Topological Phases of the Spin-1/2 Ferromagnetic-Antiferromagnetic Alternating Heisenberg Chain with Frustrated Next-Nearest-Neighbour Interaction

Kazuo Hida (Saitama University)
Ken’ichi Takano (Toyota Technological Institute)
Hidenori Suzuki (Nihon University)

1 Introduction

Spin $1/2$ ferro($J_F$)-antiferro($J_A$) alternating Heisenberg chain

\[ H = \sum_{l=1}^{L} \left( J_F S_{2l-1} S_{2l} + J_A S_{2l} S_{2l+1} \right) \]

Ground State: continuously connected to Haldane state as $J_F \rightarrow -\infty$

\[ H \xrightarrow{J_F \rightarrow -\infty} \sum_{l=1}^{L} J \hat{S}_l \hat{S}_{l+1} \]

\[ \left( \hat{S}_l = S_{2l-1} + S_{2l} : \text{“building block”}, \quad J = \frac{J_A}{4} \right) \]

Spin-$1/2$ edge spin

KH (1992)
Add ferromagnetic next-nearest neighbour interaction ⇒ frustration ($J_L < 0$)

$$\mathcal{H} = \sum_{l=1}^{L} (J_F S_{2l-1} S_{2l} + J_A S_{2l} S_{2l+1}) + \sum_{l=1}^{2L} J_L S_l S_{l+2}.$$ 

- $|J_L| \ll J_A$ or $|J_F| \ll J_A$: Haldane GS
- $|J_F|, |J_L| \gg J_A$: Ferromagnetic GS

Material with this structure

Cu$^{II}$Cl($O$-$mi$)$_2$(μ-Cl)$_2$


Ferromagnetic GS
1. Ferromagnetic Phase (F)
2. Haldane phase (H) edge spin 1/2
3. Ferromagnetic-nonmagnetic phase boundary
   \[ J_F = -\frac{2J_A J_L}{2J_L + J_A} \]
   • \( J_L/J_A = -m/2 \) (special point)
     AF short range correlation
   • \( J_L/J_A \neq -m/2 : \)
     long range spiral correlation \( k = \frac{2\pi}{L} \)
1. Infinite series of intermediate spin gap phases $I_{S_e}$
   edge spin $S_e = 1/2, 1, 3/2, 2, ..$

2. Exact ground state at the “special points” on the ferromagnetic-nonmagnetic phase boundary
   $(J_L/J_A = -m/2)$
   edge spin $S_e = (m - 1)/2$

Representative points of $I_{S_e}$ phases
2 Intermediate Spin Gap Phase

Scaled gap \( L\Delta E \)
(PBC : Numerical diagonalization)

- Weak size-dependence around \( J_F \sim -1.3 \)
- \( L\Delta E \) increases with size on both sides

Phase transition between two different spin-gap phases

Haldane phase

Intermediate spin gap phase
Open chain (DMRG)

$\Rightarrow$ Quasi-degenerate GS in nonmagnetic phases

- Haldane phase: Edge spins 1/2 (Kennedy triplet)
- Intermediate phase: Quasi-degeneracy remains

$\downarrow$

Local magnetization in the intermediate phase

$S_{\text{tot}}^z = 2$, quasi-ground state

$J_F = -1.5$, $J_L = -1.4$, $J_A = 1$

$L = 72$

$M_l \equiv \sum_{k=1}^{l} \langle S_k^z \rangle$

Edge spin-1 on both ends
Add extra spins on both ends to compensate the edge spins

Scaled gap

- Haldane phase: Finite gap
- Intermediate phase: quasi-degeneracy
  $\Rightarrow$ edge spins not compensated.

in original open chains
- Haldane phase: edge spin $S_e = 1/2$
- Intermediate phase: edge spin $S_e = 1 \Rightarrow 'I_1 phase'
For larger $J_L$: add $L_e$ $S = 1/2$ spins ferromagnetically.
• $I_{Se}$ phase: Edge spin $S_e$ in open chain
• Large $J_L \Rightarrow$ large ferromagnetic clusters
  $\Rightarrow$ large edge spin
3 Relation with exact solutions on the phase boundary

- \( J_L/J_A = -m/2 \) (special point: D. V. Dmitriev et al. PRB 56 (1997) 5985.)

Exact solution with antiferromagnetic short range correlation

Local magnetization

\[
M_I \equiv \sum_{k=1}^{l} \langle S_{k}^{z} \rangle
\]

"Special point" : representative of \( I_{S_e} \) phase \( S_e = (m - 1)/2 \)

\( m = 2, 3, \ldots, \infty \) ⇒ Infinite series of \( I_{S_e} \) phases
4 Nature of Intermediate Phases
[Equivalence of $I_{S_e}$ and $I_{S_e+1}$ phases]

- Phases with integer $S_e$ and half-odd-integer $S_e$ are different phases.
- $I_{S_e+1/2}$ phase is always present between $I_{S_e}$ and $I_{S_e+1}$ phases
  $\Rightarrow$ All $I_{S_e}$ phases can be distinguished in the present model.
- Successive phase transitions between TWO topologically distinct ground states with integer and half-odd-integer edge spin
[Valence bond picture of I\(_{Se}\) phases]

Expected valence bond structure of I\(_1\) phase (open chain \(S_e = 1\))

Two end spin added (\(S_e = 1, L_e = 2\))

To stabilize this VBS structure, add antiferromagnetic bonds between \(S_{2l}\) and \(S_{2l+3}\)

\[\begin{align*}
J_{ad}, J_A, J_F \rightarrow \infty : &\quad \text{Isolated dimers on } J_{ad} - \text{bonds} \\
\text{Gap does not close down to} &\quad J_{ad} = 0.
\end{align*}\]
Spin-spin correlation

- $\langle S_{2l} S_{2l+1} \rangle$ ($J_A$-bond) is the largest correlation even in $I_1$ phase (absolute value decreases)
- $\langle S_{2l} S_{2l+3} \rangle$ increases in $I_1$ phase

Valence bond structure

Superposition of valence bond states consistent with edge spins including long range singlet pairs

- etc.
5 Summary

1. Ferromagnetic phase
2. Haldane phase
3. Infinite series of $I_{S_e}$ phases with edge spin $S_e$
   - Strong ferromagnetic NNN interaction
     $\Rightarrow I_{S_e}$ phases with increasing $S_e$.
     Large $J_L \Rightarrow$ Large ferromagnetic cluster
     $\Rightarrow$ Large edge spin
   - Bulk ground states are classified into TWO topologically distinct phases with integer and half-odd-integer edge spins.
   - VBS-structure : superposition including long range singlet pairs
4. Exact solutions on the phase boundary (Dmitriev et al.)
   - $\frac{J_L}{J_A} = -\frac{m}{2}$ (special point) Representative of $I_{(m-1)/2}$ phase
5. Future Problems

- Characterization by entanglement spectrum.