Bound states and $E_8$ symmetry effects in perturbed quantum Ising chains

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First experimental evidence of $E_8$-symmetry

Quantum criticality in an Ising chain:

Experimental evidence for emergent $E_8$ 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

\[ |\psi_0\rangle = \lim_{\tau \to \infty} \frac{e^{-H\tau} |\psi_i\rangle}{\|e^{-H\tau} |\psi_i\rangle\|} \]
Real time evolution

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

- 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
  \[ | \uparrow \uparrow \ldots \uparrow > \text{ or } | \downarrow \downarrow \ldots \downarrow > \]

- Phase transition to a paramagnetic state \[ | \rightarrow \rightarrow \ldots \rightarrow > \]
at QCP \[ | h_{xc} | = J/2, \]

[Coldea10]
Excitations

- Elementary excitation
  - domain wall or kink (ferromagnetic phase)
  - spin flip (paramagnetic phase)

- Excitation gap closes at $h_c$

- Experimentally not possible to create one kink

Spin flip $\rightarrow$ two freely moving kinks

[Coldea10]
Longitudinal field

- Breaks the two-fold degeneracy of the ferromagnetic state
- Opens up a gap
- Moves the minimum gap to higher longitudinal field
- Confines the kinks into bound states

\[ H_L = -h^z \sum_n S_n^z \]
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 $E_8$ symmetry

- Close to the QCP
  - solvable by CFT

8 bound state masses
(and sums of them)

- $m_i / m_1$
  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
Excitations-Bound state masses
(between analytical solvable points)

- Minimum gap at zero bound state momenta
- Many bound states close to $E=J$ for $h_x \ll J$, $h_z \ll J$
- 8 bound states close to $E=0$ for $h_x \approx J/2$, $h_z \ll J$
The goal with our work

1. 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 $\text{CoNi}_2\text{O}_6$

3. Simulate the excitation spectra for the model of $\text{CoNi}_2\text{O}_6$ around $h_x=J/2$
Increasing longitudinal field

- Bound state spaced further apart
- Weight of continuum decreases
E₈ bound states

$J=1.83 \text{ meV, } h_x=J/2$

$m_1 \approx JC(2h/J)^{8/15}$, with $C = 4.40490858/0.7833$ [Fateev 94]

- Surprisingly good agreement to strong long. fields
Gap minimum

- Gap minimum indicates 3D phase transition
- Gap minimum moved far away
  - Good agreement with RPA calculations $h^x \approx h_c^x + 1.42\text{meV}(2h^z/J)^{4/7} \approx 1.12\text{ meV}$

[Carr, Tsvelik 03]
Cobalt niobate $\text{CoNi}_2\text{O}_6$

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

[Coldea 10]
3D model of $\text{CoNi}_2\text{O}_6$

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

\[ h^z = \sum_\delta J_\delta \langle S^z \rangle \]

[Lee, Kaul, Balents 10]

[Carr, Tsvelik 03]
Microscopic model of CoNi$_2$O$_6$

- Strong easy axis
  → weak XX-term still present

- Zigzag chain
  → next nearest neighbor interaction

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

Neutron scattering data

Dynamical Structure Function

\[ J' = J + J_B = 2.43 \text{ meV}, \quad h^x = 0.354 \text{ meV}, \quad h^z = 0.035 \text{ meV}, \quad J_p = 0.52 \text{ meV}, \quad J_B = 0.60 \text{ meV} \]

Varied
Fitting of parameters (low transverse field)

The microscopic model can explain the experimental data
Kinetic bound state

- Bound state stabilized by kinks moving together
- Short range interaction
- Energy gain in nn kink hopping

\[ S_n S_{n+1} + S_n S_{n+1} \]
CoNi$_2$O$_6$ close to the QCP

- Flattening of the kinetic bound state
- The relative intensity of the bound state masses are unaltered
CoNi$_2$O$_6$ close to the QCP

- Both axis rescaled by $\sim 10\%$
  - QCP moved to $h_x \approx 0.814$ meV, gap minimum moved to $h_x \approx 0.99$ meV
  - Gap minimum decreased to $E \approx 0.295$ meV

- Mass ratios unaltered
Comparison with experimental data

Experimental data

\[ B (\text{T}) \]

Experimental gap minimum \( E \approx 0.36 \text{ meV} \)

- Same general behaviour

- Experimental gap minimum \( E \approx 0.36 \text{ meV} \)
The mass ratios pass the analytical values at the critical field, not approach it at the gap minimum.
Conclusions

- The microscopic model of $\text{CoNi}_2\text{O}_6$ 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!
References

[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).