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

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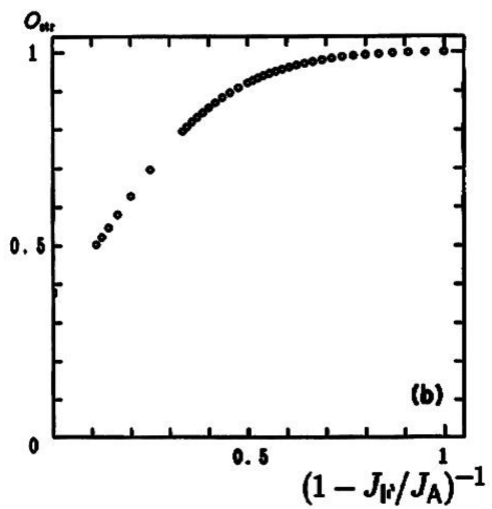
1 Introduction

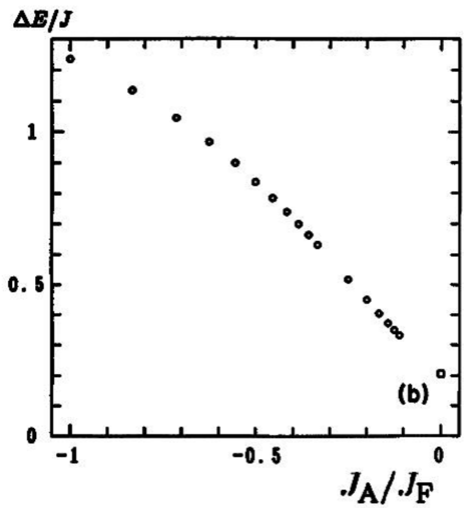
Spin 1/2 ferro($J_{\rm F}$)-antiferro($J_{\rm A}$) alternating Heisenberg chain

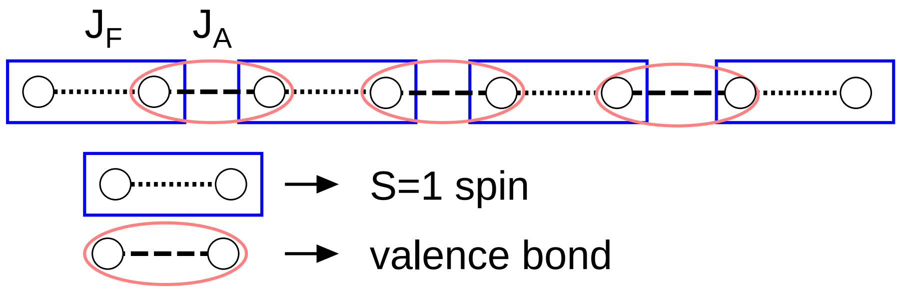
$$\mathcal{H} = \sum_{l=1}^{L} \left(J_{\rm F} \boldsymbol{S}_{2l-1} \boldsymbol{S}_{2l} + J_{\rm A} \boldsymbol{S}_{2l} \boldsymbol{S}_{2l+1} \right)$$

Ground State: continuously connected to Haldane state as $J_{\rm F} \to -\infty$

$$\mathcal{H} \overset{J_{\rm F}\to -\infty}{\Rightarrow} \sum_{l=1}^{L} J \hat{\boldsymbol{S}}_l \hat{\boldsymbol{S}}_{l+1} \quad \left(\hat{\boldsymbol{S}}_l = \boldsymbol{S}_{2l-1} + \boldsymbol{S}_{2l} : \text{“building block”}, \quad J = \frac{J_{\rm A}}{4} \right)$$





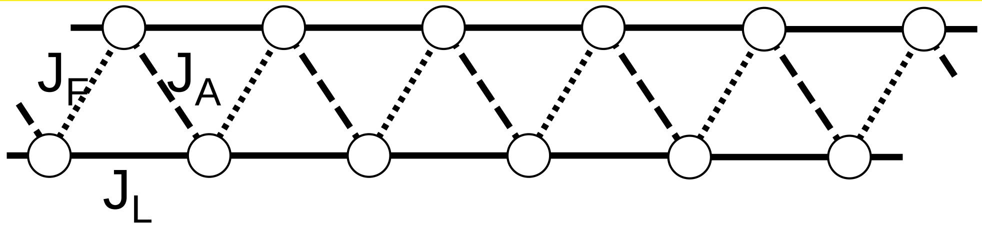


Spin-1/2 edge spin

KH (1992)

Add ferromagnetic next-nearest neighbour interaction⇒ frustration ($J_{\mathrm{L}} < 0$)

$$\mathcal{H} = \sum_{l=1}^{L} (J_{\mathrm{F}} \boldsymbol{S}_{2l-1} \boldsymbol{S}_{2l} + J_{\mathrm{A}} \boldsymbol{S}_{2l} \boldsymbol{S}_{2l+1}) + \sum_{l=1}^{2L} J_{\mathrm{L}} \boldsymbol{S}_{l} \boldsymbol{S}_{l+2}.$$



- $|J_{\mathrm{L}}| \ll J_{\mathrm{A}}$ or $|J_{\mathrm{F}}| \ll J_{\mathrm{A}}$: Haldane GS
- $|J_{\mathrm{F}}|, |J_{\mathrm{L}}| \gg J_{\mathrm{A}}$: Ferromagnetic GS

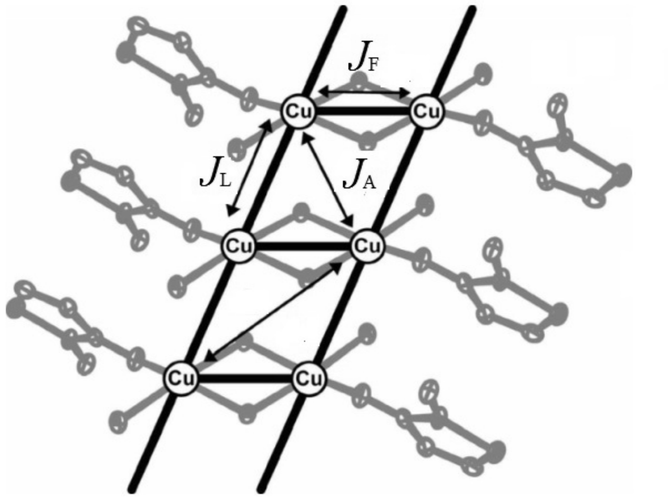
Material with this structure

Cu$^{\mathrm{II}}$Cl(O-mi)$_2$(μ-Cl)$_2$

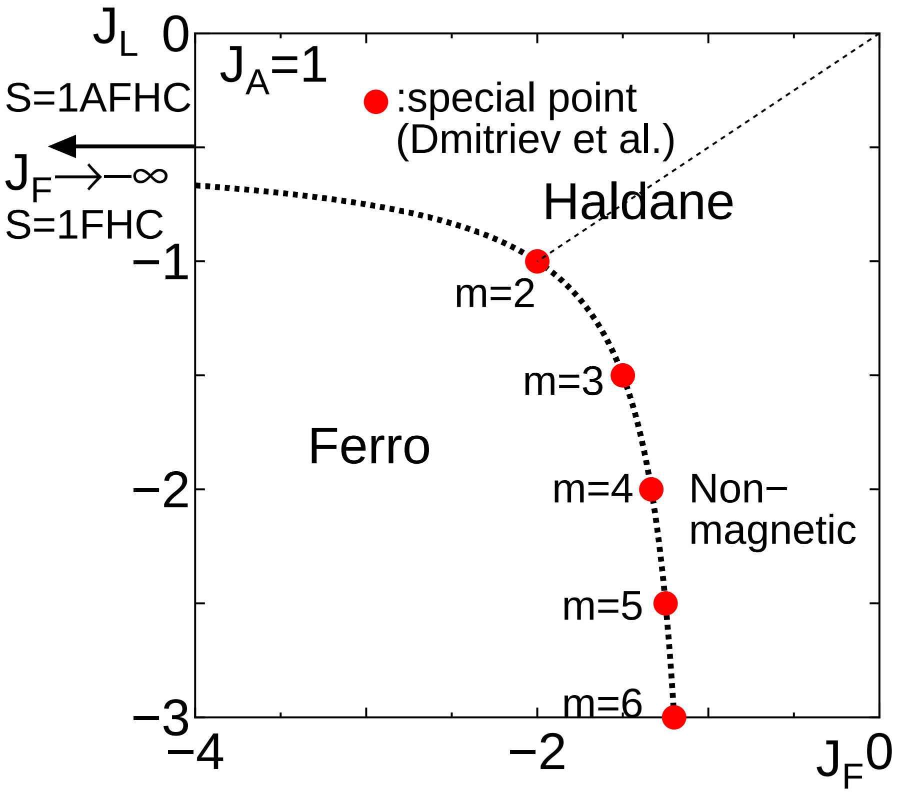
M. Kato *et al.* Eur. J. Inorg. Chem. **2011**, 495 (2011)

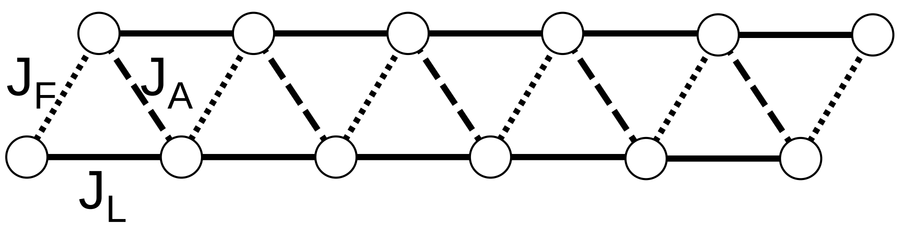
(Saitama Univ. Dept. Chem.)

Ferromagnetic GS



[Ground State Phase Diagram]
- What is known-





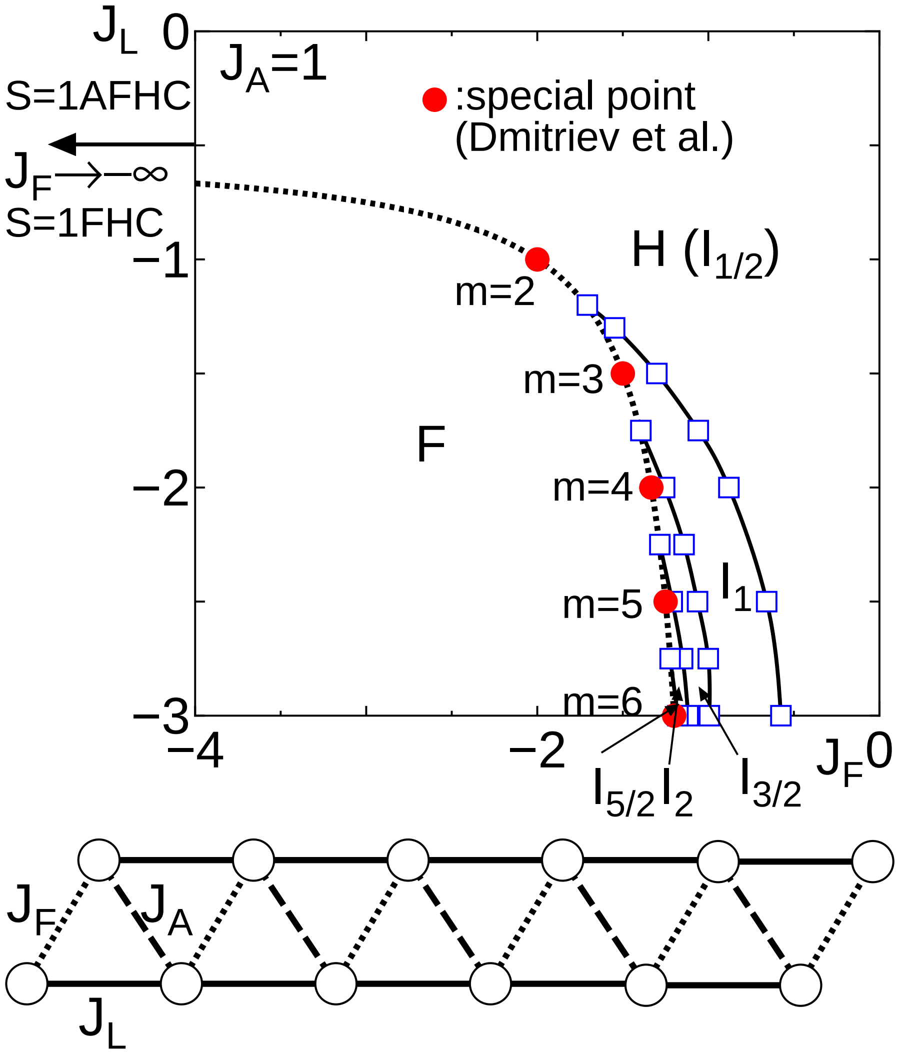
1. Ferromagnetic Phase (F)
2. Haldane phase (H) edge spin 1/2

   $J_F = 2J_L$: exact singlet dimers on J_A bonds (D. V. Dmitriev *et al.* Eur. Phys. J. B**14** (2000) 91.)
3. Ferromagnetic-nonmagnetic phase boundary

   $$J_F = -\frac{2J_A J_L}{2J_L + J_A}$$

   Nonmagnetic exact solutions (D. V. Dmitriev *et al.* Phys. Rev. **B**56 (1997) 5985.)
   - $J_L/J_A = -m/2$ (special point)
     AF short range correlation
   - $J_L/J_A \neq -m/2$:
     long range spiral correlation $k = \dfrac{2\pi}{L}$

[Ground State Phase Diagram] - What we find-

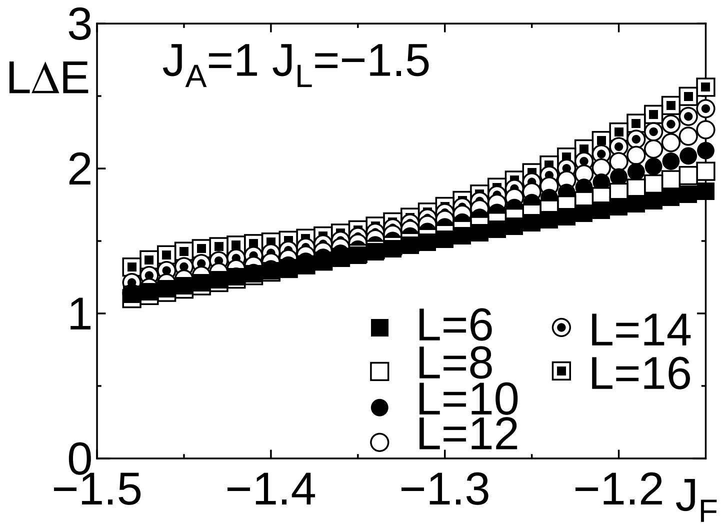


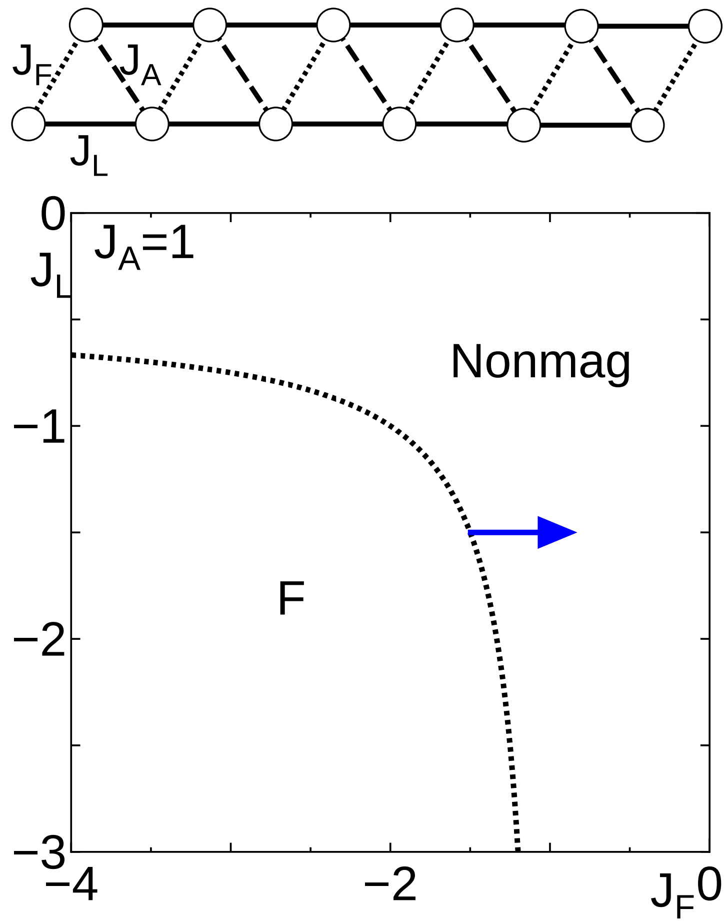
1. Infinite series of intermediate spin gap phases I_{S_e}
   edge spin $S_e = 1/2, 1, 3/2, 2, ..$
2. Exact ground state at the "special points" on the ferromagnetic-nonmagnetic phase boundary ($J_L/J_A = -m/2$)
   edge spin $S_e = (m-1)/2$
   Representative points of I_{S_e} phases

2 Intermediate Spin Gap Phase

Scaled gap $L\Delta E$

(PBC : Numerical diagonalization)





- Weak size-dependence around $J_{\mathrm{F}} \sim -1.3$
- $L\Delta E$ increases with size on both sides

$\Rightarrow$

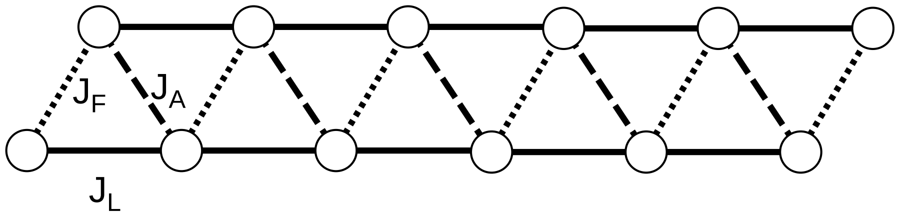
Phase transition between two different spin-gap phases

Haldane phase

$\Updownarrow$

Intermediate spin gap phase

Open chain (DMRG)



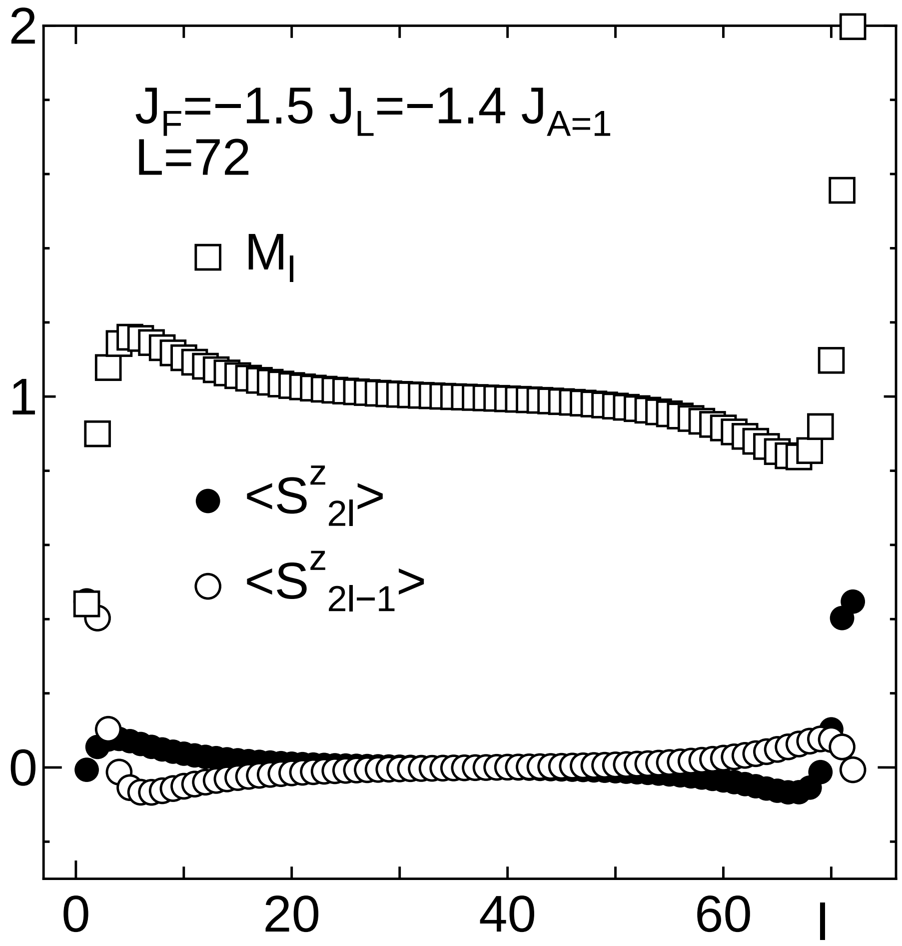
⇒Quasi-degenerate GS in nonmagnetic phases

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

⇓

Local magnetization in the intermediate phase

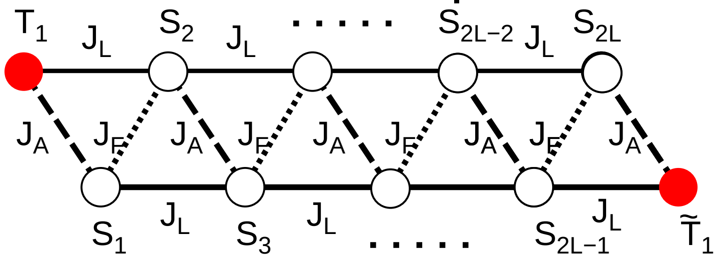
$S^z_{\text{tot}} = 2$, quasi-ground state

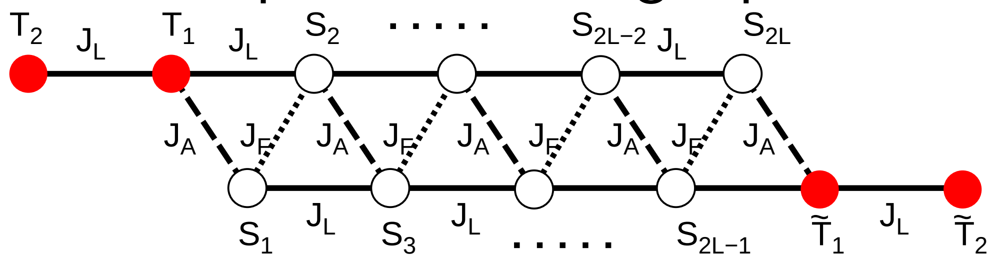


$$M_l \equiv \sum_{k=1}^{l} \langle S^z_k \rangle$$

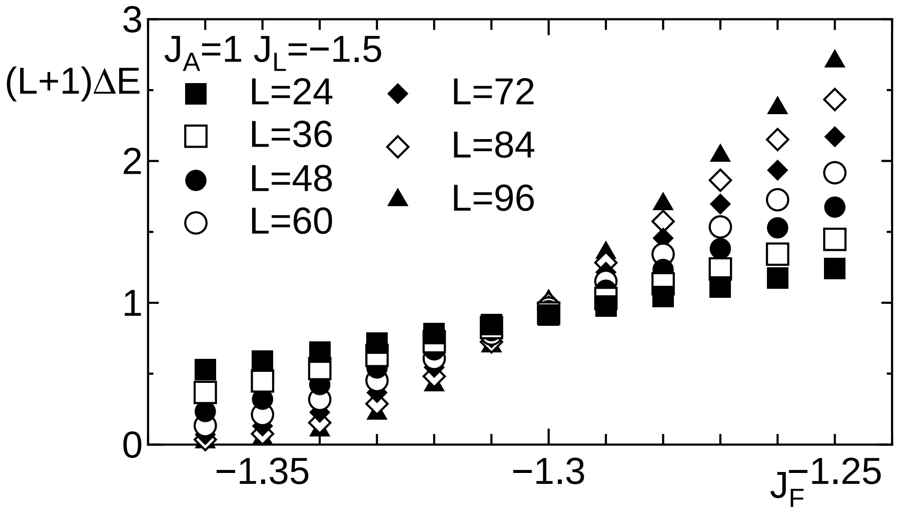
Edge spin-1 on both ends

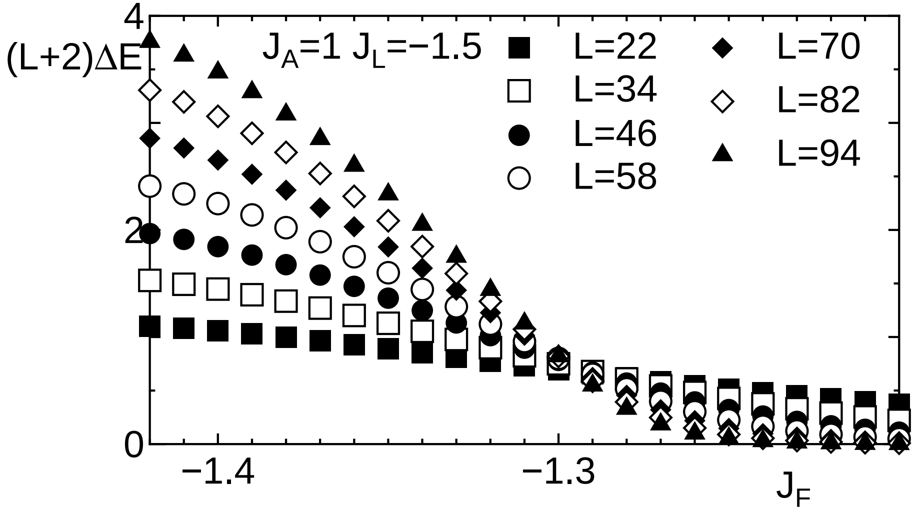
Add extra spins on both ends to compensate the edge spins





Scaled gap





- Haldane phase : Finite gap
- Interm.phase : quasi-degeneracy

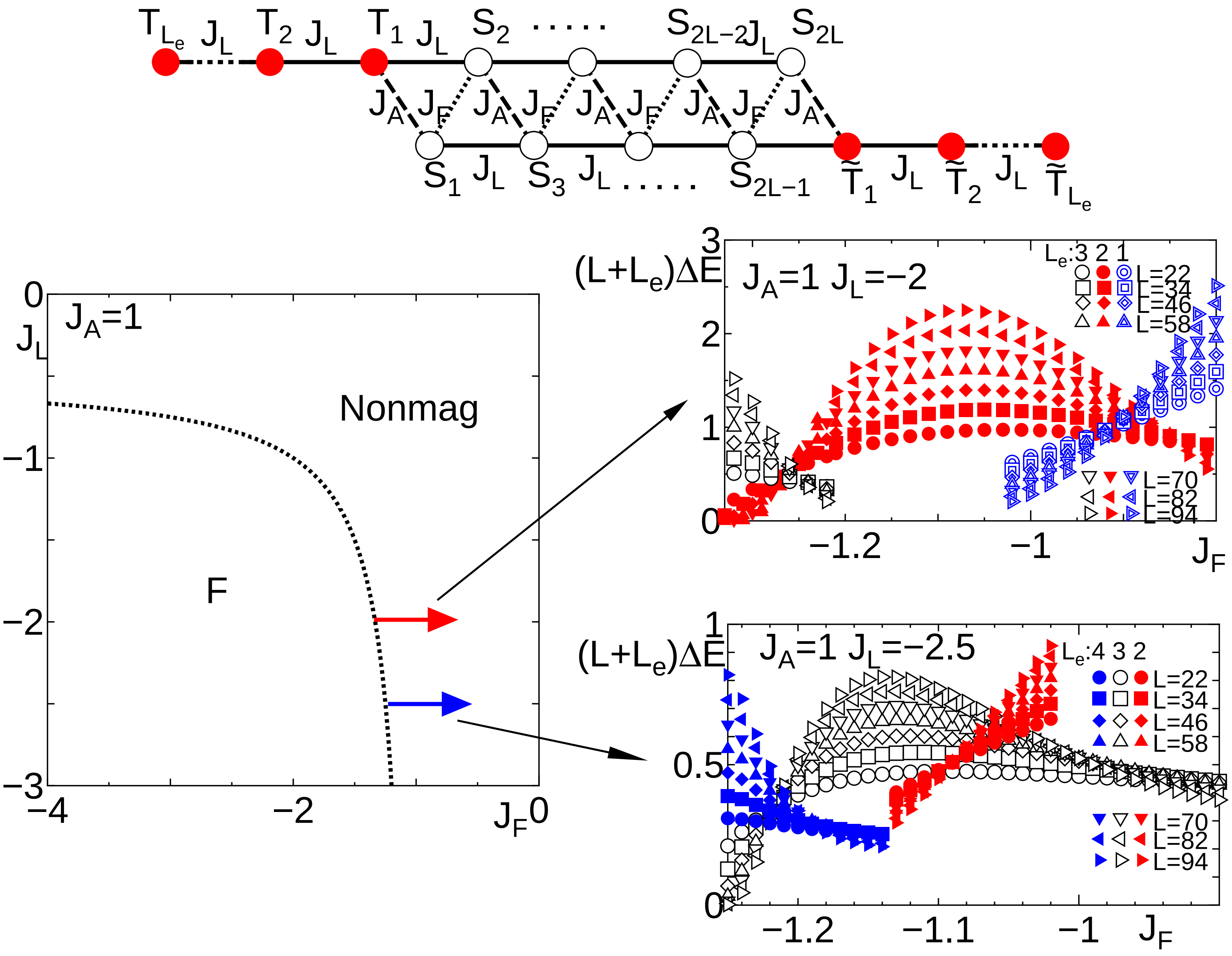
  ⇒ edge spins not compensated.

- Haldane phase : quasi-degeneracy

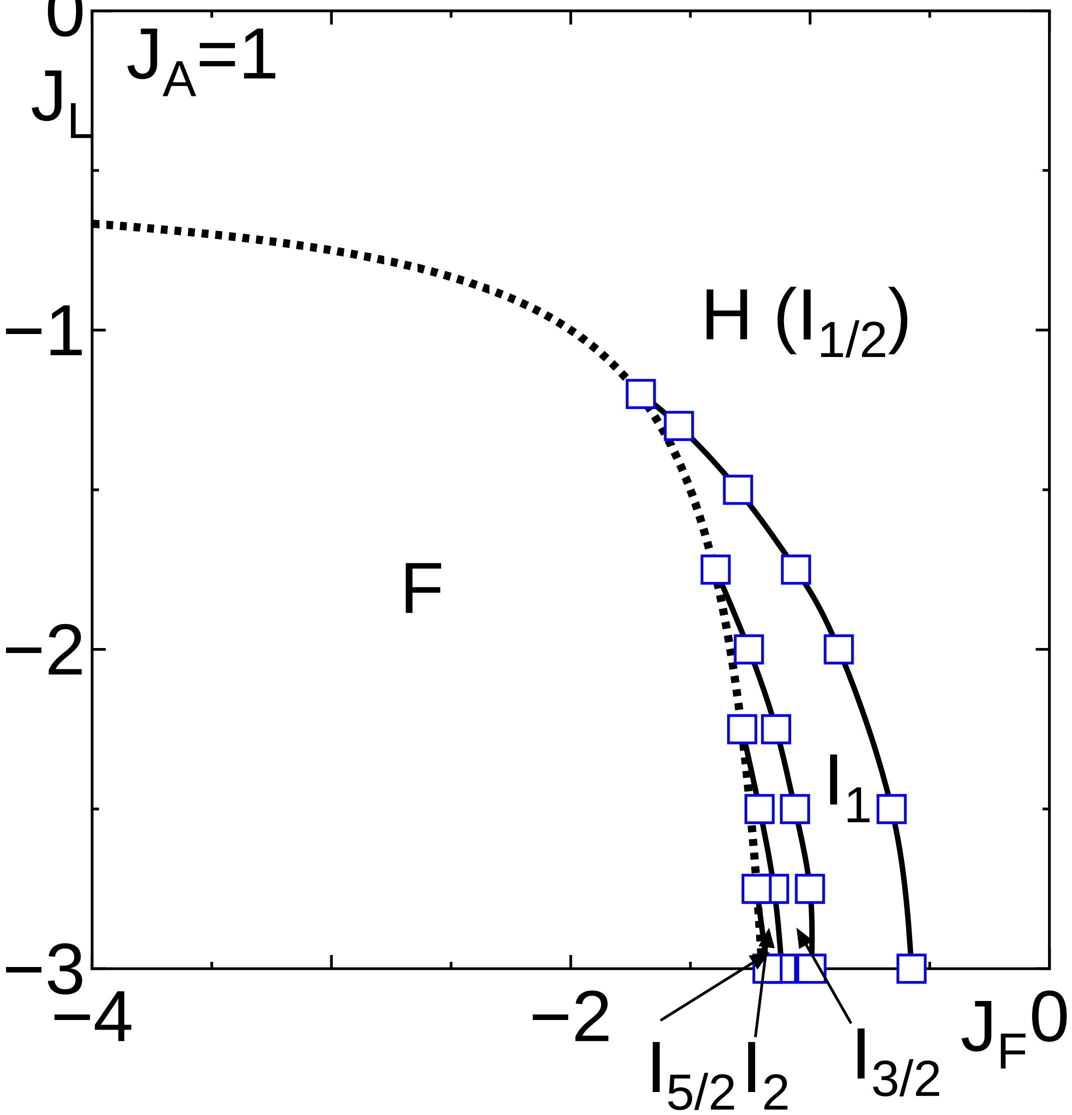
  ⇒ edge spins not compensated.
- Intermediate Phase : Finite gap

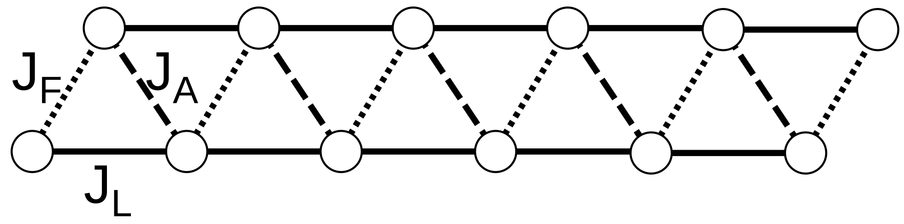
in original open chains
- Haldane phase : edge spin $S_{\mathrm{e}} = 1/2$
- Intermediate phase : edge spin $S_{\mathrm{e}} = 1$ ⇒ 「I_1 phase」

For larger $J_{\rm L}$: add $L_{\rm e}$ $S=1/2$ spins ferromagnetically



[Ground State Phase Diagram]



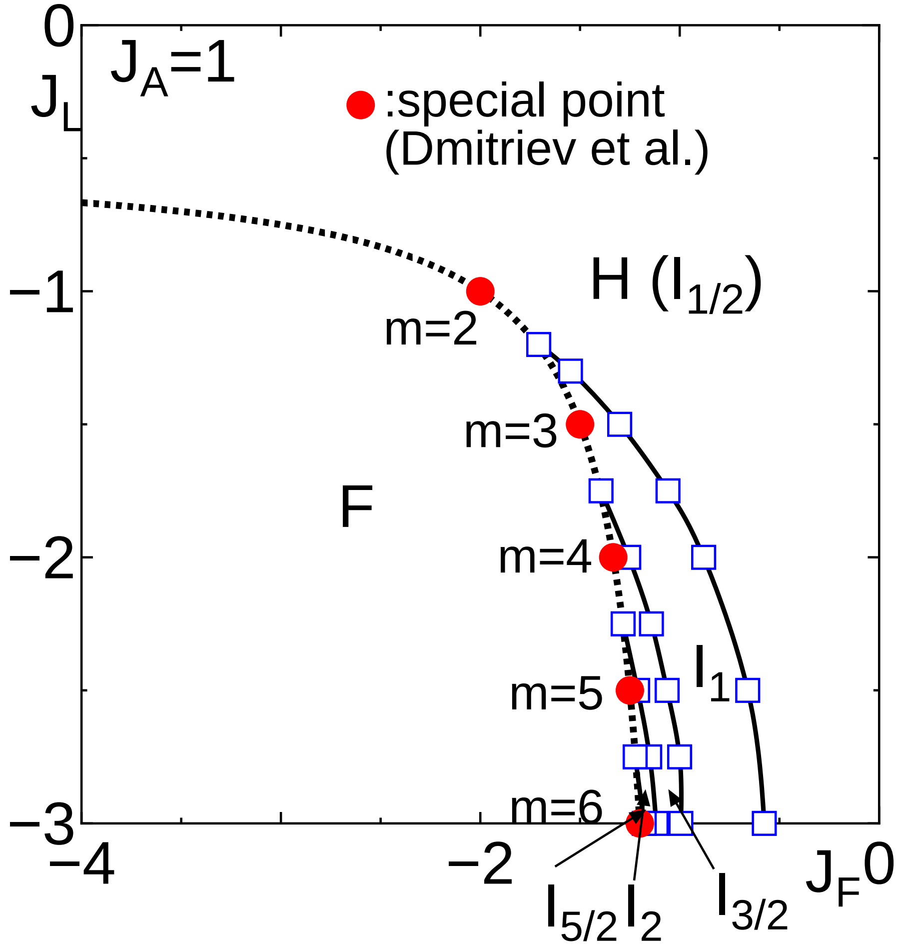


- I_{S_e} phase : Edge spin S_e in open chain
- Large $J_L \Rightarrow$ large ferromagnetic clusters
  $\Rightarrow$large edge spin

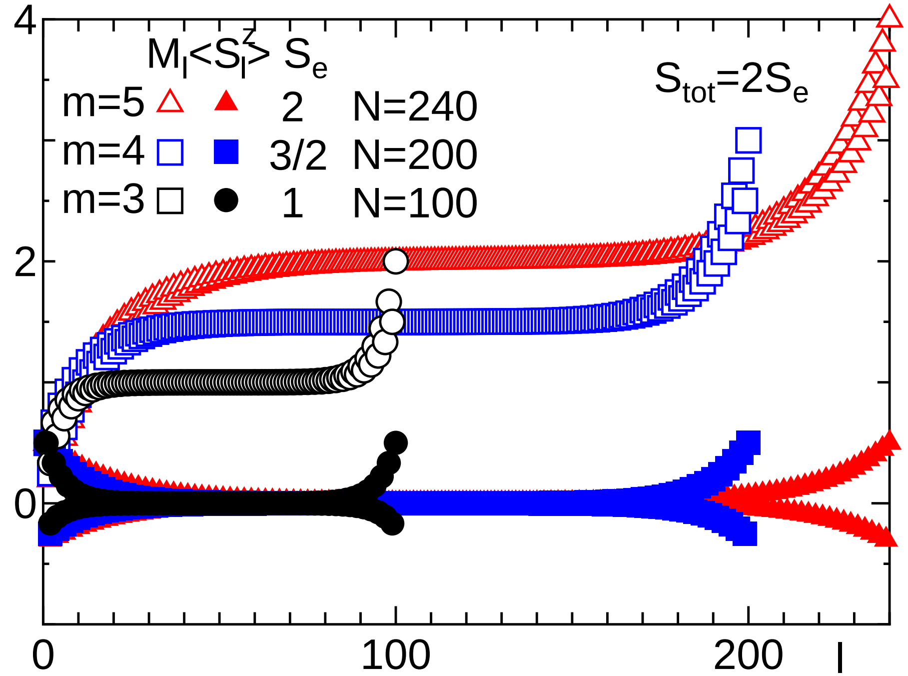
3 Relation with exact solutions on the phase boundary

- $J_{\rm L}/J_{\rm A} = -m/2$ (special point: D. V. Dmitriev *et al.* PRB**56** (1997) 5985.)

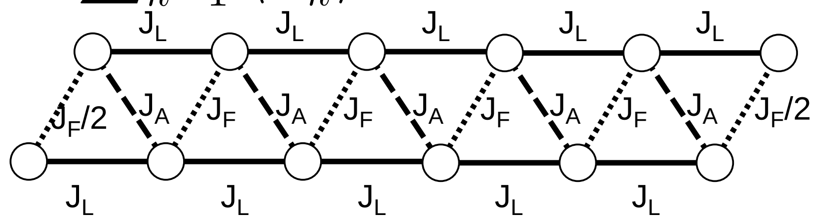
Exact solution with antiferromagnetic short range correlation



Local magnetization



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

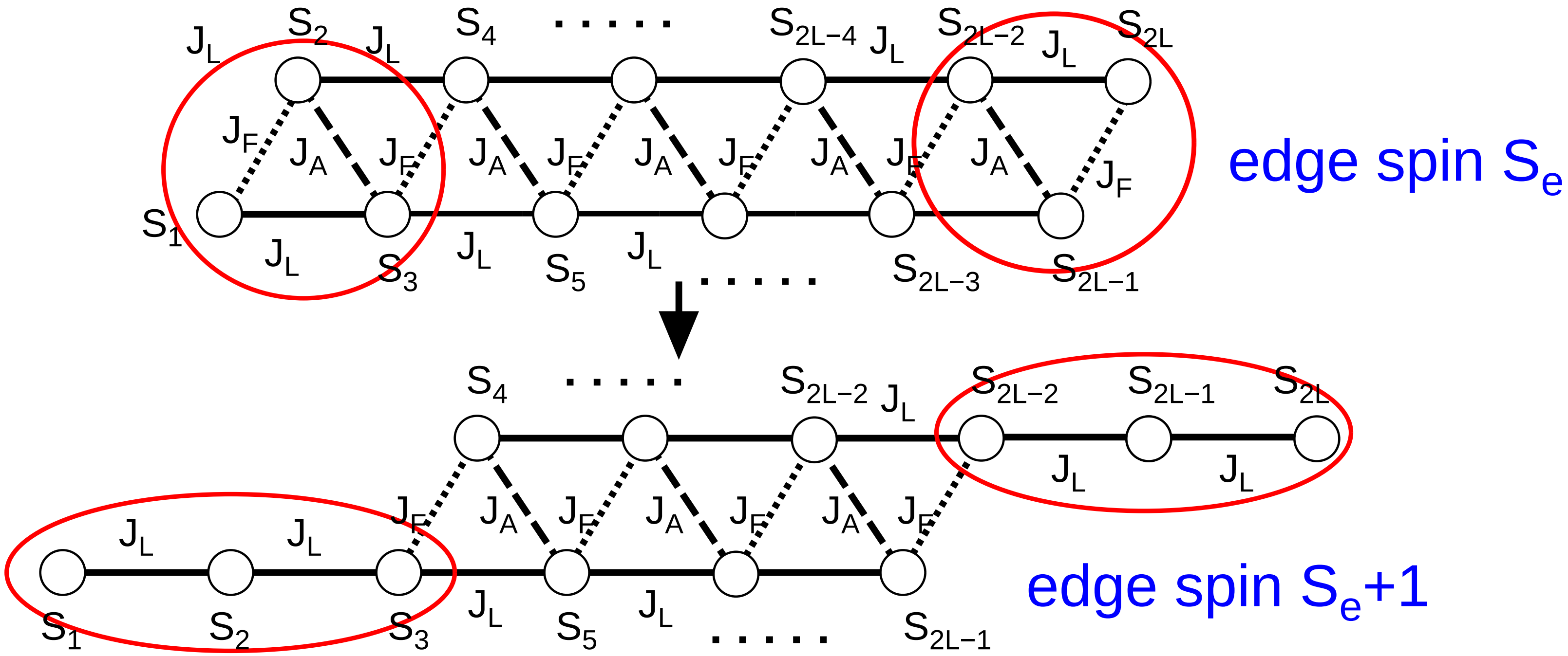


"Special point" : representative of I_{S_e} phase $S_{\rm e} = (m-1)/2$

$m = 2, 3, ..., \infty \Rightarrow$ Infinite series of I_{S_e} phases

4 Nature of Intermediate Phases

[Equivalence of $\mathrm{I}_{S_\mathrm{e}}$ and $\mathrm{I}_{S_\mathrm{e}+1}$ phases]

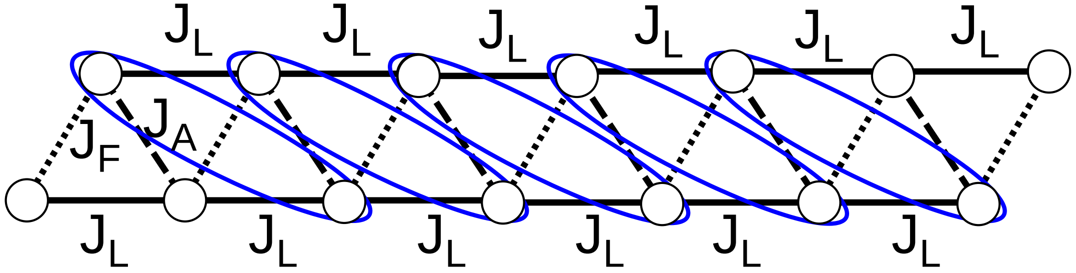


Bulk part remains the same

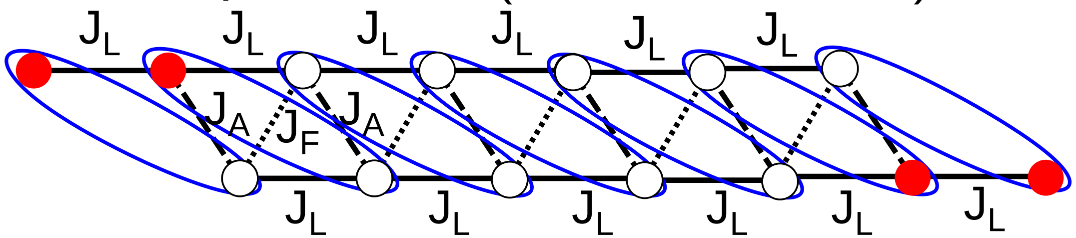
- Phases with integer S_e and half-odd-integer S_e are different phases.
- $\mathrm{I}_{S_\mathrm{e}+1/2}$ phase is always present between $\mathrm{I}_{S_\mathrm{e}}$ and $\mathrm{I}_{S_\mathrm{e}+1}$ phases
  $\Rightarrow$ All $\mathrm{I}_{S_\mathrm{e}}$ phases can be distinguished in the present model.
- Successive phase transitions between TWO topologically distinct ground states with integer and half-odd-integer edge spin

[Valence bond picture of $\mathrm{I}_{S_\mathrm{e}}$ phases]

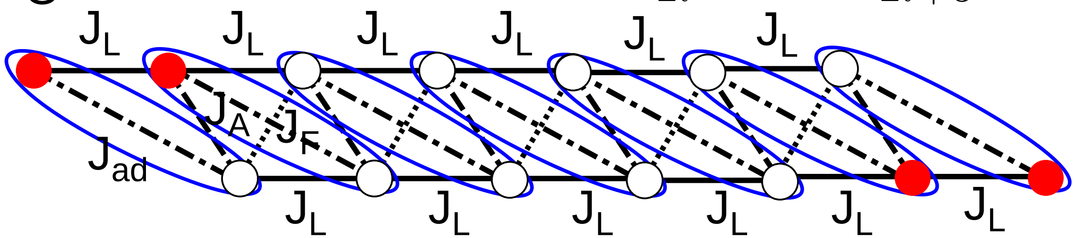
Expected valence bond structure of I_1 phase (open chain $S_\mathrm{e} = 1$)



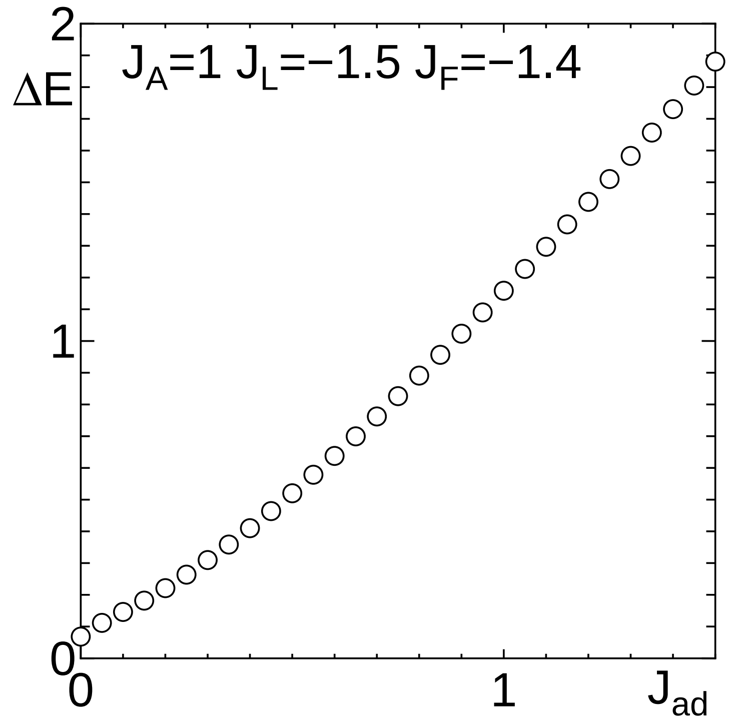
Two end spin added ($S_\mathrm{e} = 1$, $L_\mathrm{e} = 2$)



To stabilize this VBS structure, add antiferromagnetic bonds between $\boldsymbol{S}_{2l}$ and $\boldsymbol{S}_{2l+3}$

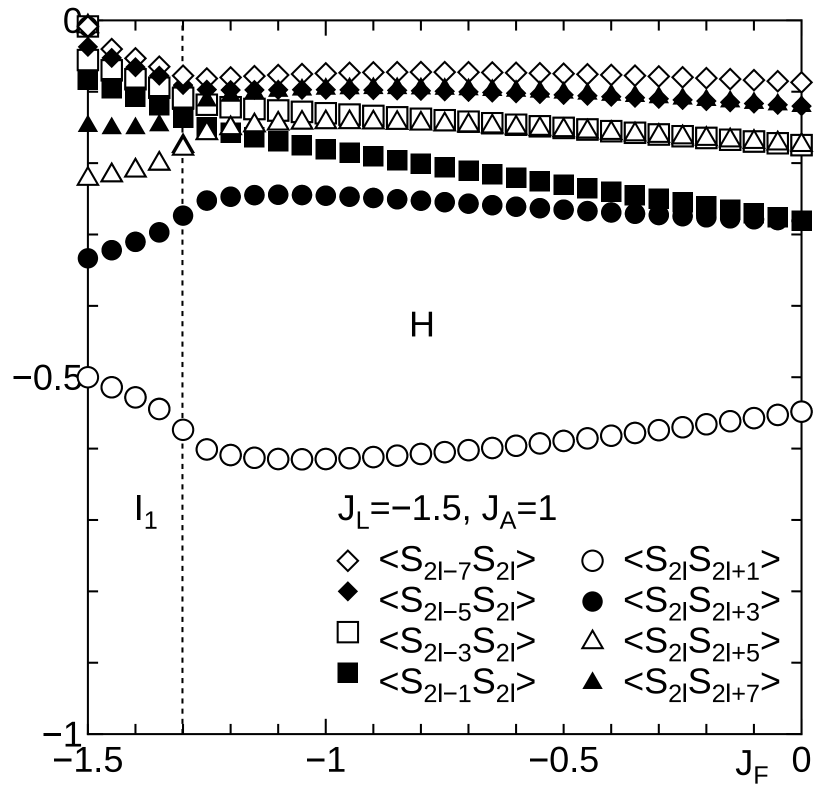


J_ad-dependence of energy gap



- $J_\mathrm{ad} \to \infty$: Isolated dimers on J_ad-bonds
- Gap does not close down to $J_\mathrm{ad} = 0$.

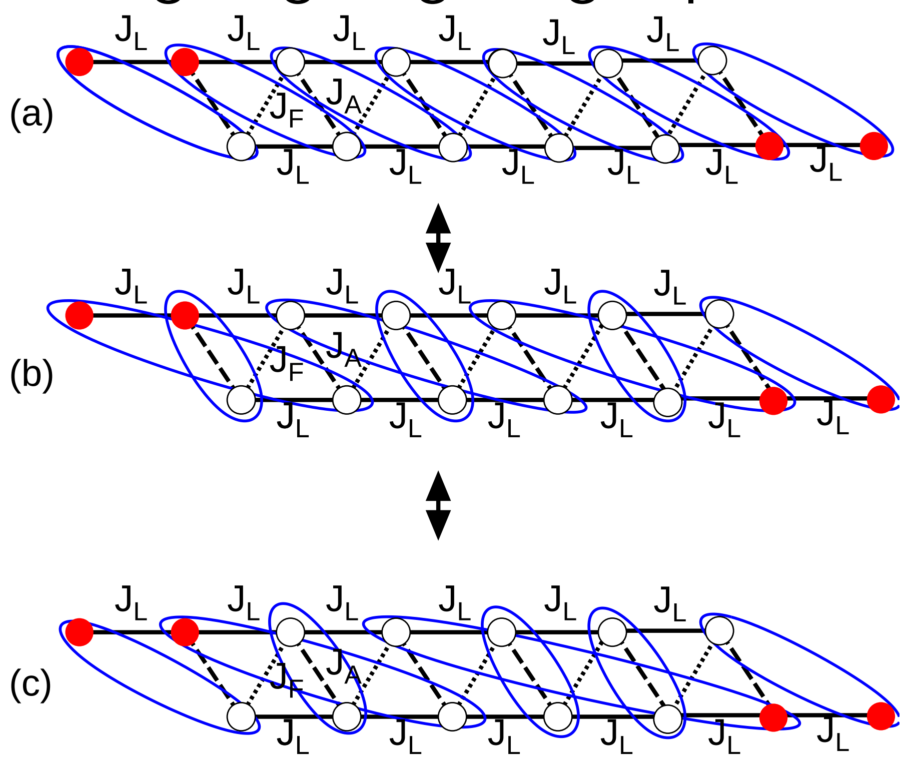
[Spin-spin correlation]



- $\langle \boldsymbol{S}_{2l}\boldsymbol{S}_{2l+1}\rangle$ ($J_{\rm A}$-bond) is the largest correlation even in I_1 phase (absolute value decreases)
- $\langle \boldsymbol{S}_{2l}\boldsymbol{S}_{2l+3}\rangle$ increases in I_1 phase

[Valence bond structure]

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

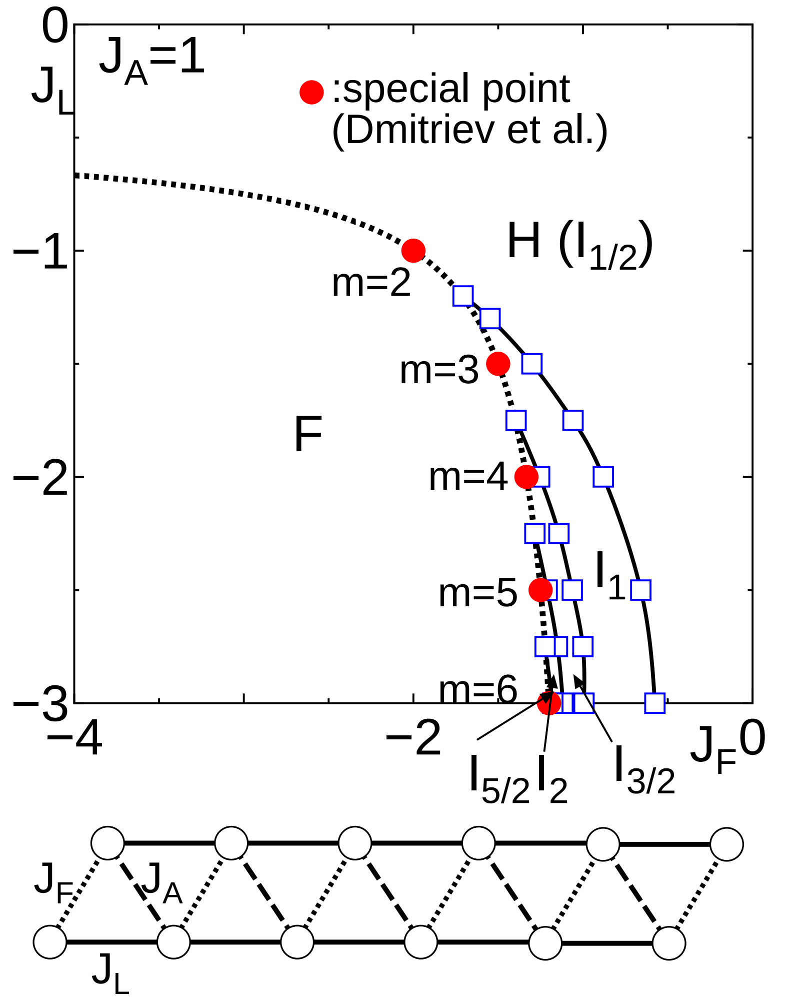


etc.

5 Summary

1. Ferromagnetic phase
2. Haldane phase
3. Infinite series of $\mathrm{I}_{S_\mathrm{e}}$ phases with edge spin S_e
   - Strong ferromagnetic NNN interaction
     $\Rightarrow$ $\mathrm{I}_{S_\mathrm{e}}$ 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

[Ground State Phase Diagram]



4. Exact solutions on the phase boundary (Dmitriev *et al.*)
   - $\dfrac{J_\mathrm{L}}{J_\mathrm{A}} = -\dfrac{m}{2}$ (special point) Representative of $\mathrm{I}_{(m-1)/2}$ phase

5. Future Problems

- Characterizaton by entanglement spectrum.
- Spin-1 case : Spiral short range order near ferromagnetic phase (S. Sahooa *et al.* arXiv:1305.6848.