Dynamically dominant excitations of string solutions in the $S=1/2$ antiferromagnetic Heisenberg chain in a magnetic field

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Spin-1/2 antiferromagnetic Heisenberg chain

The spin-1/2 antiferromagnetic Heisenberg chain in a magnetic field

\[ \mathcal{H} = J \sum_x S_x \cdot S_{x+1} - H S^z. \]

It exhibits interesting quantum many-body effects:

Fractionalization, spin liquid, quantum criticality, ...

which have inspired modern concepts for strongly correlated systems.

This system is an excellent platform to make precise comparisons between

- quasi-1D antiferromagnets
- Exact solutions using the Bethe ansatz [1].

Very long history! But, properties have not been fully understood...

\[ S(k,\omega) \text{ in a magnetic field} \]

The Bethe ansatz

Bethe wavefunction: \[ \Phi(x_1, \cdots x_M) = \sum_P \exp \left\{ i \left( \sum_j k_{P} x_j + \sum_{j < l \atop P_j > P_l} \phi_{PjP_l} \right) \right\}, \]

where \(k\) and \(\phi\) are determined so that this wavefunction becomes an eigenstate of the Hamiltonian under periodic boundary conditions.

Bethe equation:

\[
L \theta(\Lambda_j) = 2\pi I_j + \sum_{l \neq j} \theta \left( \frac{\Lambda_j - \Lambda_l}{2} \right), \quad j = 1, \cdots, M, \\
\theta(x) = 2 \arctan(x), \quad \Lambda_j = \cot \left( \frac{k_j}{2} \right), \quad 2 \cot \left( \frac{\phi_{j,l}}{2} \right) = \cot \left( \frac{k_j}{2} \right) - \cot \left( \frac{k_l}{2} \right). \\
I_j = \begin{cases} \text{integer} & \text{, if } L - M \text{ is odd} \\ \text{half-odd integer} & \text{, if } L - M \text{ is even} \end{cases}, \quad |I_j| \leq \frac{L - M - 1}{2}.
\]

Once a set of \(\{I_j\}\) is given, an eigenstate is obtained.

Dynamically dominant excitations for $S^{zz}(k, \omega)$ and $S^{-+}(k, \omega)$

Spinless Fermions

- psinon $\psi$
- antipsinon $\psi^*$

- hole
- particle
Dynamically dominant excitations for $S^{zz}(k,\omega)$ and $S^{-+}(k,\omega)$

\[ S^{zz}(k,\omega) \{ I_j \} \quad \text{psinon } \psi \quad \text{antipsinon } \psi^* \]

\[ S^{zz}(k,\omega) \quad \psi\psi^* \text{ excitation [2,3]} \]

\[ S^{-+}(k,\omega) \{ I_j \} \quad \text{2}\psi \text{ excitation [3]} \]

\[ S^{zz}(k,\omega) = \sum_i \langle k, \epsilon_i | S_k^{zz} | \text{G.S.} \rangle^2 \delta(\omega - \epsilon_i). \]

\[ S^{-+}(k,\omega) = \sum_i \langle k, \epsilon_i | S_k^{+-} | \text{G.S.} \rangle^2 \delta(\omega - \epsilon_i). \]

Dynamically dominant excitations for $S^+(k,\omega)$

$1\psi^* [3-7], 2\psi^* [8]:$

$$S^+(k,\omega) = \sum_i |\langle k,\varepsilon_i | S^+_k | \text{G.S.} \rangle|^2 \delta(\omega-\varepsilon_i).$$

\[\Delta S^z=-1\]

\[\begin{align*}
\{I_j\} & \quad \text{1$\psi^*$ excitation} \\
\{I_j\} & \quad \text{2$\psi^*$ excitation}
\end{align*}\]

\[\begin{align*}
S^z/L=1/8 & \quad \text{low field} \quad \leftarrow & \quad H & \quad \rightarrow & \quad \text{high field} \\
S^z/L=1/4 & \quad \text{low field} \quad \leftarrow & \quad H & \quad \rightarrow & \quad \text{high field} \\
S^z/L=3/8 & \quad \text{low field} \quad \leftarrow & \quad H & \quad \rightarrow & \quad \text{high field}
\end{align*}\]

Psinon ($\psi$) carries $S^z=+1/2$.

Antipsinon ($\psi^*$) carries $S^z=-1/2$.

Zero field

Spinon which carries $S^z=+1/2$.

\[
\begin{align*}
S^+(k,\omega) & \sim |\langle \text{Exc.}(S^z+1)|S^+|G.S.(S^z)\rangle|^2 : \Delta S^z = +1 \quad \cdots \quad 2\psi \text{ excitations} \\
S^{zz}(k,\omega) & \sim |\langle \text{Exc.}(S^z)\rangle|S^z|G.S.(S^z)\rangle|^2 : \Delta S^z = 0 \quad \cdots \quad \psi\psi^* \text{ excitations} \\
S^-(k,\omega) & \sim |\langle \text{Exc.}(S^z-1)|S^-|G.S.(S^z)\rangle|^2 : \Delta S^z = -1 \quad \cdots \quad 2\psi^* \text{ excitations}
\end{align*}
\]

Missing spectral weight in $S^-(k,\omega)$

$S^z/L = 1/8$

$\Delta S^z = -1$

1$\psi^*$

2$\psi^*$

low field

$S^-(k,\omega) (H=0)$

Real-$\Lambda$ solutions

$S^z/L = 1/4$

$H \approx 0$

Complex-$\Lambda$ solutions

$S^-(k,\omega) [r+i1+i2]$

$S^z/L = 0.025$

$S^z/L = 3/8$

$H \approx 0$

(string solutions)

$S^-(k,\omega) [r]$

$S^z/L = 0$

$S^z/L = 0.025$
Solutions with a string

String solutions with one string are specified by two sets of \( \{I_j\} \): \( \{I^R_j\} \) for real rapidities and \( \{I^I_j\}(j=1) \) for complex rapidities.

Real \( \Lambda_j \)

Complex \( \Lambda_j \)

\( \{I^R_j\} \) for real rapidities

\( \{I^I_1\} \) for complex rapidities

\( \psi^* \) \hspace{2cm} \psi \hspace{2cm} \text{QP for the string}
**$S(k,\omega)$ in a magnetic field in 1D**

Dynamically dominant excitations in $S(k,\omega)$ in $L=2240$

Excitations which satisfy more than 80% of sum rules in $L=320$

- 2-string solutions
- $2\psi^*$
- $1\psi^*$
Comparison with experimental results on CuPzN

Experimental results observed in the quasi-one-dimensional antiferromagnet \( \text{Cu(C}_4\text{H}_4\text{N}_2)(\text{NO}_3)_2 \) (CuPzN) in a magnetic field [9] were well explained.

Comparison with experimental results on CuPzN

Experimental results on CuPzN [9]

Present result

Comparison with experimental results on CPC

Experimental results observed in the quasi-one-dimensional antiferromagnet CuCl₂ · 2N(C₅D₅) (CPC) in a magnetic field [10] were also well explained.

Behaviors of dynamical structure factors $S^{+-}(k, \omega)$, $S^{zz}(k, \omega)$, and $S^{+}(k, \omega)$ of the $S=1/2$ antiferromagnetic Heisenberg chain in a magnetic field have been investigated using exact Bethe-ansatz solutions.

- **2-string solutions** form a well-defined continuum in $S^{+-}(k, \omega)$.
- This continuum reduces to the des Cloizeaux-Pearson mode in the zero-field limit and the bound states of overturned spins near the saturation field.
- **Psinon** ($\psi$) and **antipsinon** ($\psi^*$) can be naturally interpreted as quasiparticles (QPs) in $H$ carrying $S^z = +1/2$ and $S^z = -1/2$, respectively.
- Experimental results on quasi-1D antiferromagnets (CuPzN and CPC) in a magnetic field were reasonably explained.

Not only $\psi$ ($S^z = +1/2$) and $\psi^*$ ($S^z = -1/2$) but also **QP for a 2-string** ($S^z = -1$) plays an important role for dynamical properties in a magnetic field.