Antiferromagnetic spin-S chains with exactly dimerized ground-states

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Scope

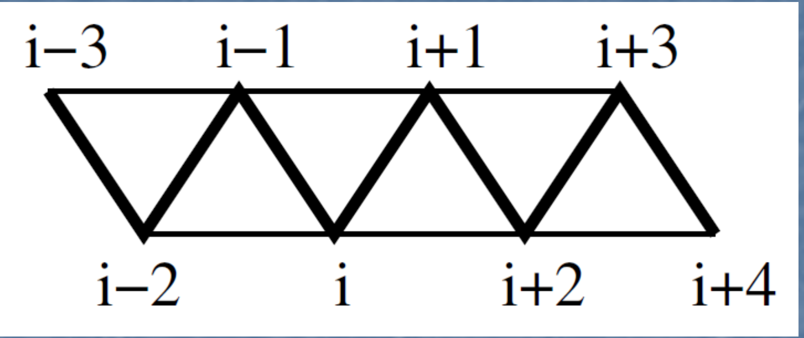
- The spin-1/2 J_1-J_2 chain
  → Majumdar-Ghosh point and dimerization
  → Some generalizations
- Three-site interaction
  → microscopic origin of three-site interaction
  → exactly dimerized ground states for any S
- Spin-1 case
  → phase diagram
- Conclusions

The spin-1/2 J_1-J_2 chain

$$\mathcal{H}_{J_1-J_2} = \sum_i (J_1 \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \vec{S}_i \cdot \vec{S}_{i+2})$$

Majumdar-Ghosh point

$$J_2 = J_1/2$$

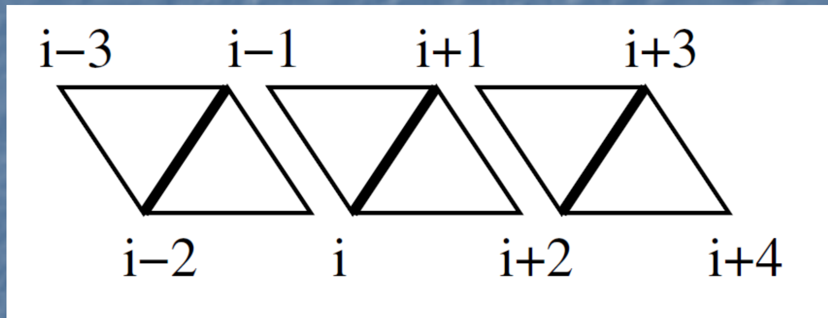


$$|\psi_{\mathrm{even,odd}}\rangle = \prod_{i \ \mathrm{even,odd}} |S(i,i+1)\rangle, \quad |S(i,i+1)\rangle = \mathrm{singlet}$$

Exact ground-states

Eigenstates

$$\mathcal{H}_{J_1-J_2} = \sum_{i \text{ odd}} \left(J_1 \vec{S}_i \cdot \vec{S}_{i+1} + \frac{J_1}{2}(\vec{S}_i + \vec{S}_{i+1}) \cdot \vec{S}_{i-1} + \frac{J_1}{2}(\vec{S}_i + \vec{S}_{i+1}) \cdot \vec{S}_{i+2}\right)$$



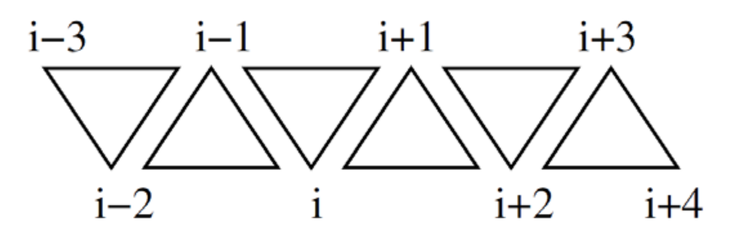
$$(S_i^\alpha + S_{i+1}^\alpha)|S(i,i+1)\rangle = 0, \quad \alpha = x, y, z$$

$$\mathcal{H}_{J_1-J_2}|\psi_{\text{odd}}\rangle = \frac{N}{2}\left(-\frac{3}{4}J_1\right)|\psi_{\text{odd}}\rangle$$

Idem for the even case

Lowest energy

$$\mathcal{H}_{J_1-J_2} = \sum_i \frac{J_1}{2}(\vec{S}_i \cdot \vec{S}_{i+1} + \vec{S}_i \cdot \vec{S}_{i+2} + \vec{S}_{i+1} \cdot \vec{S}_{i+2}) = \sum_i \mathcal{H}_{\triangle}(i)$$



$$E_0(\mathcal{H}_{\triangle}(i)) = -\frac{3}{4}\frac{J_1}{2}$$

$$\Rightarrow E_0(\mathcal{H}_{J_1-J_2}) \geq \sum_i E_0(\mathcal{H}_{\triangle}(i)) = -\frac{3}{4}\frac{J_1}{2}N = E_{\text{odd}}$$

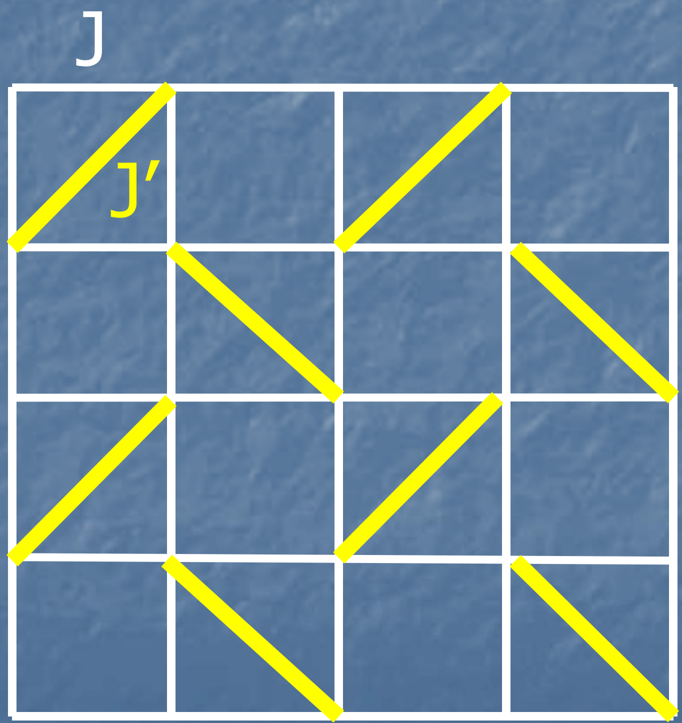
$$\Rightarrow E_0(\mathcal{H}_{J_1-J_2}) = E_{\text{odd}}$$

Phase diagram

Experimental realization: $CuGeO_3$ (?)

2D, arbitrary S generalization

Shastry-Sutherland model (1981)



Product of singlets on J' bonds
= GS if J/J' not too large.

Variational bound:

J/J'<1/2 for S=1/2

J/J'<2(1+S) for S≥1

1D, larger S generalization?

- Simple (but naive) idea: J_1-J_2 spin-S model
  → eigenstates? YES
  → lowest-energy? NO
- Klein's model

$$\mathcal{H}_{\rm Klein} = -\sum_i P^{i,i+1,i+2}_{S_{tot}=S}$$

$$P^{i,i+1,i+2}_{S_{tot}=S} = \prod_{\sigma\neq S} \frac{(\mathbf{S}_i + \mathbf{S}_{i+1} + \mathbf{S}_{i+2})^2 - \sigma(\sigma+1)}{S(S+1) - \sigma(\sigma+1)}$$

Very complicated, hence not realistic, for S>1/2

Back to Hubbard

- Standard 1D Hubbard model at half-filling

  → $S=1/2$ J_1-J_2 chain with $J_1 = O(t^2/U)$ and $J_2 = O(t^4/U)$

- Two-orbital 1D Hubbard model, 2 e^-/site

  → $S=1$ extended Heisenberg model with 4 types of terms

  $J_1\, S_i.S_{i+1}$ with $J_1 = O(t^2/U)$

  $$\left.\begin{array}{l} J_2\, S_i.S_{i+2} \\ J_{Biq}\, (S_i.S_{i+1})^2 \\ J_3\, [(S_{i-1}.S_i)(S_i.S_{i+1}) + h.c.] \end{array}\right\} \quad J_2,\, J_{Biq},\, J_3 = O(t^4/U)$$

Three-site interaction

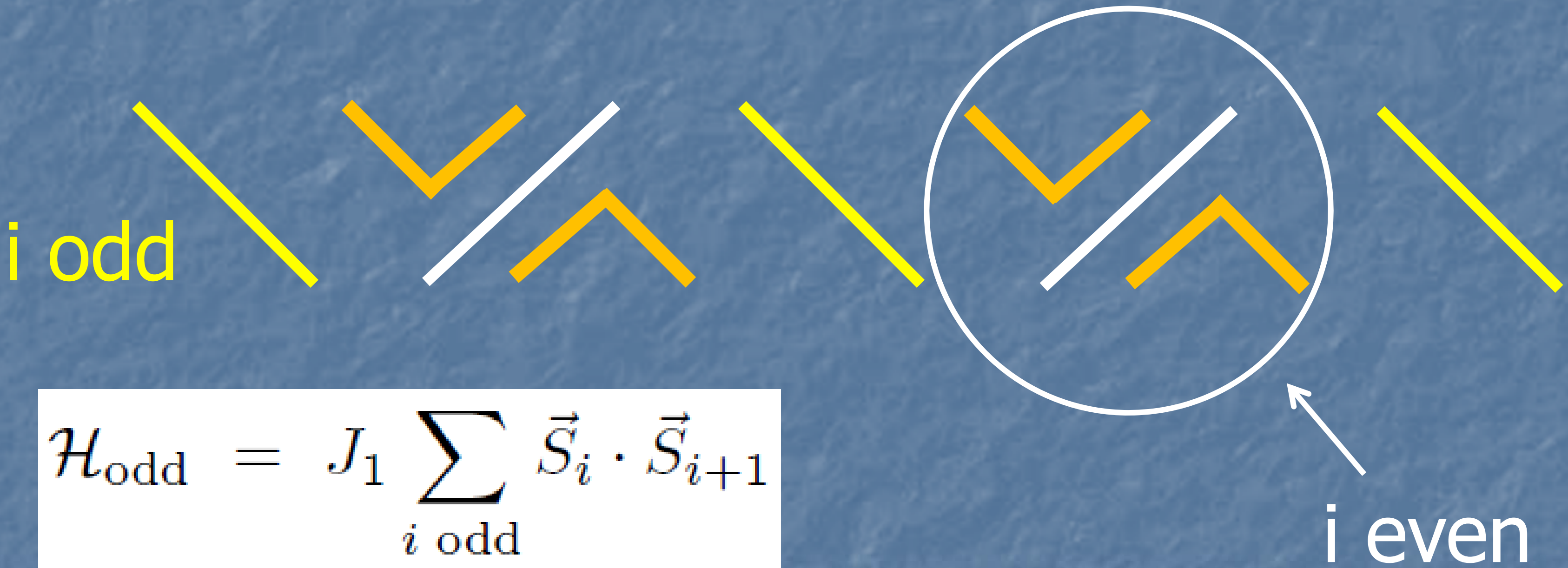
$$\mathcal{H}_{J_1-J_3} = J_1 \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + J_3 \sum_i \left[(\vec{S}_{i-1} \cdot \vec{S}_i)(\vec{S}_i \cdot \vec{S}_{i+1}) + \mathrm{h.c.} \right]$$

- Reduces to J_1-J_2 model with $J_2=J_3/2$ for S=1/2
  → generalization of S=1/2 J_1-J_2 chain

F. Michaud, F. Vernay, S. Manmana, FM, PRL 2012

Dimerized eigenstates I

$$\mathcal{H}_{J_1-J_3} \;=\; \mathcal{H}_{\mathrm{odd}} + \mathcal{H}_{\mathrm{even}}$$



$$\mathcal{H}_{\mathrm{odd}} \;=\; J_1 \sum_{i\ \mathrm{odd}} \vec{S}_i \cdot \vec{S}_{i+1}$$

$$\mathcal{H}_{\mathrm{odd}}|\psi_{\mathrm{odd}}\rangle = -N\frac{J_1}{2}S(S+1)|\psi_{\mathrm{odd}}\rangle$$

Dimerized eigenstates II

$$\mathcal{H}_{\text{even}} = J_1 \sum_{i \text{ even}} \vec{S}_i \cdot \vec{S}_{i+1}$$

$$+ \; J_3 \sum_{i \text{ even}} \left[(\vec{S}_{i-1} \cdot \vec{S}_i)(\vec{S}_i \cdot \vec{S}_{i+1}) + \text{h.c.} \right] + \left[(\vec{S}_{i+1} \cdot \vec{S}_{i+2})(\vec{S}_i \cdot \vec{S}_{i+1}) + \text{h.c.} \right]$$

$$(\vec{S}_i \cdot \vec{S}_{i+1})(\vec{S}_{i-1} \cdot \vec{S}_i)|\psi_{\text{odd}}\rangle = -S(S+1)\; \vec{S}_i \cdot \vec{S}_{i+1}\; |\psi_{\text{odd}}\rangle$$

$$\vec{S}_i \cdot \vec{S}_{i+1}|\psi_{\text{odd}}\rangle = \sum_{\sigma,\sigma'} C_{\sigma,\sigma'} |T_\sigma(i-1,i)\rangle |T_{\sigma'}(i+1,i+2)\rangle \prod_{j \text{ odd}}{}' |S(j,j+1)\rangle$$

$$\Rightarrow \quad (\vec{S}_{i-1} \cdot \vec{S}_i)(\vec{S}_i \cdot \vec{S}_{i+1})|\psi_{\text{odd}}\rangle = [1 - S(S+1)]\; \vec{S}_i \cdot \vec{S}_{i+1}\; |\psi_{\text{odd}}\rangle$$

Dimerized eigenstates III

$$\mathcal{H}_{\text{even}}|\psi_{\text{odd}}\rangle = (J_1 - (4S(S+1)+2)J_3) \sum_{i \text{ even}} \vec{S}_i \cdot \vec{S}_{i+1}|\psi_{\text{odd}}\rangle$$

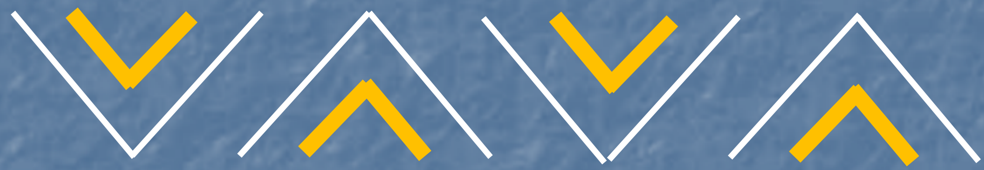
If $$\frac{J_3}{J_1} = \frac{1}{4S(S+1)-2}$$

then $$\mathcal{H}_{\text{even}}|\psi_{\text{odd}}\rangle = 0$$

hence $$\mathcal{H}_{J_1-J_3}|\psi_{\text{odd}}\rangle = -N\frac{J_1}{2}S(S+1)|\psi_{\text{odd}}\rangle$$

Lowest energy

$$\mathcal{H}_{J_1-J_3} = J_1 \sum_i \mathcal{H}_i$$

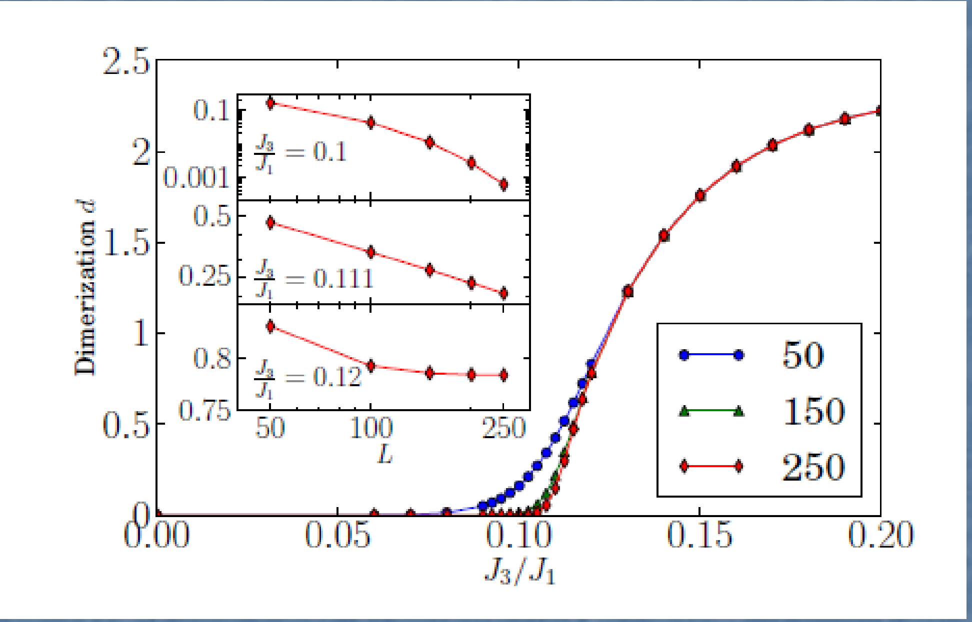


$$\mathcal{H}_i = \frac{1}{2}(\vec{S}_{i-1}\cdot\vec{S}_i + \vec{S}_i\cdot\vec{S}_{i+1}) + \frac{1}{4S(S+1)-2}[(\vec{S}_{i-1}\cdot\vec{S}_i)(\vec{S}_i\cdot\vec{S}_{i+1}) + \text{h.c.}]$$

$$E_0(\mathcal{H}_i) = -\frac{S(S+1)}{2}$$

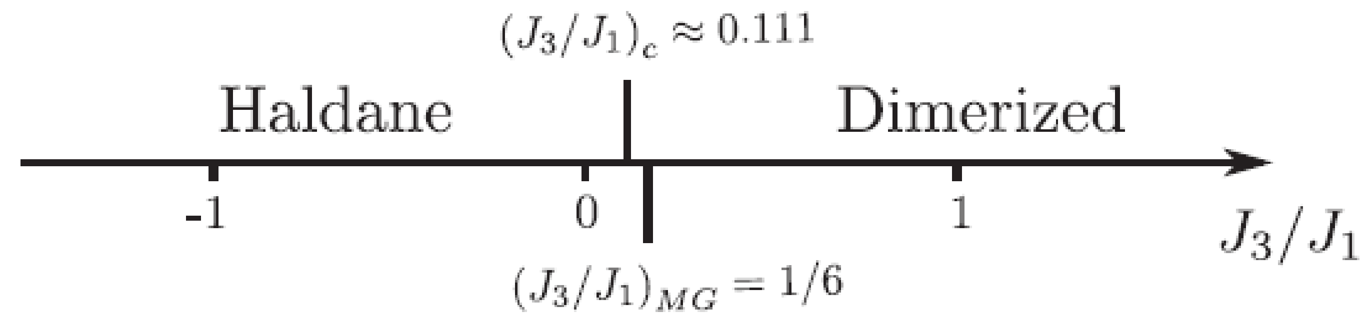
$$\Rightarrow E_0(\mathcal{H}_{J_1-J_3}) = E_{\text{odd}}$$

Spin-1: phase diagram

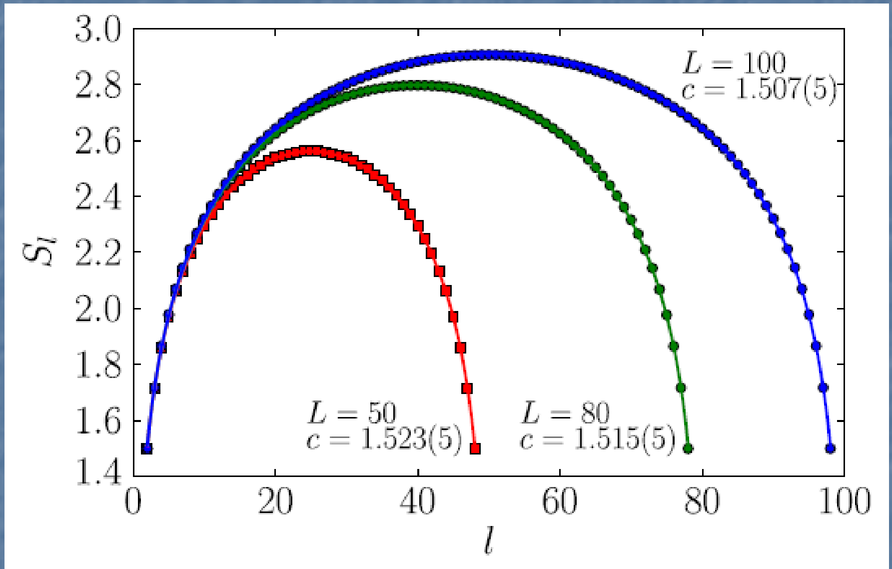


DMRG dimerization

$$d = \left| \langle \vec{S}_i . \vec{S}_{i+1} - \vec{S}_{i-1} . \vec{S}_i \rangle \right|$$



Critical point : $(J_3/J_1)_c \approx 0.111$



$$S_\ell = \frac{c}{3} \ln\left[\frac{L}{\pi} \sin\left(\frac{\pi\ell}{L}\right)\right] + g_{\mathrm{PBC}}$$

Calabrese-Cardy

- Central charge: c=3/2
- Wess-Zumino-Witten model with k=2
- Same universality class as bilinear-biquadratic model with $J_{Biq}=-J_1$

Experimental implications

$J_3/J_1=1/(S(S+1)-2)$ is small for $S>1/2$:

1/6 (S=1), 1/13 (S=3/2), 1/22 (S=2)

$(J_3/J_1)_c$ even smaller (see poster Michaud)

- Realistic close to Metal-Insulator transition
- Other terms of same order (J_2, biquadratic)

→ check their effect or make them small

Conclusions/Perspectives

- New route to dimerization in spin-S chains
  → 'realistic' 3-site interaction
  → exactly dimerized ground state for $J_3/J_1=1/(4S(S+1)-2)$
- S>1 (see poster Frédéric Michaud)
  → $(J_3/J_1)_c$ very small
  → higher order WZW models with k=2S and central charge c=3S/(S+1)