Bound states and E₈ symmetry effects in perturbed quantum Ising chains

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First experimental evidence of E₈ - symmetry

Quantum criticality in an Ising chain:

Experimental evidence for emergent E8 Symmetry

[Coldea 10] R. Coldea, D. A. Tennant, E. M. Wheeler, E. Wawrzynska, D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl and K. Kiefer, **Science** 326, 177 (2010).

Theoretically derived in a 2D classical Ising model

Integrals of motion and S-matrix of the (scaled) T=T_c Ising model with magnetic field

[Zamolodchikov 89] A. B. Zamolodchikov, Int. J. Mod. Phys. A 4, 4235 (1989).

Time Evolving Block Decimation (TEBD)

- Numerical simulation of 1D quantum system
- Based on a matrix product state (MPS) representation
- Descendant of the DMRG algorithm
- Ground state by time evolution in imaginary time

$$|\psi_0\rangle = \lim_{\tau \to \infty} \frac{e^{-H\tau} |\psi_i\rangle}{||e^{-H\tau} |\psi_i\rangle||}$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Dynamical structure function – neutron scattering data

$$S(q,\omega) = \sum_{x} \int_{-\infty}^{\infty} dt e^{-iqx} e^{i\omega t} C(x,t)$$
$$C(x,t) = \langle \psi_0 | S_x^-(t) S_0^+(0) | \psi_0 \rangle$$

Computationally hard to simulate long enough times

- Calculate C(x,t) for every 10th time steep and interpolate its value between
- "Light-cone" like spread of the entanglement
- Linear prediction

Quantum Ising chain

$$H = -J\sum_{n} S_n^z S_{n+1}^z - h^x \sum_{n} S_n^x$$

J > 0 favors a ferromagnetic state
 | ↑↑ ... ↑> or | ↓↓ ... ↓>



Excitations



←● ●→ [Coldea10]

Longitudinal field

- Breaks the two-fold degeneracy of the ferromagnetic state
- Opens up a gap
- Moves the minimum gap to higher longitudinal field

$$H_L = -h^z \sum_n S_n^z$$

Confinement into bound states

- Ferromagnetic interchain coupling
- A longitudinal field

confines the kinks into bound states
 splits up the excitation continuum

Analytical solution

- At low transverse field and small bound state momentum
- 1 D Schrödinger equation with a linear confining potential



Energy levels are the zeros of the Airy function

Analytical solution - Hidden E₈ symmetry

- Close to the QCP
 - solvable by CFT
 - 8 bound state masses (and sums of them)



- <u>mi∕ m</u>1
 - 1.000 1.618 ← golden ratio
 - 1.989 2.405
 - 2.956 3.218
 - 3.891 4.783

"Spinon jets"

- Additional bound state
- High energy bound state kinks far apart
- Energetically favorable to flip intermediate spin
- Two new kinks
- Each one forms a bound state with one original

➡ Continuum in the excitation spectra



The goal with our work

- Simulate the excitation spectra for the transverse Ising chain in a longitudinal field around h_x=J/2
- 2. Derive an accurate microscopic model of CoNi₂O₆
- Simulate the excitation spectra for the model of CoNi₂O₆ around h_x=J/2

Longitudinal field



- Increasing longitudinal field
- Bound state spaced further apart
- Weight of continuum decreases



Surprisingly good agreement to strong long. fields



- Gap minimum indicates 3D phase transition
 - Gap minimum moved far away [Carr, Tsvelik 03] - Good agreement with RPA calculations $h^x \approx h_c^x + 1.42 m eV (2h^z/J)^{4/7} \approx 1.12 m eV$

Cobalt niobate CoNi₂O₆

- Ising spins on each Co(2+) ion
- Weakly coupled zigzag ferromagnetic chains



<u>3D model of CoNi₂O₆</u>

- Perpendicular plane has triangular structure
- Ferrimagnetic structure
- Magnetic ordered at low temperature

$$h^z = \sum_{\delta} J_{\delta} \langle S^z \rangle$$

[Carr, Tsvelik 03]



Microscopic model of CoNi₂O₆

- Strong easy axis
- ➡ weak XX-term still present
 - Zigzag chain
- next nearest neighbor interaction

$$H = -J' \sum_{n} S_{n}^{z} S_{n+1}^{z} - h^{x} \sum_{n} S_{n}^{x} - h^{z} \sum_{n} S_{n}^{z}$$
$$- J_{p} \sum_{n} \left(S_{n}^{x} S_{n+1}^{x} + S_{n}^{y} S_{n+1}^{y} \right) + J_{B} \sum_{n} S_{n}^{z} S_{n+2}^{z}.$$

Fitting of parameters (low transverse field)



Fitting of parameters (low transverse field)



The microscopic model can explain the experimental data

Kinetic bound state

Bound state stabilized by kinks moving together

Kinetic bound state
Short range interaction

 Energy gain in nn kink hopping

$$S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+$$



CoNi₂O₆ close to the QCP



- Flattening of the kinetic bound state
- The relative intensity of the bound state masses are unaltered



Both axis rescaled by ~ 10%

- QCP moved to hx ≈ 0.814 meV, gap minimum moved to hx ≈ 0.99 meV

- Gap minimum decreased to $\text{E}\approx0.295~\text{meV}$

• Mass ratios unaltered



Same general behaviour

0

- Experimental gap minimum E ≈ 0.36 meV



 The mass ratios passes the analytical values at the critical field, not approach it at the gap minimum

Conclusions

- The microscopic model of CoNi₂O₆ reproduce the experimental data well
- Mass ratios follow straight lines through the analytical values at the critical field strength
- Improved experiments should be as likely to detect higher bound states as in a pure QIC.

Thank You!

<u>References</u>

[Coldea 10] R. Coldea, D. A. Tennant, E. M.Wheeler, E. Wawrzynska,

D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl and K. Kiefer, **Science** 326, 177 (2010).

[Zamolodchikov 89] A. B. Zamolodchikov, Int. J. Mod. Phys. A 4, 4235 (1989).

[Lee, Kaul, Balents 10] S. Lee, R. K. Kaul, and L. Balents, (2010), **Nature Physics** published online.

[Carr, Tsvelik 03] S. T. Carr and A.M. Tsvelik, Phys. Rev. Lett. 90, 177206 (2003).

[Fateev 94]]V. A. Fateev, Phys. Lett. B 324, 45 (1994).

[Rutkevich 08] S. B. Rutkevich, J. Stat. Phys. 131, 917-939 (2008).