Symmetry, topology, and magnets: Neutrons with a twist

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Symmetry is familiar but topology is also important

Remarkable properties can emerge

Hidden order

Quasicrystals

Symmetry in particle physics

Supersymmetry implies relationships between the fundamental building blocks

Topological states in nature

Vortex is a familiar topological state

Applying topological quantum states

Topological quantum computer
Unexpected symmetries and topologies govern the remarkable properties in quantum materials.
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…

These can carry fractional quantum numbers
- Anderson’s RVB state
- Fractional quantum Hall effect

• Puzzle 15 is split into sectors

• 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 higher 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

\[ H = \sum_{<ij>} [J_{ij}^{z} S_{i}^{z} S_{j}^{z} + J_{ij}^{xy} \left( S_{i}^{x} S_{j}^{x} + S_{i}^{y} S_{j}^{y} \right)] + g \mu_{B} B \sum_{i} S_{i}^{z} \]
Magnets are simulators for many quantum systems

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

\[
V_{ij} = J_{ij}^z
\]

spin flop phase has ODLRO

\[
< a_i^+ a_j^- > \propto < S_i^x S_j^x > + < S_i^y S_j^y >
\]

chemical potential

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

Particle density NS-\langle M \rangle

- \[ S_i^z = \frac{1}{2} - a_i^+ a_i \]
- \[ S_i^x = \frac{a_i^+ + a_i}{2} \]
- \[ S_i^y = \frac{i(a_i^+ + a_i)}{2} \]
- \[ S_i^+ = a_i^-; S_i^- = a_i^+ \]
Neutrons are the most powerful probe of the energy levels and wavefunctions.

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

**Thermoelectric devices**

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

\[ H = J \sum_i S^z_i S^z_{i+1} + h S^x_i = J \sum_i S^z_i S^z_{i+1} + \frac{h}{2} (S^+_i + S^-_i) \]

• Field \( h < h_c \)
  • Two ground states
  ...
  \[ \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \cdots \]
  ...
  \[ \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \downarrow \cdots \]

• Excitations are pairs of kinks
  ...
  \[ \uparrow \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow \uparrow \cdots \]
  ...
  \[ \uparrow \uparrow \uparrow \downarrow \downarrow \uparrow \uparrow \uparrow \cdots \]
  ...
  \[ \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \uparrow \cdots \]

• Field \( h > h_c \)
  • One ground state
  ...
  \[ \cdots \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \rightarrow \cdots \]

• Excitation is spin flip
  ...
  \[ \cdots \rightarrow \rightarrow \leftarrow \leftarrow \rightarrow \rightarrow \cdots \]

“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 temperature

• Order parameter

\[ Q = (0, 0.34(1), 0) \]

\[
\begin{array}{c|c|c|c|c}
\text{Field (T)} & 4.0 & 4.5 & 5.0 & 5.5 & 6.0 \\
\hline
\text{Counts (10^3/sec)} & 0 & 1 & 2 & & \\
\end{array}
\]

\[ \Delta(h) \]

\[ \text{domain-wall quasiparticles} \]
\[ \text{flipped-spin quasiparticles} \]

\[ h_C \]

\[ \text{Transverse Field } h \]
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.

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

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

- Ising resonances
- Kink confinement


G. Mussardo
Intensities and energies follow the E8 predictions

- Modes are observable

- E8 exceptional Lie group give the energy gaps (masses)
  - $m_1 = C h^8_{2/15}$, $C \approx 4.4$
  - $m_2/m_1 = 2 \cos(\pi/5)$
  - And intensities

- Golden Ratio
  - $E_8$ ratio
  - $2 \cos(\pi/5)$
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.

<table>
<thead>
<tr>
<th>Particles in the standard model</th>
</tr>
</thead>
<tbody>
<tr>
<td>u, c, t, γ</td>
</tr>
<tr>
<td>d, s, b, g</td>
</tr>
<tr>
<td>ν_e, ν_μ, ν_τ, Z^0</td>
</tr>
<tr>
<td>e, μ, τ, w^±</td>
</tr>
</tbody>
</table>
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

- $\alpha, \beta, \gamma, \delta, \nu$ critical exponents
- Universality classes: symmetry and dimensionality of system
- Scaling laws e.g. $\gamma = \nu(2 - \eta)$

\[
\begin{align*}
C &\sim |T - T_C|^{-\alpha} \quad \text{Heat capacity} \\
M_0 &\sim (T_C - T)^{\beta} \quad (T < T_C) \quad \text{Order parameter} \\
\chi &\sim |T - T_C|^{-\gamma} \quad \text{Susceptibility} \\
B &\sim M^{\delta} \quad \text{Critical field} \\
\zeta &\sim |T - T_C|^{\nu} \quad \text{Correlation length}
\end{align*}
\]

Near criticality, in the "critical region", $\zeta$ 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
Probing directly the Quantum Critical Volume in space and time

Material KCuF3 realizes a spin $\frac{1}{2}$ 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,
Universal theories for Luttinger liquid and Energy/Temperature scaling confirmed
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

Spinons are stabilised by a Berry’s phase and are special to \( S = 1/2, 3/2, \ldots \)

\[ \hat{H} = J_{||} \sum_r \vec{S}_{r,l} \cdot \vec{S}_{r+1,l} + J_{\perp} \sum_{l,\delta} \vec{S}_{r,l} \cdot \vec{S}_{r,l+\delta} \]
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, …

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

Quantum wires should be very important in the future

Giant thermal conductivity
Superconductivity
Tensor network theory calculates properties

Cuts at constant wavevector

Constant Energy
Tensor network theory calculates properties of data and DMRG.
Tensor network theory calculates properties

**Cuts at constant wavevector**

**Constant Energy**

$T=150K; J=30.24\text{meV}$
Tensor network theory calculates properties
Tensor network theory calculates properties
How to get fractional states in 3D: Deconfinement of magnetic monopoles

Trick to get deconfined defects in 3D comes from ice

Effective spin-1/2 pyrochlore Dy$_2$Ti$_2$O$_7$. 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

\[ S \approx \frac{N}{2} k \ln \frac{3}{2} \]

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

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

Break ice rule in adjacent tetrahedra
Energy cost ~2K
String forms in random walk
Energy cost $\sim 2K$
String is tensionless
Energy cost ~2K

Castelnovo, C., Moessner, R. and Sondhi, S.L.
Onsager’s Ion Diffusion in Water

E $\parallel [001]$

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

\[ \langle \tilde{B}_i^\alpha (x) \tilde{B}_j^\beta (0) \rangle \propto \delta_{\alpha\beta} \frac{3 x_i x_j - r^2 \delta_{ij}}{r^5} \]

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

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.

- $\mathbf{M}$ efficiently carries $\mathbf{B}$ field
- $\mathbf{H}$ falls as $1/r^5$

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

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

Emergent Monopoles Gas

$1/r^2$ interacting gas
Monopole plasmas are highly controlable and can do non-equilibrium experiments

- See monopole recombination time scales
- Screening transition
Monopoles can flow in artificial circuits
With quantum tunneling emergent electrodynamics is expected

\[
\langle \tilde{B}_i^\alpha (x) \tilde{B}_j^\beta (0) \rangle \propto \delta_{\alpha \beta} \frac{3x_i x_j - r^2 \delta_{ij}}{r^5} \\
\langle \tilde{B}_i^\alpha (k) \tilde{B}_j^\beta (-k) \rangle \propto \delta_{\alpha \beta} \left( \delta_{ij} - \frac{q_i q_j}{q^2} \right)
\]

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

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

CoNb2O6
Radu Coldea (Oxford)
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.
• For CoNb2O6 details don't matter near quantum critical point
Near gapless – WZNW QCP

- Fictitious flux confinement in ladders
- M. Greiter PRB66, 054505 (2002)

- Quantum critical behaviour
- WZNW QCP
- Cyclic exchange strength
  - \( J_{\text{cyc}} = J_\perp / 3 \)

- Confinement like quark pairs to mesons
Wess Zumino Novikov Witten state is seen in spin ladders

\[ WZNW \text{ QCP} \]

- Asymptotic confinement
- “quarks pair into mesons”

\[ \text{Threshold gap } Q_{\perp}=0 \]