Scattering Neutrons from Magnons, Spinons, Solitons, and Breathers

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- Neutron Scattering and 1D magnetism
- Spin-1 chains
- Toward Quantum Criticality
  - strongly interacting dimers (PHCC)
  - Quantum critical spin-1/2 chain
- Field Effects at Criticality
  - $H>0$: Extended Critical phase
  - $h_s>0$: From spinons to solitons
- Conclusions
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Neutron Scattering and 1D Magnetism
Magnetic Neutron Scattering

\[ \hbar Q = p_i - p_f \]

\[ \hbar \omega = E_i - E_f \]

The scattering cross section is proportional to the Fourier transformed dynamic spin correlation function

\[ S^{\alpha \beta}(Q, \omega) = \frac{1}{2\pi\hbar} \int dt \ e^{-i\omega t} \frac{1}{N} \sum_{RR'} e^{iQ(R-R')} \langle S^\alpha_R(t) S^\beta_{R'}(0) \rangle \]
NIST Center for Neutron Research
\[
S^{\alpha\beta}(Q, \omega) = \frac{1}{2\pi\hbar} \int dt \, e^{-i\omega t} \frac{1}{N} \sum_{RR'} e^{iQ \cdot (R-R')} < S^{\alpha}_{R}(t) S^{\beta}_{R'}(0) >
\]
Better Instrumentation at Existing Sources

[Graph showing neutron flux and energy distribution with annotations for 2 cm and 4 cm distances]

Jose A. Rodriguez, NIST
20+20 Channel MACS detection system
Spallation Neutron Source at ORNL, TN

Neutrons + B>30 Tesla

One of 18 instruments
Magnons and their decay in spin-1 chains
Neutrons Create magnons in spin-1 chain

\[ \text{NENP} = \text{Ni}(\text{C}_2\text{H}_8\text{N}_2)_2\text{NO}_2\text{ClO}_4 \]

Ma et al. PRL (1992)
Spin-correlation function of the $S=1$ antiferromagnetic Heisenberg chain at $T=0$

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The correlation function $\rho(l) = \langle S_i S_{i+l} \rangle$ is calculated for the spin-1 Heisenberg antiferromagnetic chain ($H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}, \vec{S}_{N+1} = \vec{S}_1$) at the ground state. Using the Monte Carlo method of Hirsch, Sugar, Scalopino, and Blankenbecler, we find that $\rho(l)$ decays exponentially in contrast to the $S = \frac{1}{2}$ case where $\rho(l)$ decays algebraically. This fact coincides with Haldane’s prediction and recent numerical calculations. We calculate the upper bound of elementary excitation from the structure factor using a variational method which resembles the Feynman theory for elemen-

FIG. 5. Elementary excitation $\epsilon(q)$ and $g(q)$ defined in (13) for $S=1$ AFH chain in units of $J$. Circles are elementary excitation with total spin one and momentum $q$ of the $N=14$ chain which is taken from the Parkinson and Bonner’s table in Ref. 6. Crosses are $g(q)$ for the $N=32$ chain.

\[
\epsilon(q) = \frac{[\epsilon(q) + \epsilon(-q)]}{2} \leq \frac{1}{2} \frac{\langle \psi | S^z_{-q} H S^z_q + S^z_q H S^z_{-q} | \psi \rangle}{\langle \psi | S^z_{-q} S^z_q | \psi \rangle} - E_0 = \frac{1}{2} \frac{\langle \psi | [S^z_{-q}, [H, S^z_q]] | \psi \rangle}{\langle \psi | S^z_{-q} S^z_q | \psi \rangle} = \frac{J (1 - \cos q) \left[ -N^{-1} \sum_i \langle S^z_i S^z_{i+1} + S^z_i S^z_{i+1} \rangle \right]}{S(q)} = \frac{J (1 - \cos q) [\rho(1) - \rho(1)]}{S(q)} \equiv g(q)
\]
Single mode approximation for spin-1 chain

\[ \hbar \omega \text{ (meV)} \]

\[ S_{\parallel}^{\parallel}(q) \]

Ma et al. PRL (1992)

Dispersion relation

Equal time correlation function
Excitation spectra of $S = 1$ antiferromagnetic chains

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The dynamical structure factor $S(Q, \omega)$ of the $S = 1$ antiferromagnetic Heisenberg chain with length 20 at zero temperature is calculated. The lowest-energy states have the $\delta$-function peak at the region $\pi \geq |Q| > 0.3\pi$. At $|Q| < 0.3\pi$ the lowest-energy states are the lower edge of the continuum of the scattering state, the strength of which decreases for large systems. This gives a reasonable explanation for the experimental fact that no clear peak is observed at the region $Q < 0.3\pi$. This situation is more apparent for the valence-bond solid state. On the contrary for $S = \frac{1}{2}$ antiferromagnetic Heisenberg chain the lowest-energy states are always the edge of the continuum.
Neutrons Create magnons in spin-1 chain

Ma et al. PRL (1992)
Approaching Quantum Criticality
Strongly Interacting Dimers in PHCC

\((\text{C}_4\text{H}_{12}\text{N}_2)\text{Cu}_2\text{Cl}_6\) (PHCC)

\(\hat{\hbar}\omega \text{ (meV)}\)

\(2\Delta < E_{\text{max}}\)

Stone et al. PRB (2001)
Magnon decay in two-magnon continuum

**Uniform spin chain: Unbound spinons**

\[ \text{Cu(C}_4\text{H}_4\text{N}_2)(\text{NO}_3)_2 \]

Stone et al. (2003).

a Data, CuPzN H=0

\[ \tilde{\Gamma} (1/\text{meV}) \]

\[ \hbar \omega (\text{meV}) \]

\[ \tilde{q} / \pi \]
Finite T scaling at the QCP

Exact low energy scaling form is known for spin-1/2 chain:

\[
\chi''(q\omega) = \frac{\pi}{k_B T} \text{Im} \left[ \rho\left( \frac{\hbar \omega - v(q - \pi)}{4\pi k_B T} \right) \rho\left( \frac{\hbar \omega + v(q - \pi)}{4\pi k_B T} \right) \right]
\]

Here we measure the q-integrated “local” response:

\[
\chi''(\omega) = \int dq \chi''(q\omega) \sim \frac{1}{J} \tanh\left( \frac{\hbar \omega}{k_B T} \right)
\]

H. J. Schultz PRB (1986)
Local response of spin-1/2 chain

\[
\chi''(\omega) = \int dq \chi''(q\omega) \sim \frac{1}{J} \tanh \left( \frac{\hbar \omega}{k_B T} \right)
\]
Spin-$\frac{1}{2}$ chain in uniform field
Spinons in magnetized spin-$\frac{1}{2}$ chain

(XY case for simplicity)
Uniform Spin $\frac{1}{2}$ chain

Stone et al. (2003)
Uniform Spin $\frac{1}{2}$ chain

Stone et al. (2003)
Spin-$\frac{1}{2}$ chain in a staggered field
Why staggered field yields bound states

Zero field state quasi-long range AFM order

Without staggered field distant spinons don’t interact

With staggered field solitons separate “good” from “bad” domains, which leads to interactions and bound states
Spin-$\frac{1}{2}$ chain with two spins per chain unit

\[ H = \sum_n \left( J S_n \cdot S_{n+1} + D_n S_n \times S_{n+1} - \mu_B H g_n S_n \right) \]

\[ = \sum_n \left( J S_n \cdot S_{n+1} - \tilde{H} S_n^z - h_s (-1)^n S_n^x \right) \]

\[ h_s \sim \left( \frac{g_1 - g_2}{2} \right) H + \frac{1}{2J} D \times \left( \frac{g_1 + g_2}{2} \right) H \]

Xia and Riseborough (1988)

Oshikawa and Affleck (1997)
H=0 T

\[ \tilde{q} (\pi) \]

\[ \hbar \omega \text{(meV)} \]

Kenzelmann et al. (2003)
Bound states from 2-spinon continuum

\[ \tilde{q} = \pi \]

\[ \tilde{q} = 0.77\pi \]

Kenzelmann et al. (2003)
Sine-Gordon mapping of spin-1/2 chain

Effective staggered + uniform field spin hamiltonian

\[ H_{\text{eff}} = \sum_n \left( J \tilde{S}_n \cdot \tilde{S}_{n+1} - \tilde{H}\tilde{S}_n^z - h_s (-1)^n \tilde{S}_n^x \right) \]

Spin operators are represented through a phase field \( \tilde{\phi}(x, t) \) relative to incommensurate quasi-long-range order with Lagrangian density

\[ L = \frac{1}{2} \left[ \left( \partial_i \tilde{\phi} \right)^2 - \left( \partial_x \tilde{\phi} \right)^2 \right] + C h_s \cos \left( 2\pi R(H) \tilde{\phi} \right) \]

This is sine-Gordon model with interaction term proportional to \( h_s \)

Spectrum consists of

- Solitons, anti-solitons

\[ M = J A \left( \frac{\tilde{H}}{J} \right) \left( \frac{h_s}{J} \right)^{\frac{1}{2-2\pi R(\tilde{H})^2}} \]

- Breather bound states

\[ M_n = 2M \sin \left( n\pi \xi(H) / 2 \right) \]

Oshikawa and Affleck (1997)
Bound states from 2-spinon continuum

Breathers $n=1,2$ and possibly 3

$\tilde{q} = \pi$

Soliton, M

$\tilde{q} = 0.77\pi$

Kenzelmann et al. (2003)
Testing sine-Gordon predictions

Theory by Essler-Tsvelik (1998)

Kenzelmann et al. (2003)
MFT of fermions in a staggered field

\[ \mathcal{H}_{\text{MF}} = -\frac{J\gamma}{2} \sum_{i,\sigma} (c_i^\dagger c_{i+1,\sigma} + \text{H.c.}) - \frac{g_c}{2} \mu_B H \sum_{i,\sigma} \sigma n_{i\sigma} \]

\[-\frac{1}{2} (g_a \mu_B H_{\text{st}} + J\delta) \sum_{i,\sigma} (-1)^i c_{i\sigma}^\dagger c_{i\sigma}^- + \lambda \sum_i n_i,\]

\[ \mathcal{H}_{\text{MF}} = \sum_{-\pi < k \leq \pi, \sigma} \left[ \left( -J\gamma \cos(k) - \frac{\sigma}{2} g_c \mu_B H \right) c_{k\sigma}^+ c_{k\sigma}^- \right. \]

\[ -\frac{1}{2} (g_a \mu_B H_{\text{st}} + J\delta) \left( c_{k+\pi\sigma}^+ c_{k\bar{\sigma}}^- + c_{k\sigma}^+ c_{k+\pi\bar{\sigma}}^- \right) \right]. \]

\[ \epsilon_{k\sigma}^\pm = \pm \sqrt{\left( J\gamma \cos(k) + \frac{\sigma g_c}{2} \mu_B H \right)^2 + \frac{1}{4} (g_a \mu_B H_{\text{st}} + J\delta)^2}, \]

Kenzelmann, Batista, et al. (2005)
Mean Field Dispersion Relations

\[ \tilde{\hbar}\omega(q, \nu) \]

(a) \( \nu = x, y \)

(b) \( \nu = z \)
High energy bound states

Kenzelmann et al. (2005)
Conclusions

- **Single mode approximation**
  - Good for spin-1 chain when $q > 0.3\pi$
  - A versatile tool for experimentalists & theorists

- **Decay of bound state in near critical spin-1/2 bi-layer**

- **Spin-1/2 chains: Physical realization of QCP**

- **Uniform field exposes extended critical state**

- **Staggered fields**
  - inherent to multi-atom cells
  - produce rich spectrum of bound states

- **Sine-Gordon model describes**
  - Bound state energies
  - Breather intensities
  - Field dependent incommensurability

- **High-E bound states predicted & observed**
Some Challenges in Quantum Magnetism

- Identify isotropic D>1 critical phase
  - Isolated critical phase via perturbations
  - Purify known glassy quantum magnets
- “Vortex lattice” in quantum magnet
  - High field phase of spin-1/2 ladder
  - Correlations in magnetization plateau
- Structure & dynamics of quantum impurities in D>1
- Itinerant quantum magnetism
  - Frustration+low D+mobile fermions