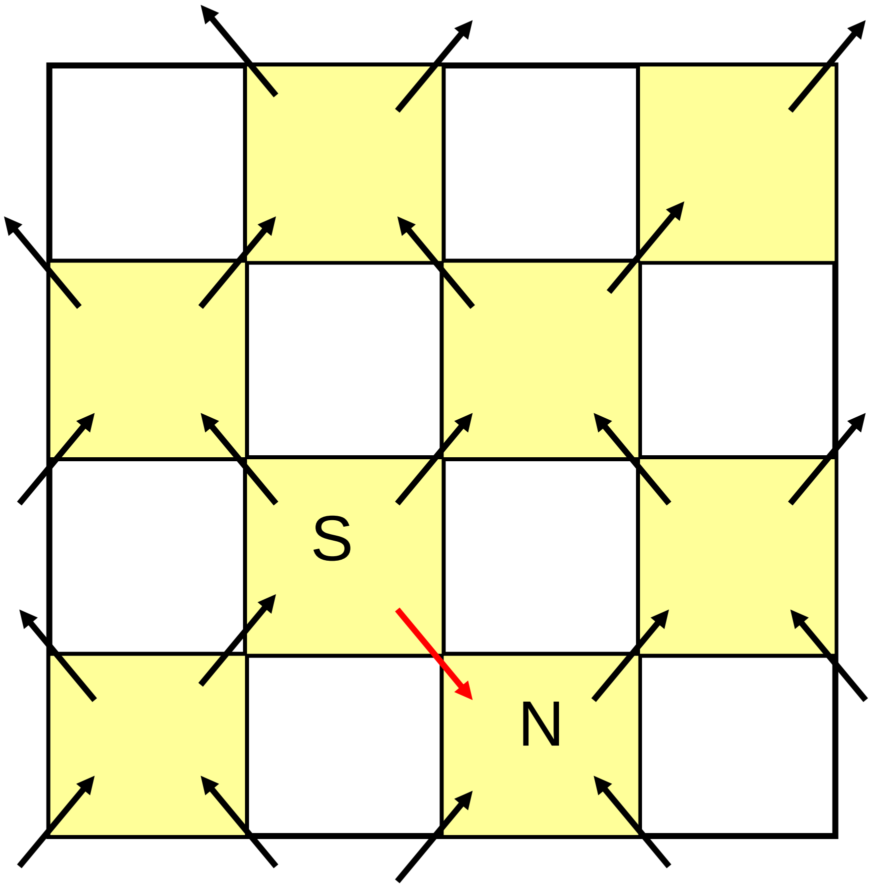
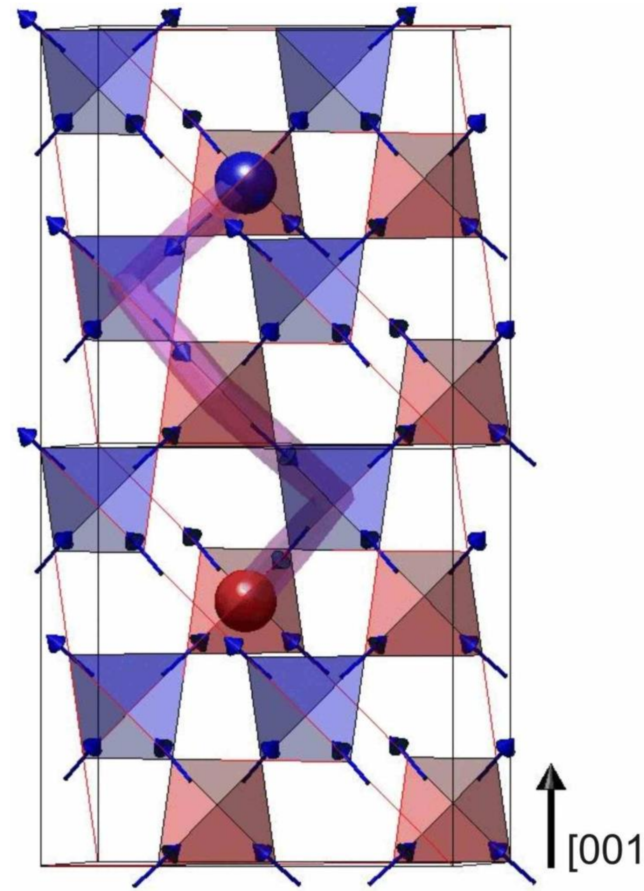
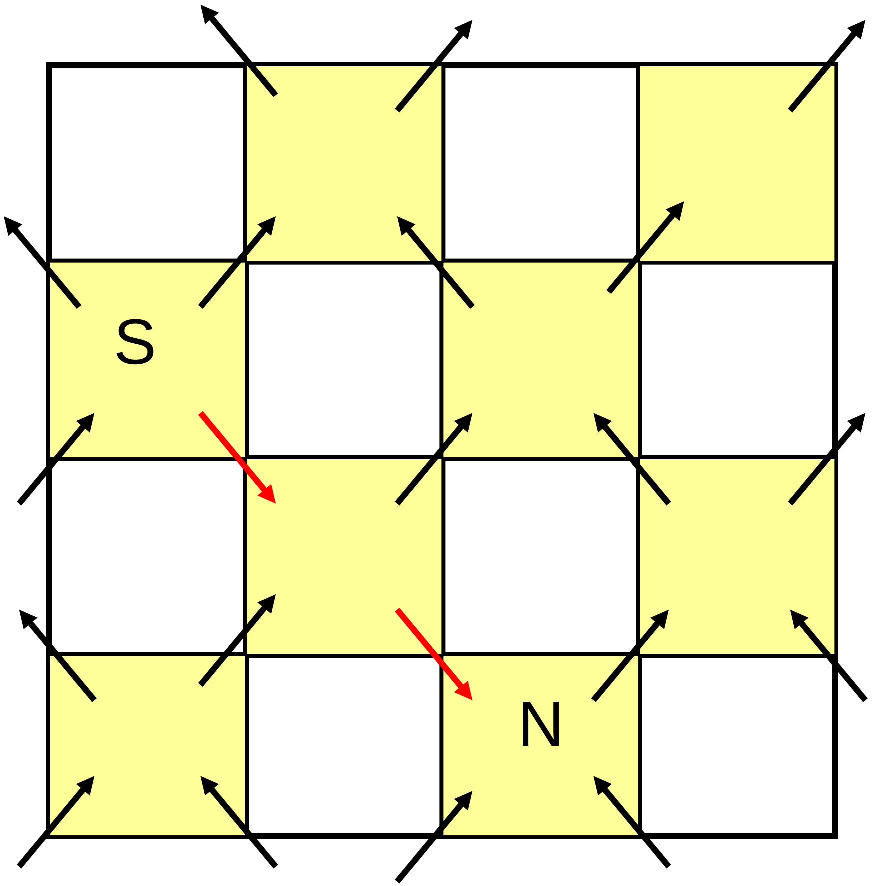
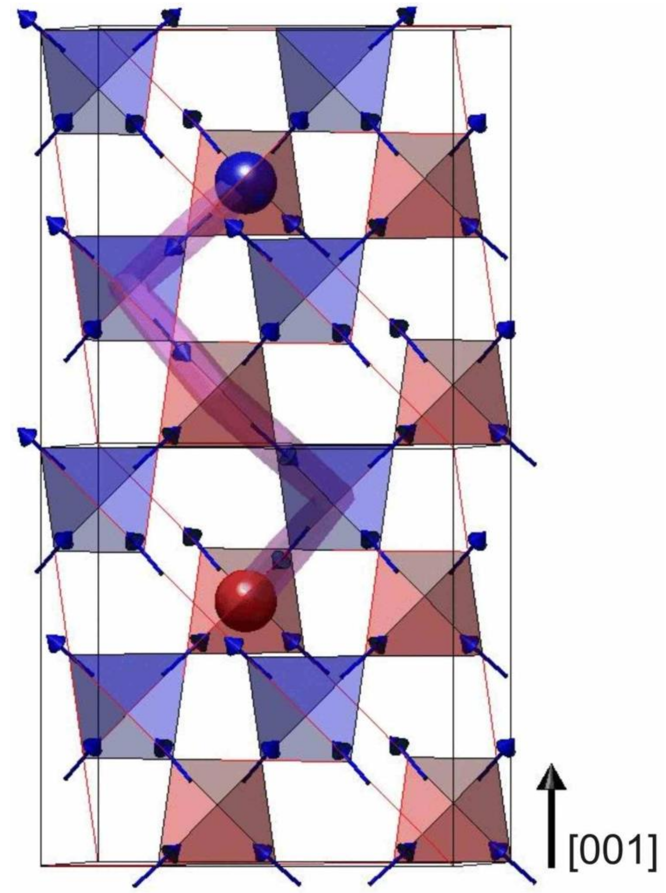


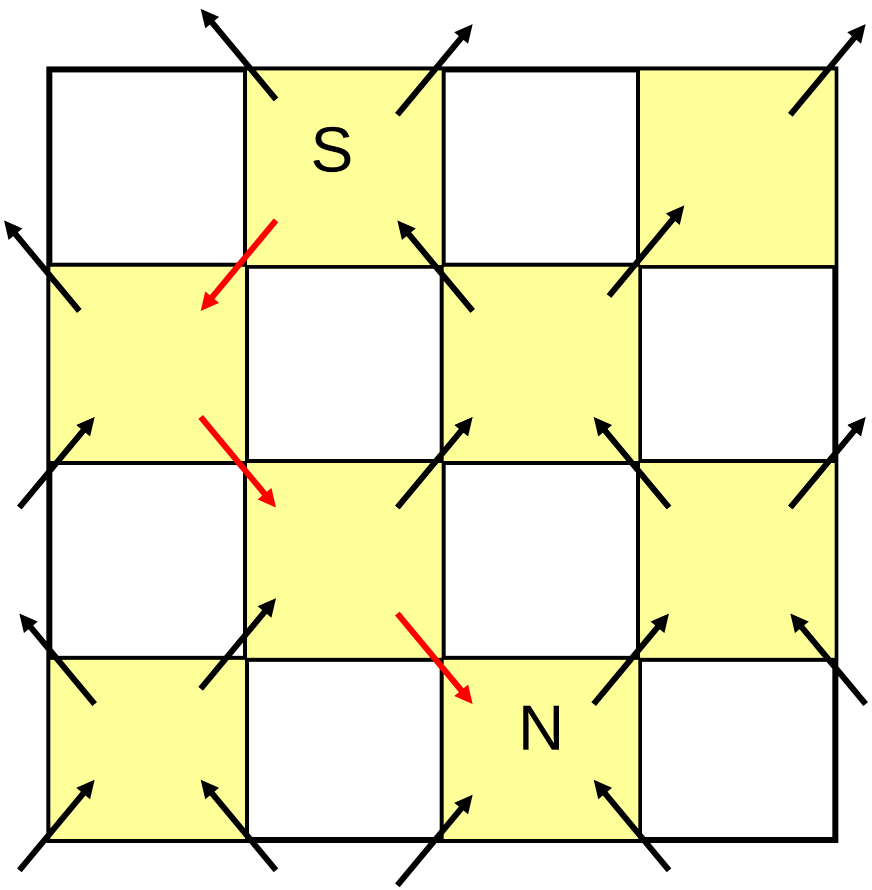


Break ice rule in adjacent tetrahedra
Energy cost ~2K

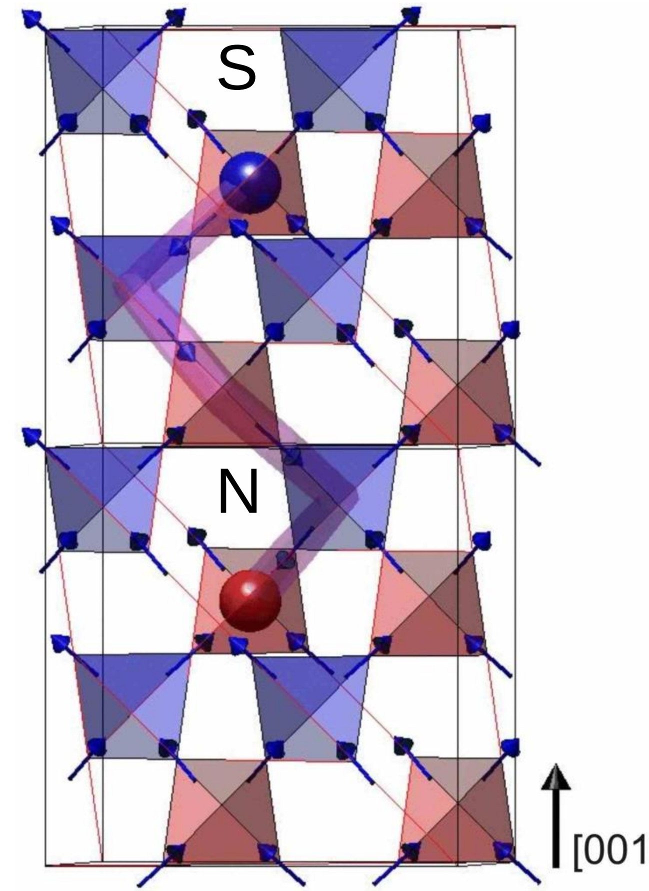




String forms in random walk
Energy cost ~2K



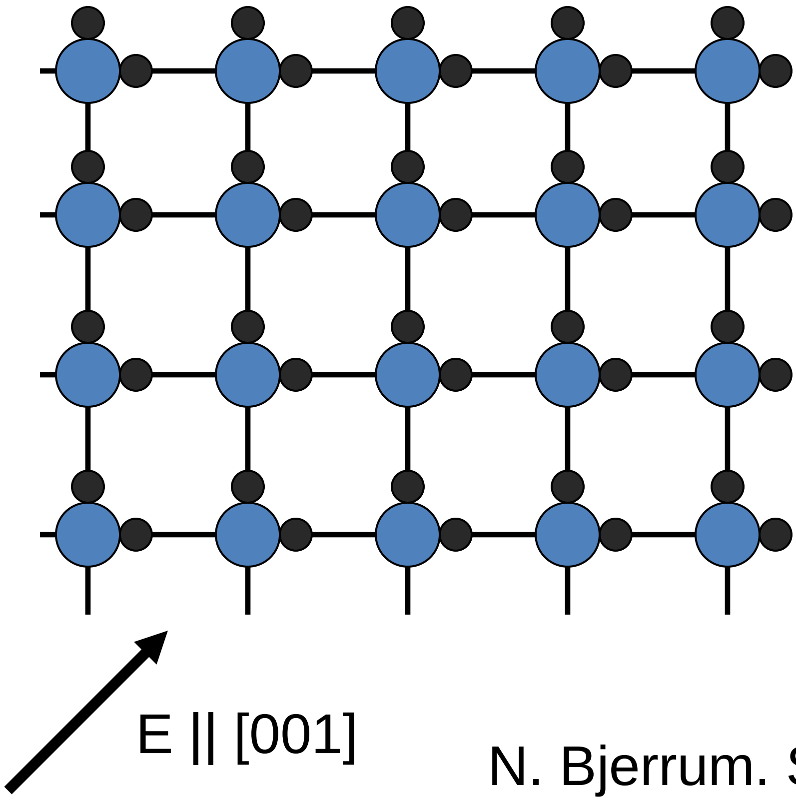
String is tensionless
Energy cost ~2K



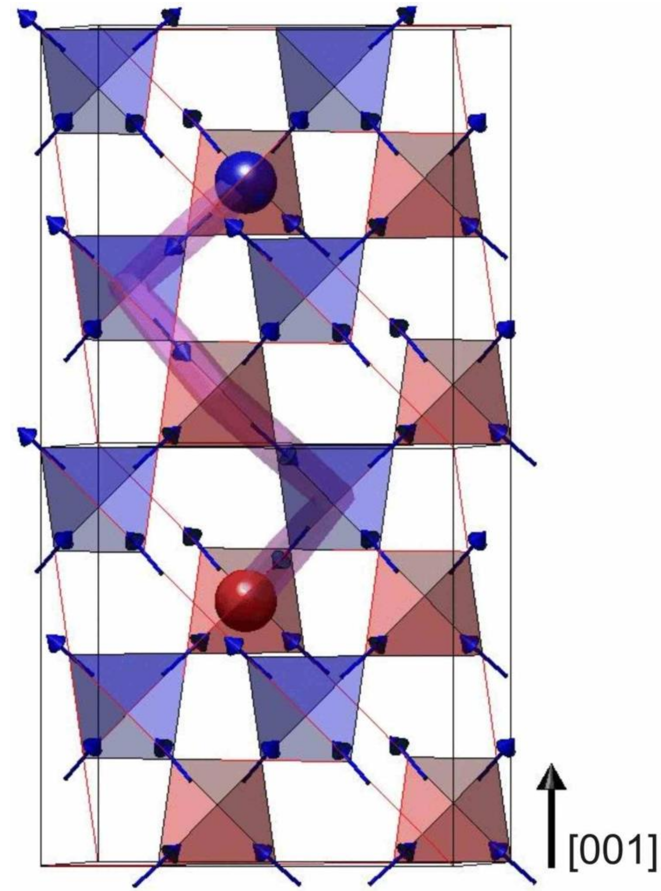
Castelnovo, C., Moessner, R. and Sondhi, S.L. "Magnetic Monopoles in Spin Ice", Nature **451**, 42-45 (2008).

Onsager's Ion Diffusion in Water

Charge movement

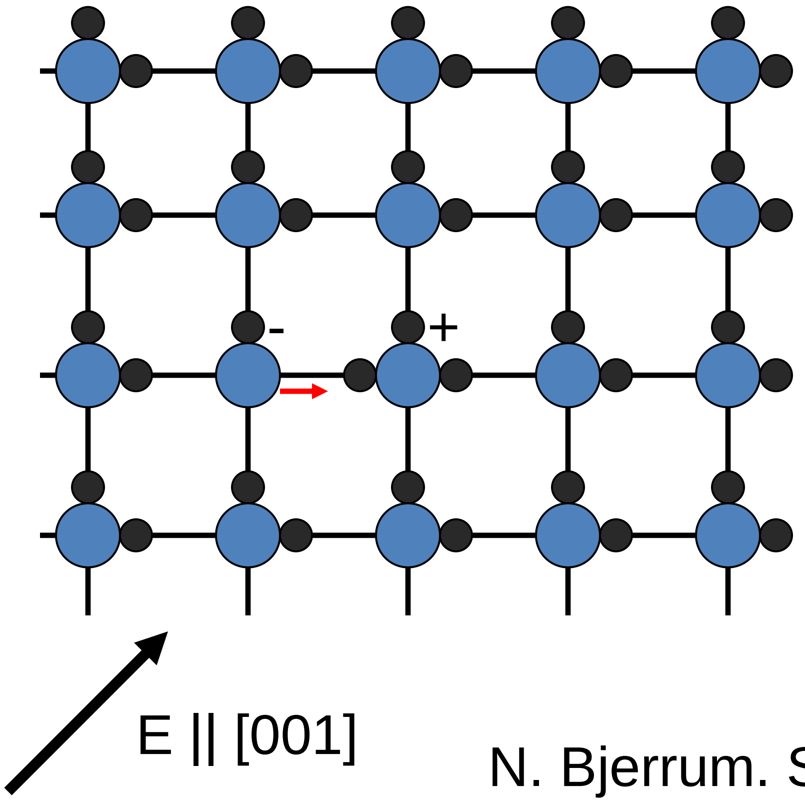


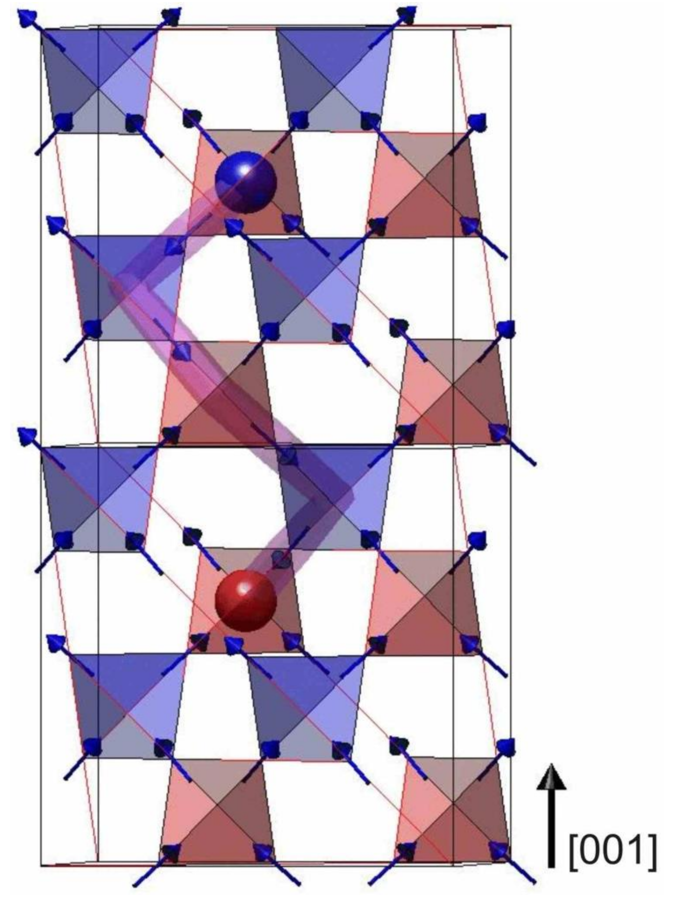
E || [001]



N. Bjerrum. Science **115**, 385 (1952)

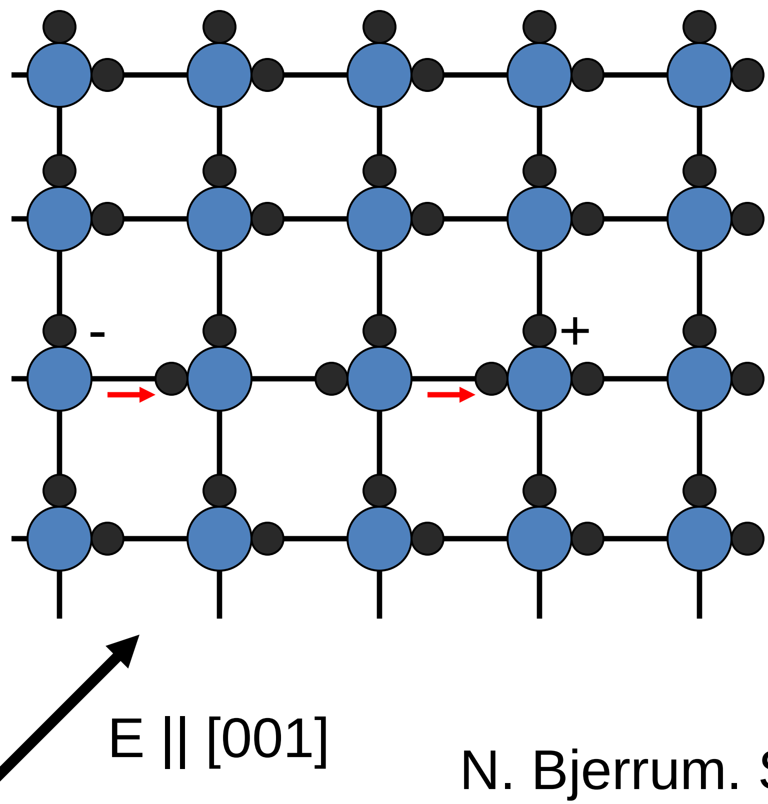
Onsager's Ion Diffusion in Water

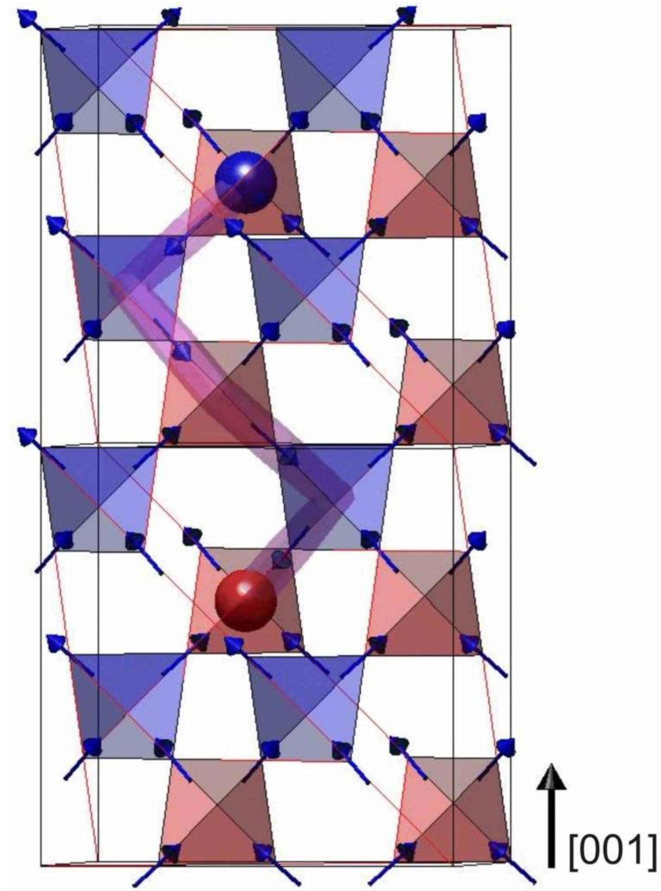




N. Bjerrum. Science **115**, 385 (1952)

Onsager's Ion Diffusion in Water

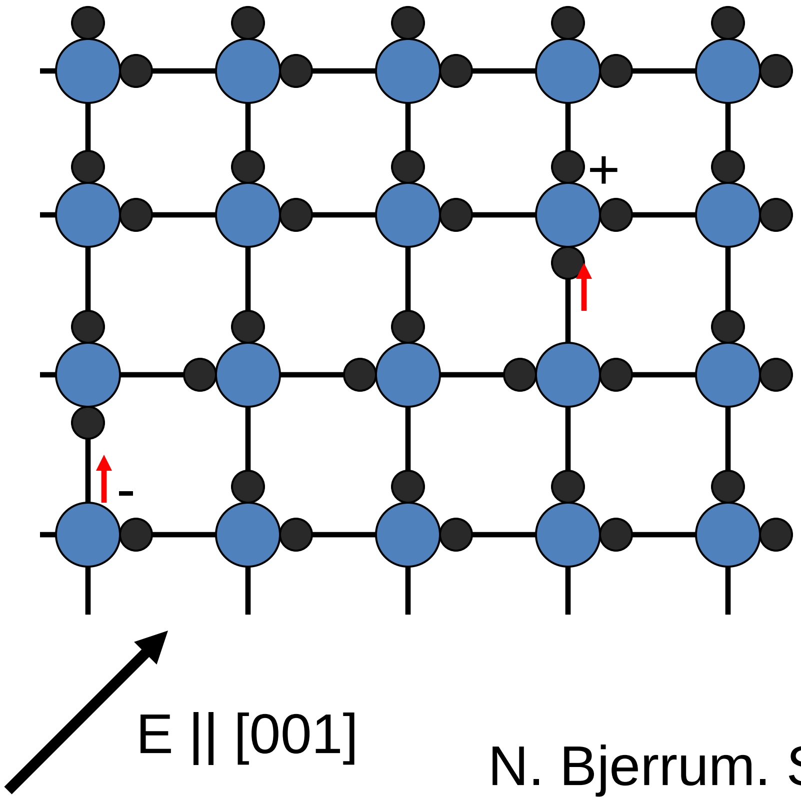


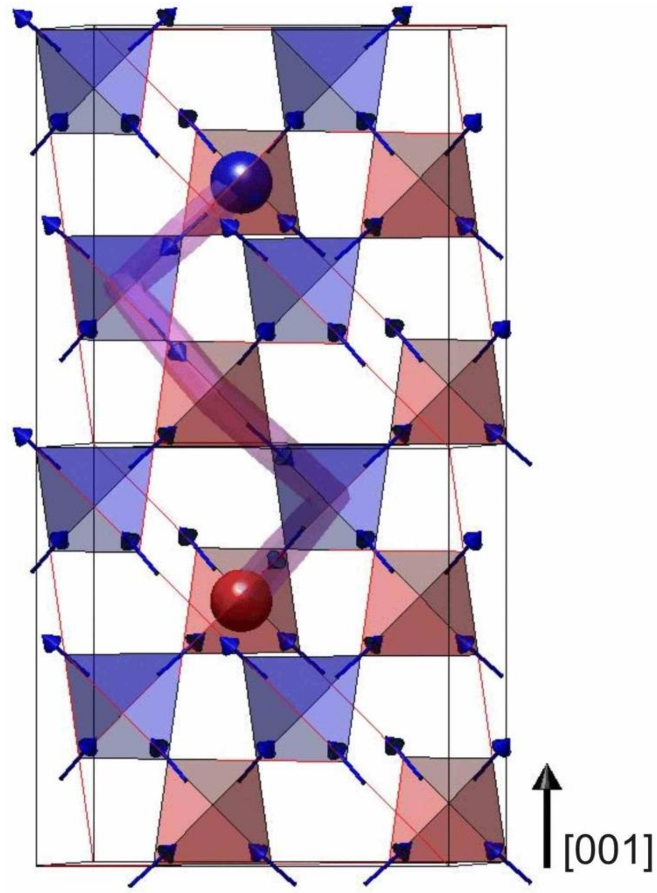


N. Bjerrum. Science **115**, 385 (1952)

Onsager's Ion Diffusion in Water

Random walks in ice

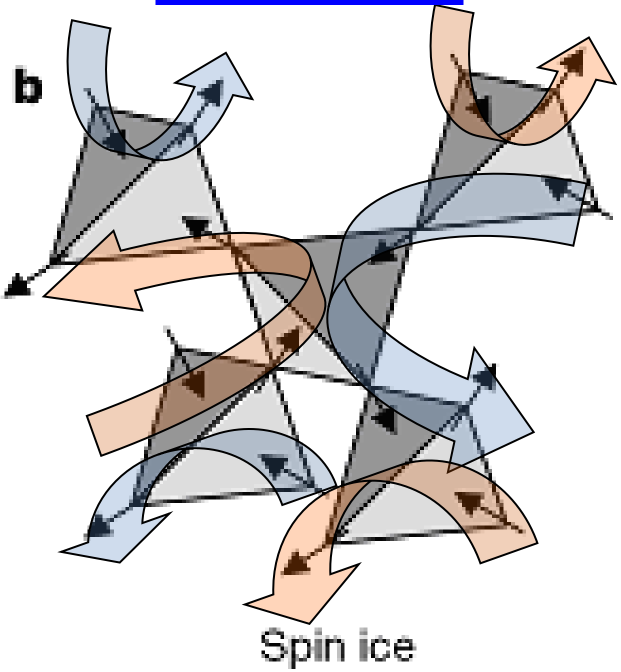


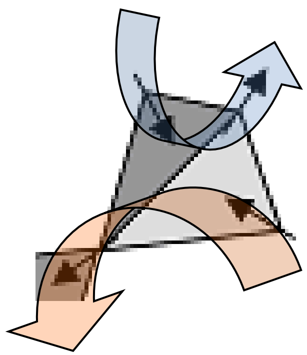


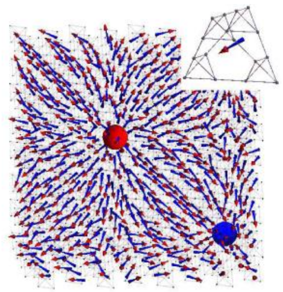
N. Bjerrum. Science **115**, 385 (1952)

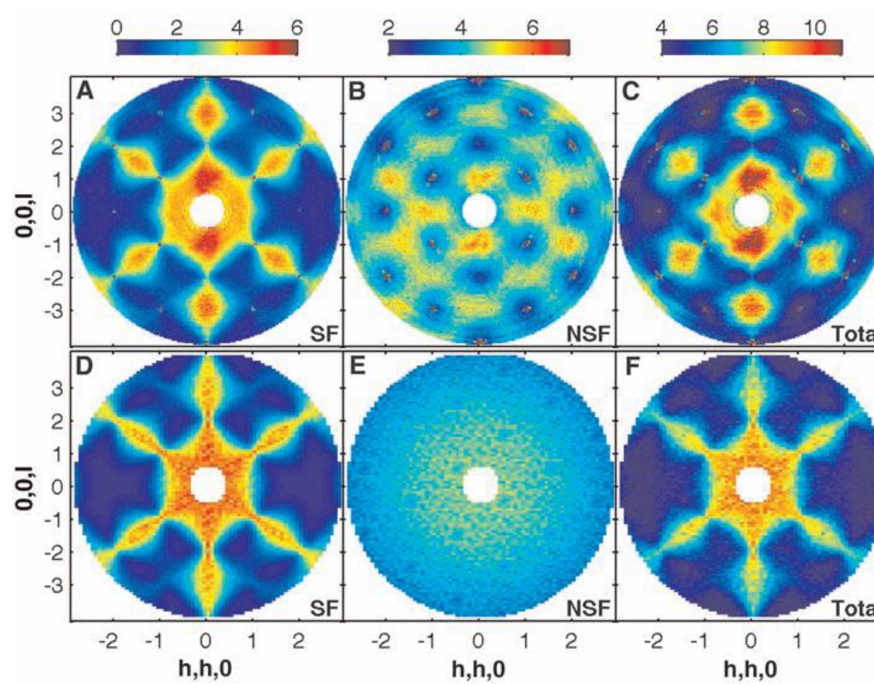
The signature behavior of emergent dipolar correlations are seen by neutrons

Dy2Ti2O7









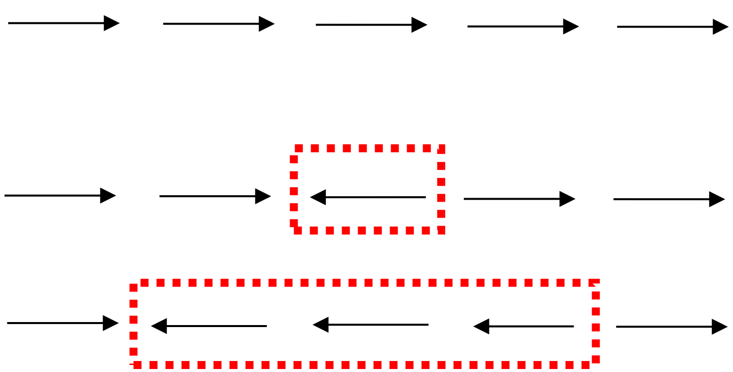
$$\left\langle \widetilde{B}_i^{\alpha}(\mathbf{x})\widetilde{B}_j^{\beta}(0)\right\rangle \propto \delta_{\alpha\beta}\frac{3x_i x_j - r^2\delta_{ij}}{r^5}$$

$$\left\langle \widetilde{B}_i^{\alpha}(\mathbf{k})\widetilde{B}_j^{\beta}(-\mathbf{k})\right\rangle \propto \delta_{\alpha\beta}\left(\delta_{ij} - \frac{q_i q_j}{q^2}\right)$$

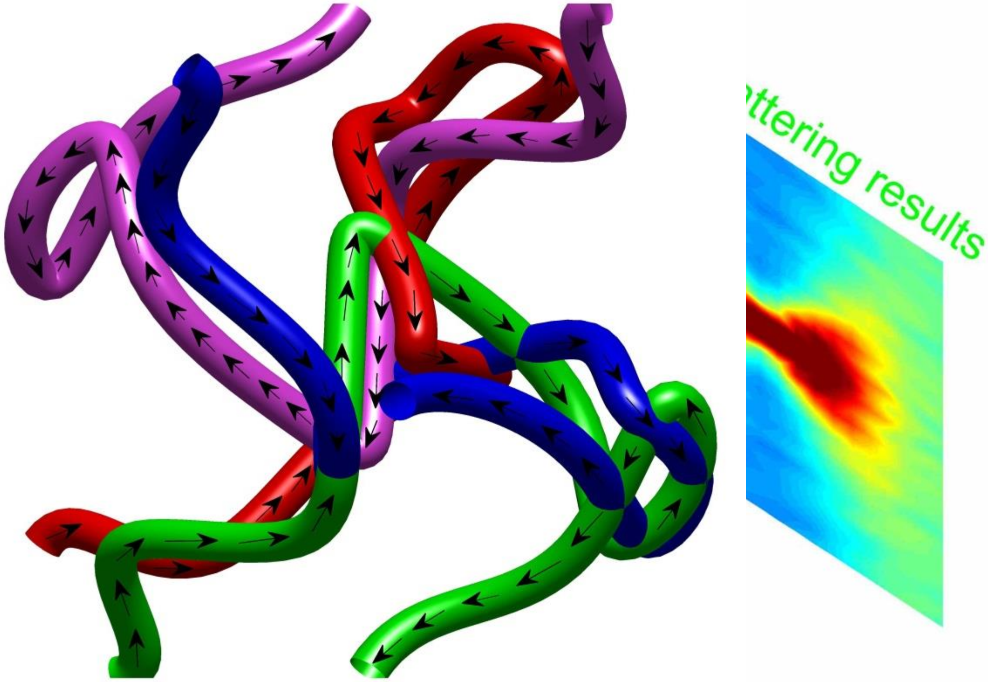
T. Fennell et al.
Science 326, 415 (2009)

Response to a magnetic field shows Dirac strings of monopoles

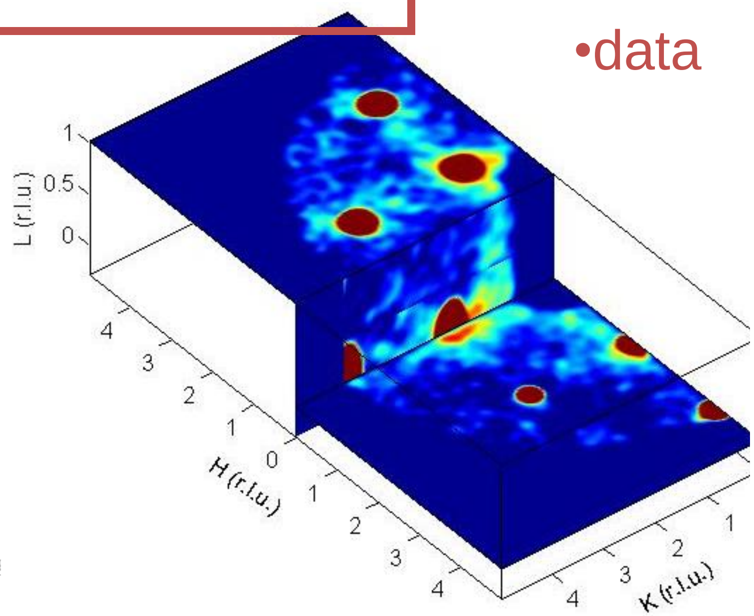
- Defects



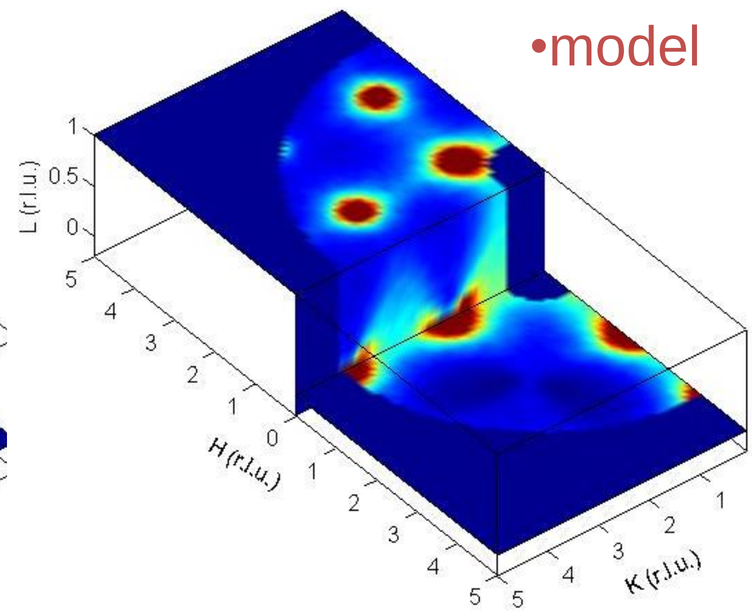
- These deconfine



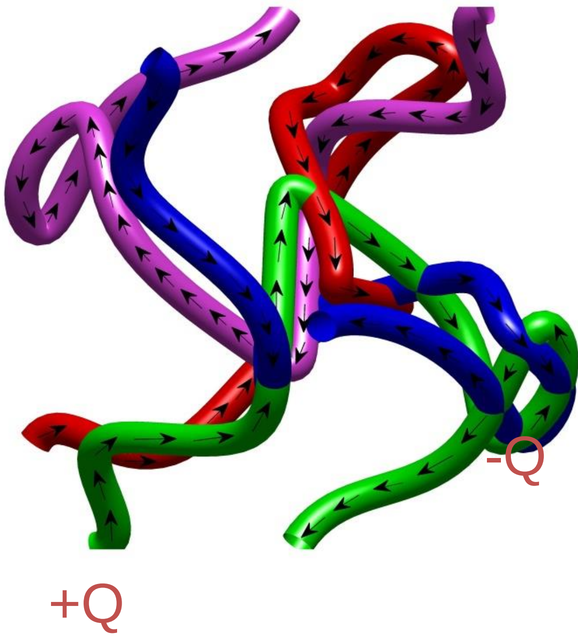
- data

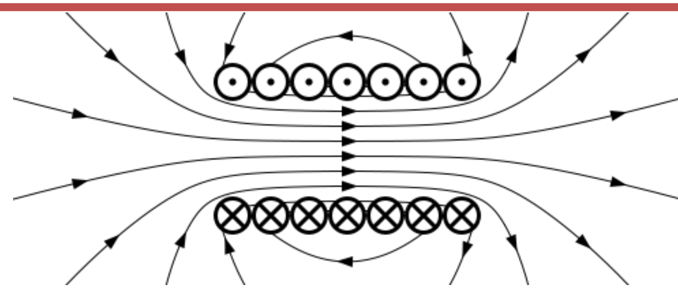


- model



Why it works : gauge fluid configurations are entropic and overcome meanfield confinement effects



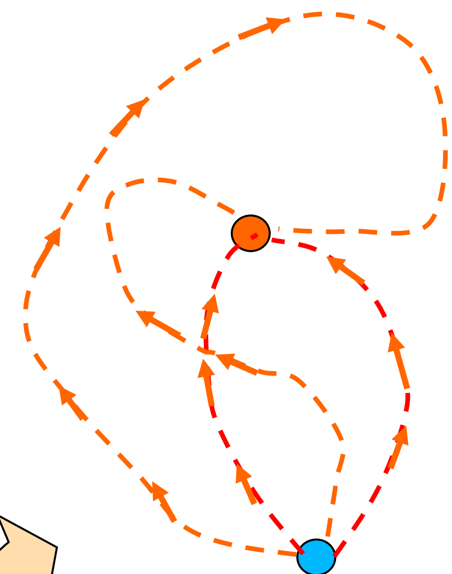


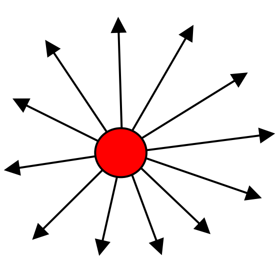
- M efficiently carries B field
- H falls as $1/r^5$

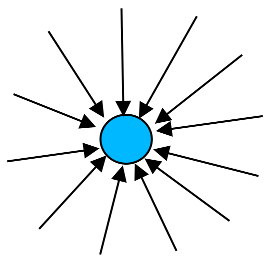
$$\mathbf{B} = \mu_0 \left(\mathbf{H} + \mathbf{M} \right)$$

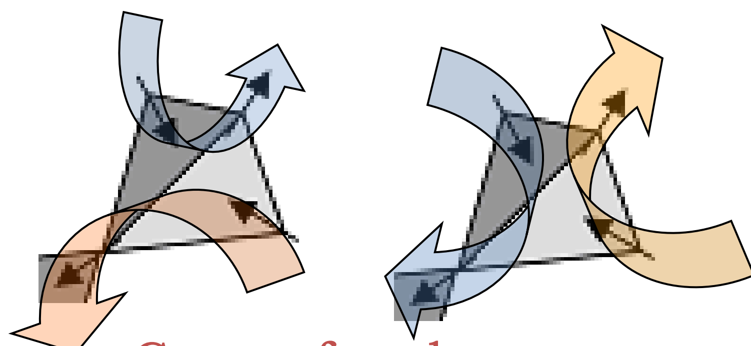
$$\nabla \cdot \mathbf{H} = -\nabla \cdot \mathbf{M} \neq 0$$

No unique path



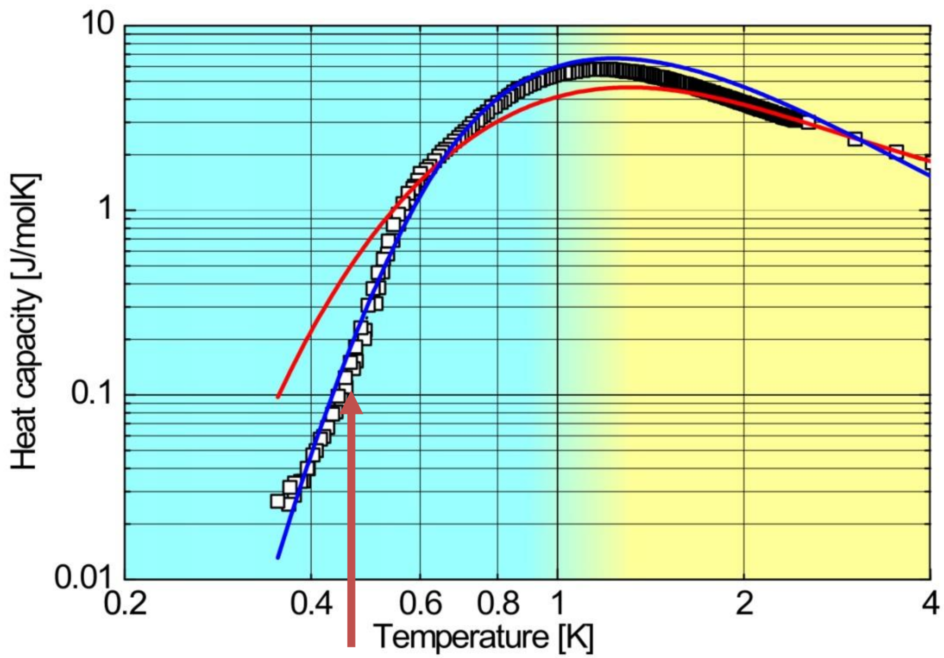






- Gauge freedom
- motifs

Energy of the monopole plasma matches inverse square law and charge

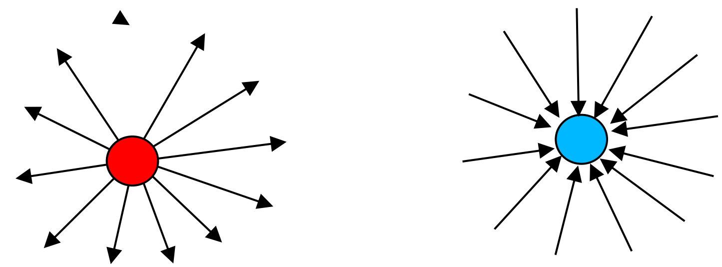


Interacting monopole gas - no adjustable parameters:

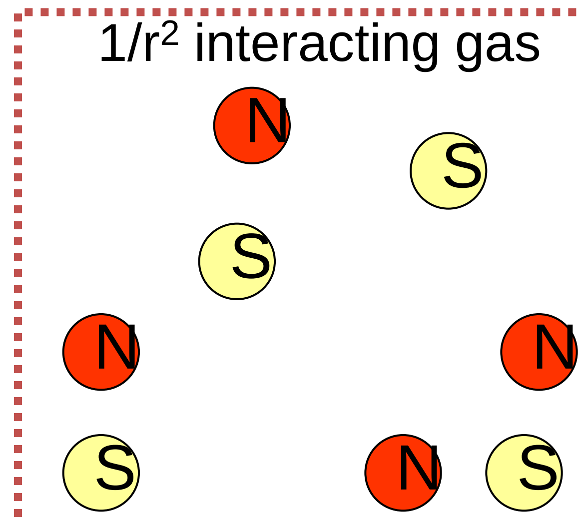
- Q directly derived from lattice
- Debye-Huckel approximation

•+Q

•-Q

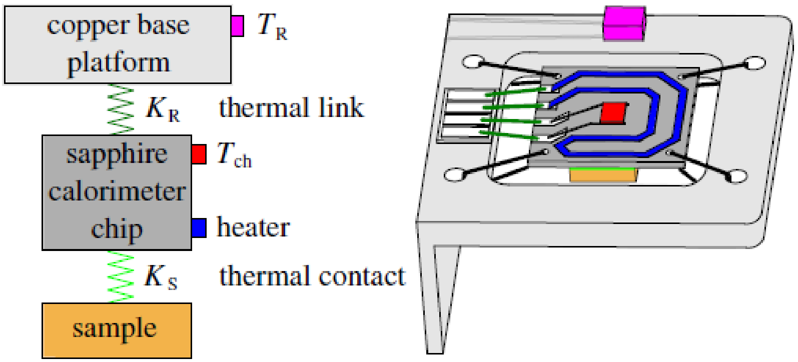


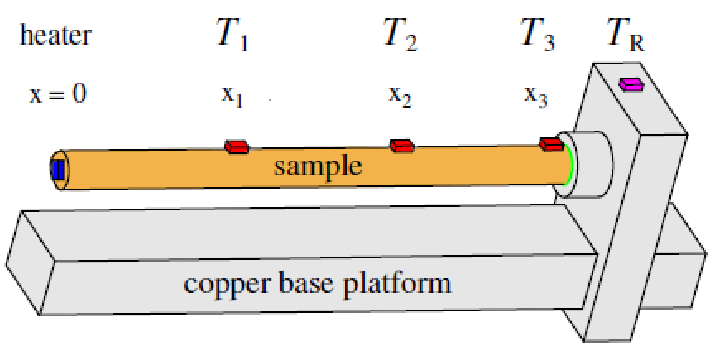
Emergent Monopoles Gas



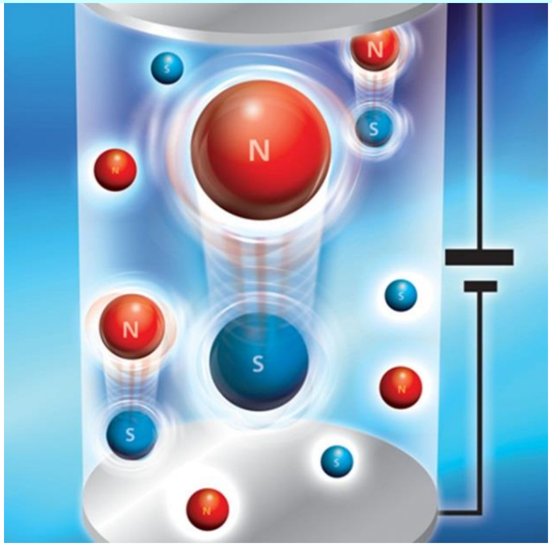
Monopole plasmas are highly controlable and can do non-equilibrium experiments

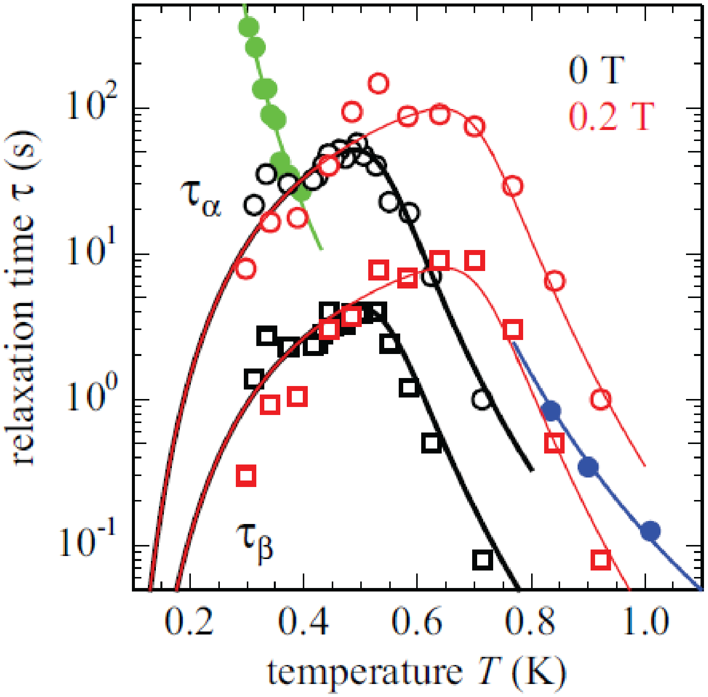
- See monopole recombination time scales
- Screening transition



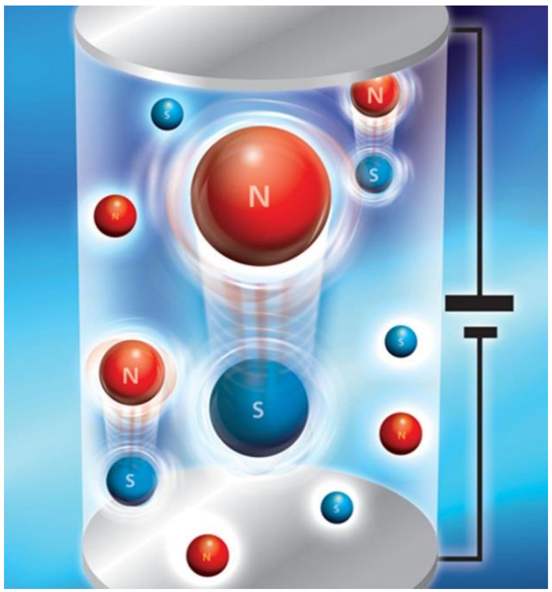


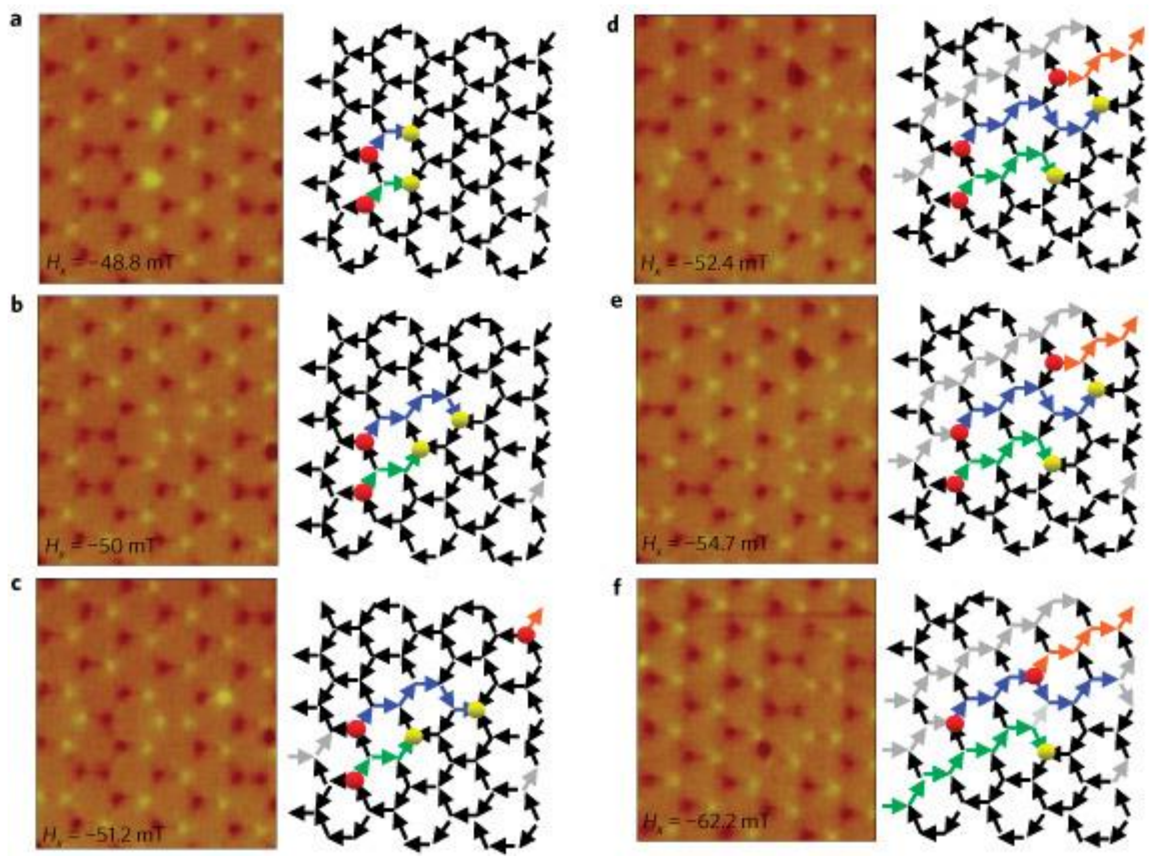
Monopoles flowing carrying magnetic charge





Monopoles can flow in artificial circuits

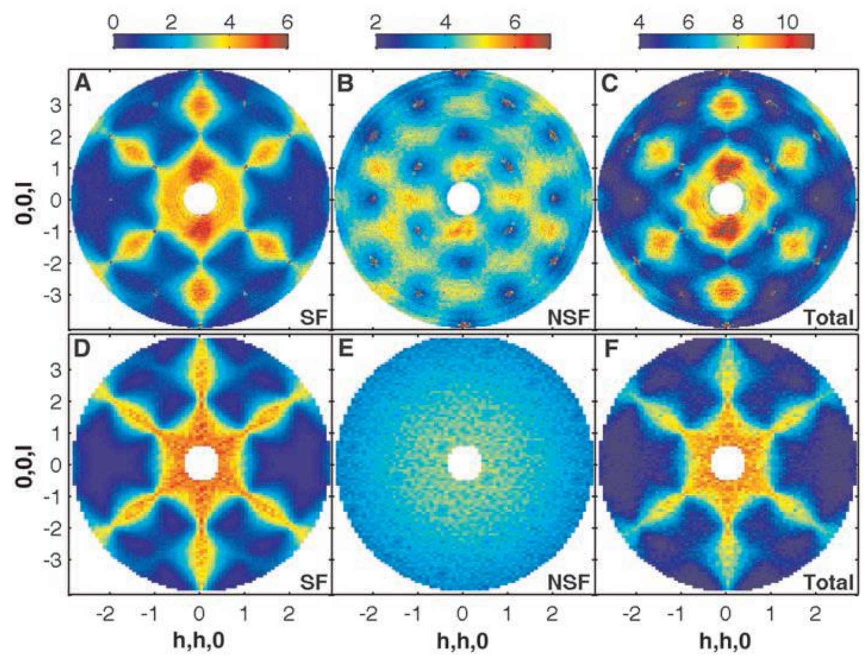




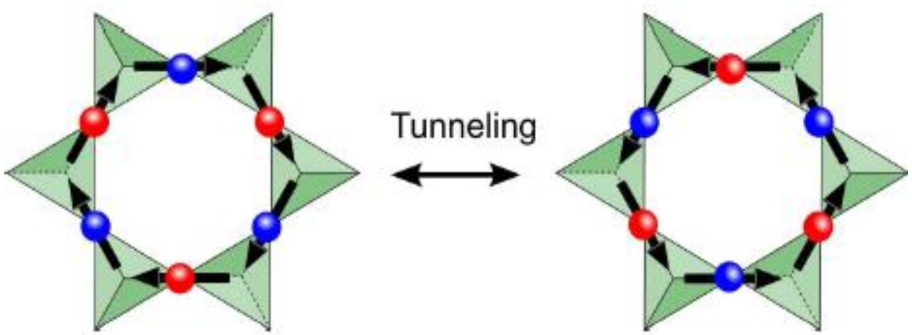
With quantum tunneling emergent electrodynamics is expected

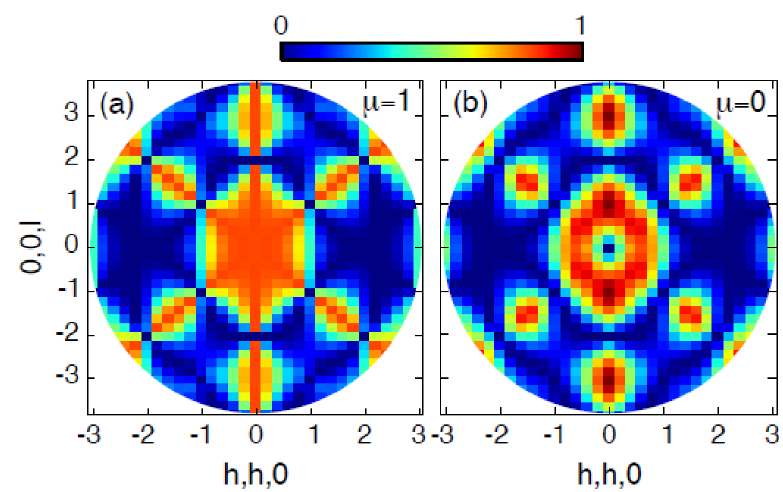
$$\left\langle \widetilde{B}_i^{\alpha}(\mathbf{x})\widetilde{B}_j^{\beta}(0)\right\rangle \propto \delta_{\alpha\beta}\frac{3x_i x_j - r^2\delta_{ij}}{r^5}$$

$$\left\langle \widetilde{B}_i^{\alpha}(\mathbf{k})\widetilde{B}_j^{\beta}(-\mathbf{k})\right\rangle \propto \delta_{\alpha\beta}\left(\delta_{ij} - \frac{q_i q_j}{q^2}\right)$$



Quantum electrodynamics
3+1 dimensions

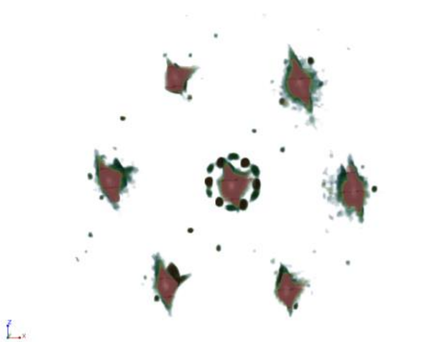




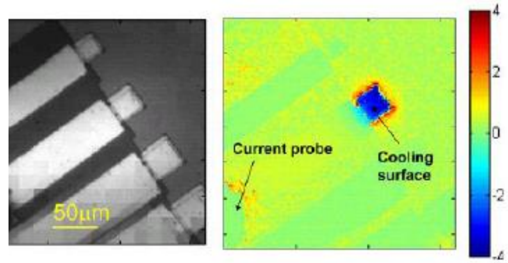
Get the analogue of photons

Coming full circle : water ice as a topological material

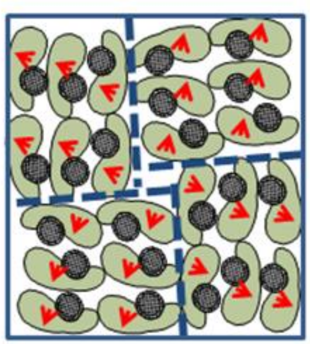
- Use large N theory to model ice
- Gain a full theoretical description



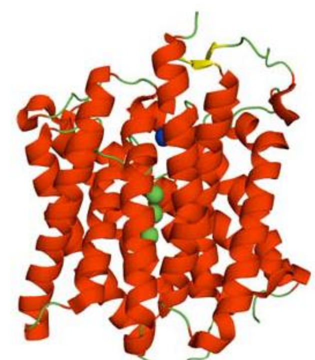
battery materials



thermoelectrics

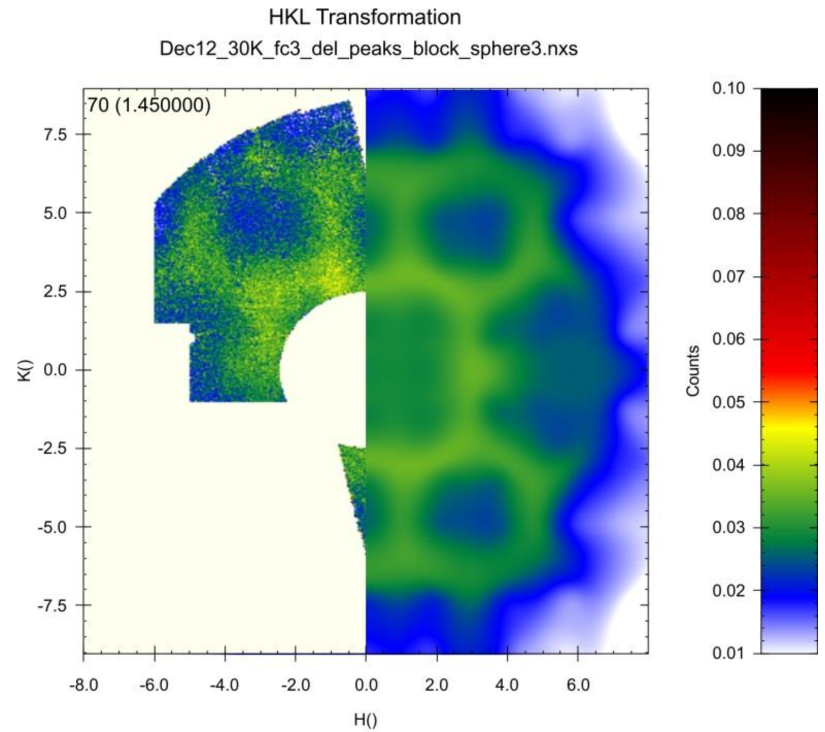


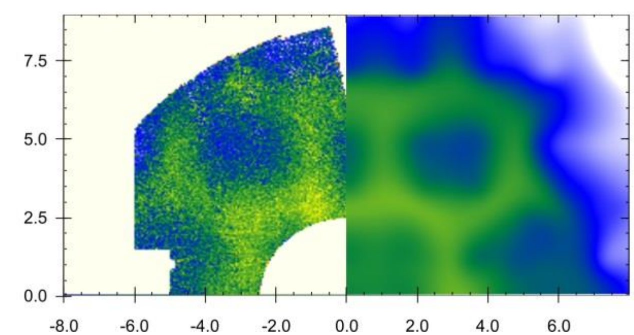
ferroelectrics



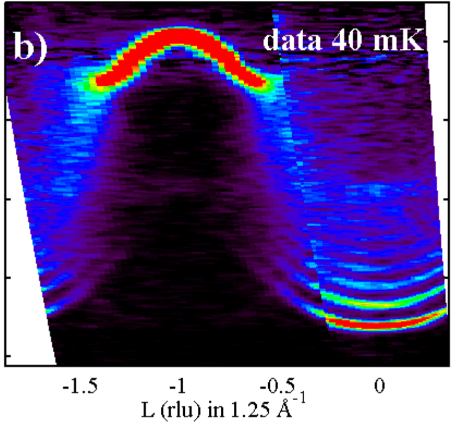
(A)

Proton transport and exchange





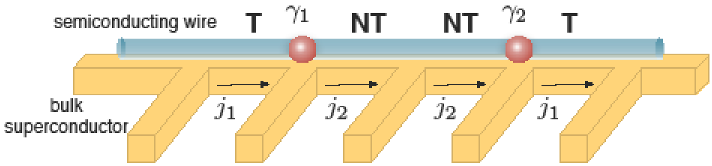
Summary and conclusion

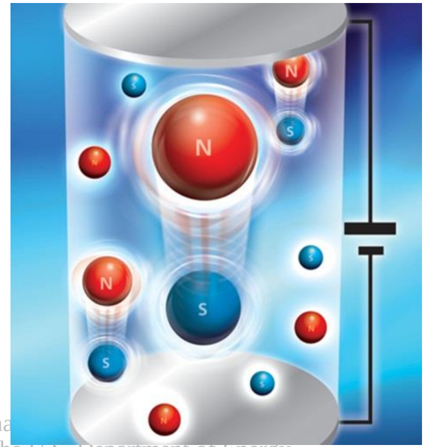


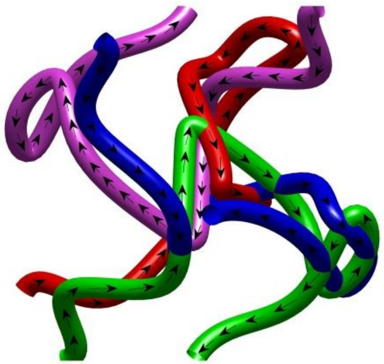
Topological ideas give a new perspective on some old problems

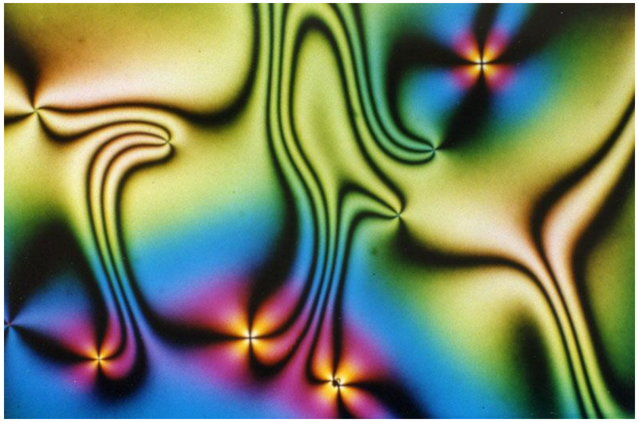
Quantum magnets provide outstanding simulations of the most complex magnetic states

Ideas from magnetism have wider impact on understanding disordered materials









Collaborators

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Dharmalingan Prabhakaran (Oxford)

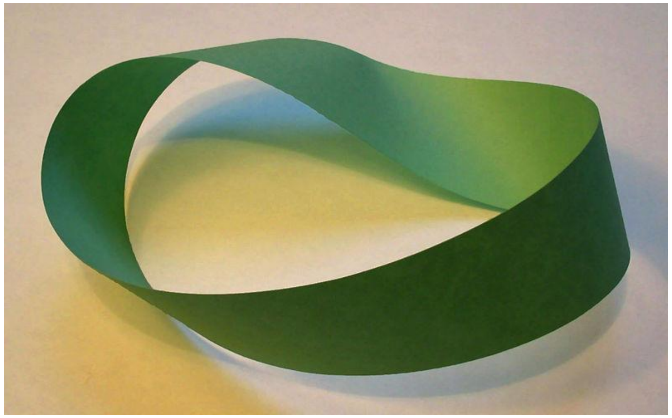
Heisenberg chains
Bella Lake (HZB)
Steve Nagler (ORNL)
Jean-Sebastian Caux (Amsterdam)
Fabian Essler (Oxford)

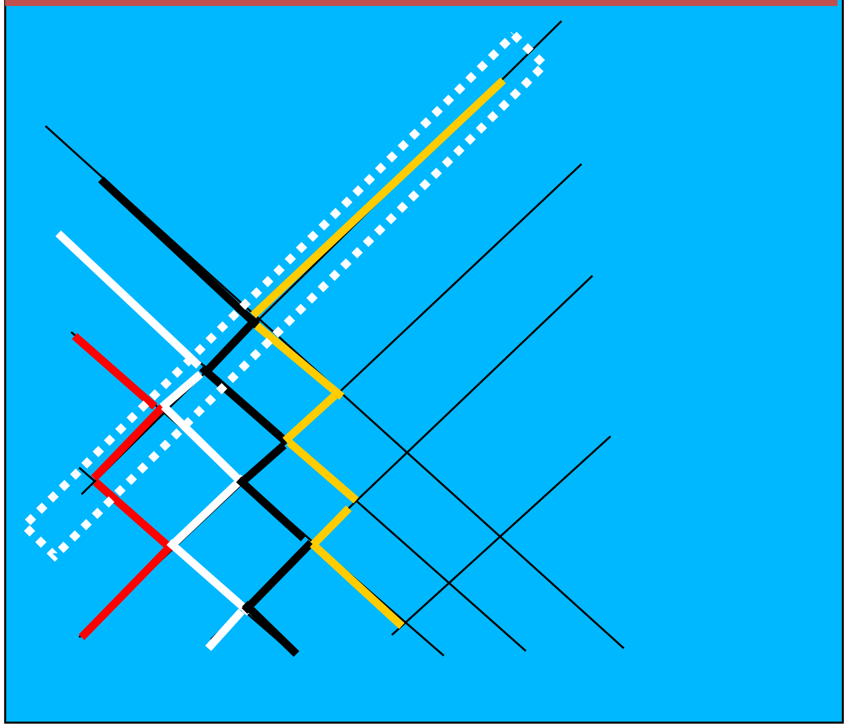
Ladders
Bella Lake (HZB)
Alexei Tsvelik (BNL)
Bernd Büchner (IFW)

Spin ice
Jon Morris (HZB)
Bastian Klemke (HZB)
Santiago Grigera (U. La Plata)
Roderich Moessner (Max-Planck I, Dresden)
Claudio Castelnovo (U London)

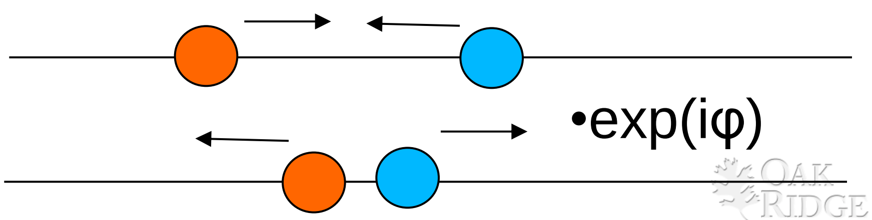
Thank you for your attention

A chain of spins is an integrable system : this gives remarkable physics

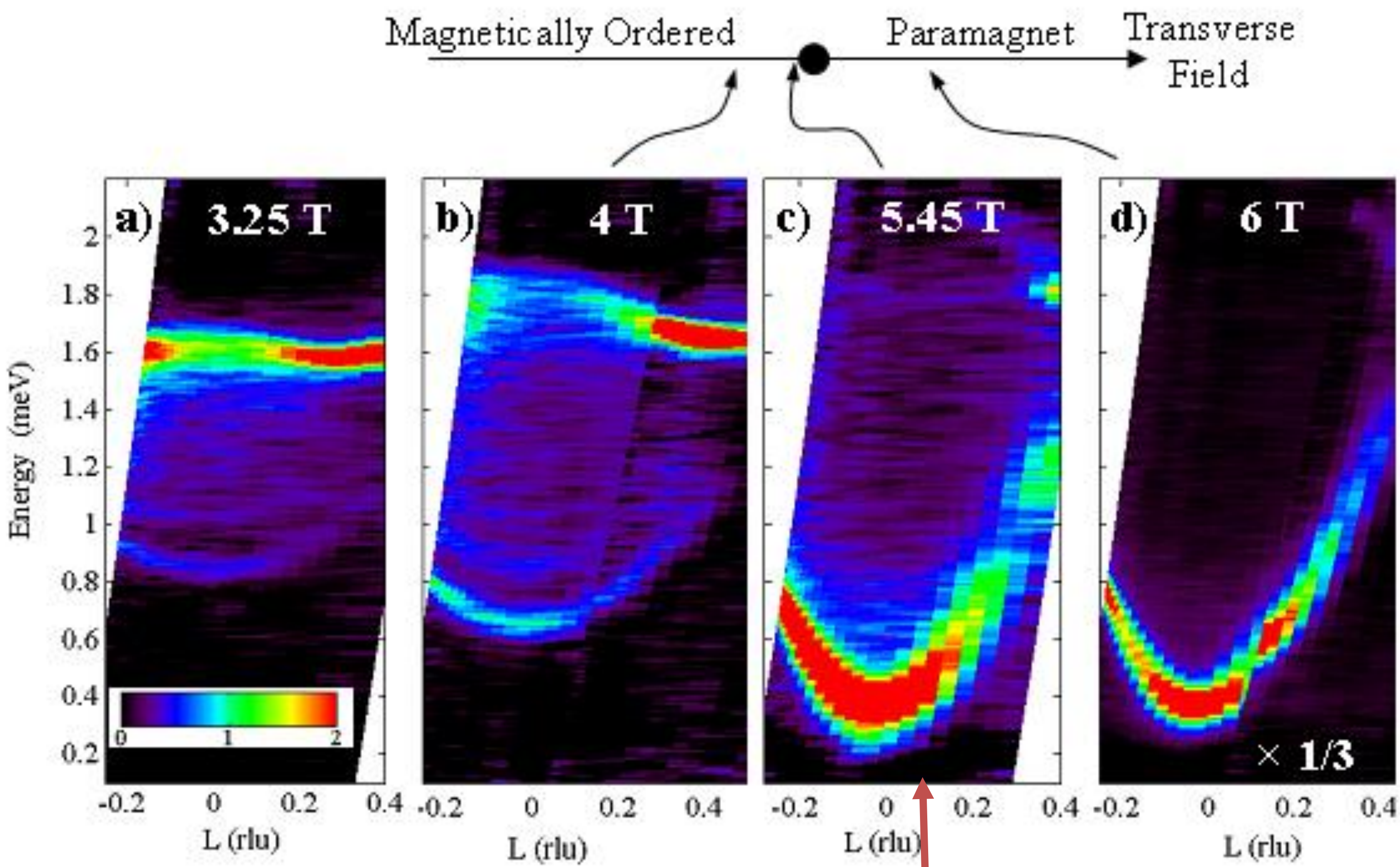




Conservation laws in an integrable quantum system



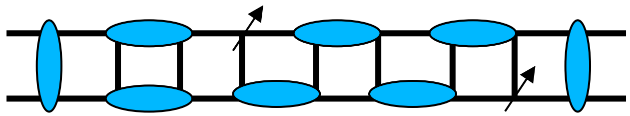
Reflections in a Kaleidoscope

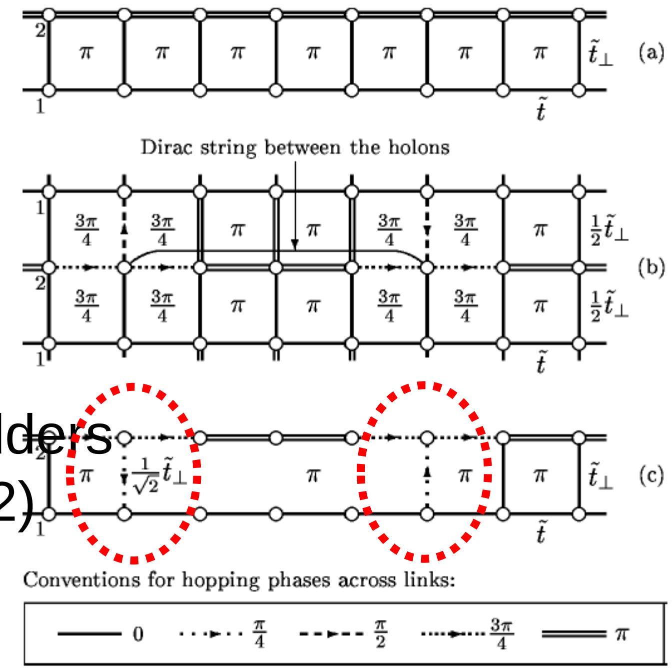


•For CoNb2O6 details don‘t matter near quantum critical point

Near gapless – WZNW QCP

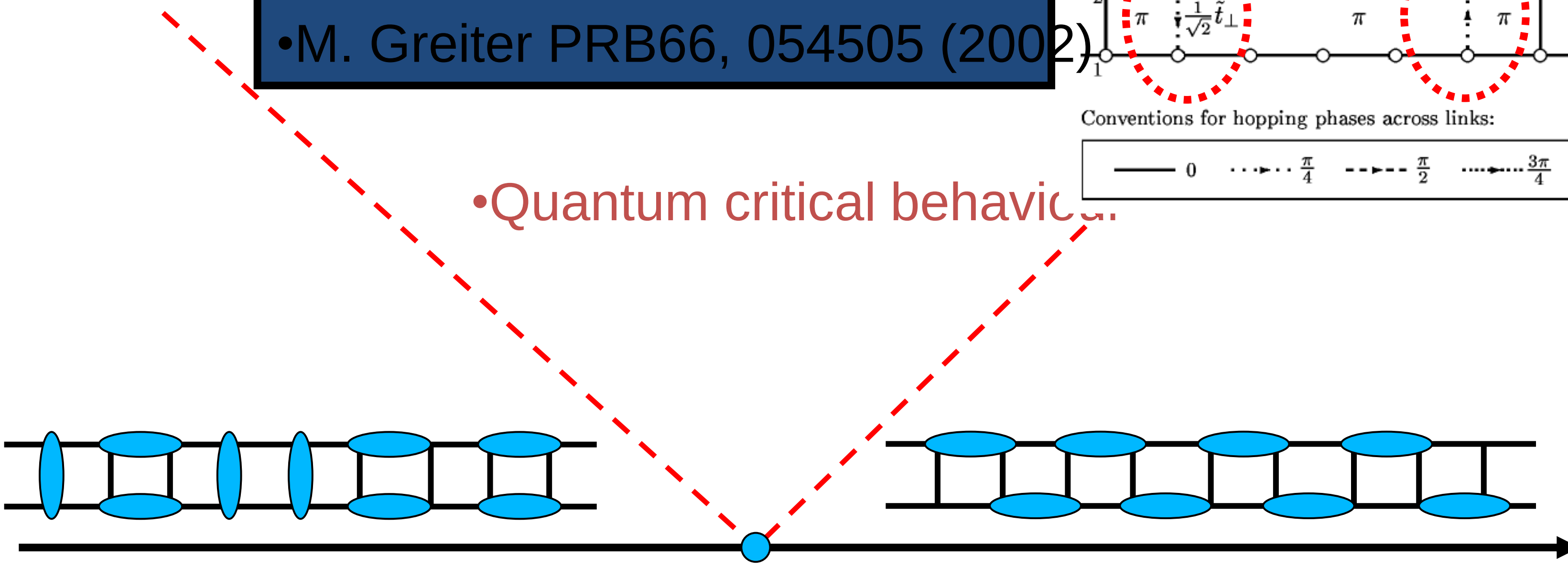
•3rd QCP in 1D : Ladder





•Ficticious flux confinement in ladders

•M. Greiter PRB66, 054505 (2002)



•Quantum critical behavior

•WZNW QCP

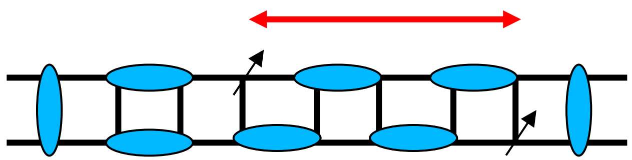
•$J_{cyc}=J_{\perp}/3$

•Cyclic exchange strength

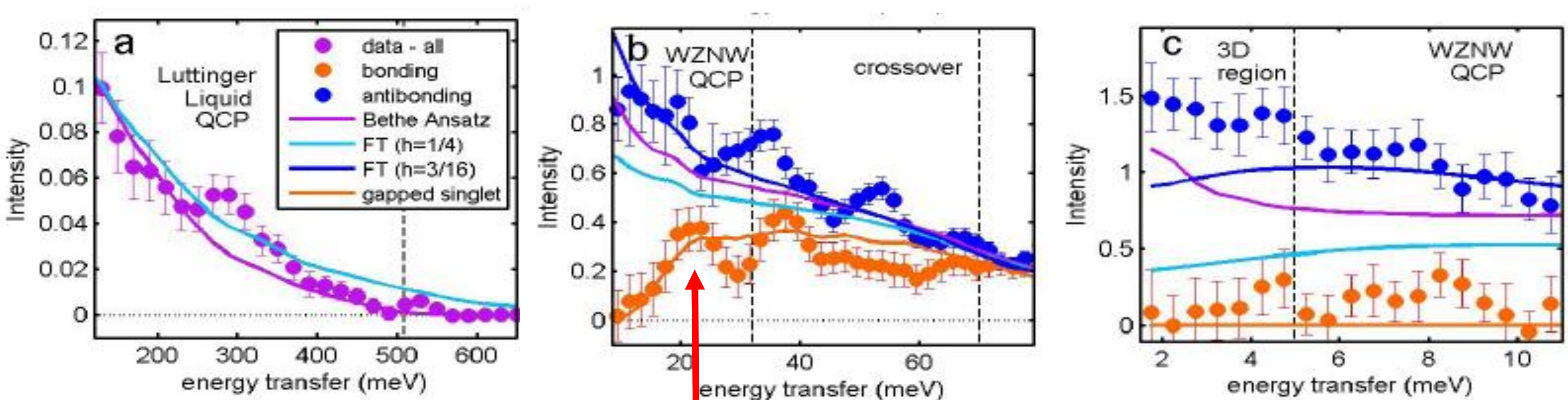
•Confinement like quark pairs to mesons

Wess Zumino Novikov Witten state is seen in spin ladders

WZNW QCP



- Asymptotic confinement
- „quarks pair into mesons“



•Threshhold gap $Q_{\perp}=0$

•Lake, Tsvelik, Notbohm, Tennant, Reehuis, Frost, Büchner, Nat. Phys. Janua