Antiferromagnetic Spin Chains

University of Florida, April 2020

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2. Goldstone modes, and spin-wave theory.
   - Using the Neel state as the broken symmetry state one might think we should be able to find spin-wave excitations which we know are gapless, and lead to power law correlations.

Outline

1. Spin-waves for 1D AFM
2. Lieb-Shultz-Mattis theorem
3. Solvable models and valence bond solid states
4. Symmetry of the VBS state

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Heisenberg model

For a 1D chain with local spin-s on each site the Heisenberg Hamiltonian can be written as:

$$\begin{aligned} H &= J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \\ &= J \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + S_i^z S_{i+1}^z, \end{aligned}$$

with

$$S^+ = \frac{1}{\sqrt{2}} \left(S^x + i S^y \right) \qquad S^- = \frac{1}{\sqrt{2}} \left(S^x - i S^y \right),$$

$$[S^i, S^j] = i \epsilon^{ijk} S^k \qquad [S^+, S^-] = S^z$$

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Anti-ferromagnetism: $J < 0$

$$|\Psi_{\text{Neel}}\rangle = |+s \ \ -s \ \ +s \ldots\rangle$$
$$H \, |\Psi_{\text{Neel}}\rangle \neq E_0 \, |\Psi_{\text{Neel}}\rangle$$
$$|\Psi_0\rangle \neq |\Psi_{\text{Neel}}\rangle$$

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Neel state spontaneously breaks the symmetry and hence would result in a Goldstone modes leading to a gapless excitations.

Holstien-Primakov transformation in AFM case

$$S_A^z = s - a^\dagger a \quad S_A^- = a^\dagger \left[s - \frac{a^\dagger a}{2} \right]^{1/2}$$

$$S_B^z = -s + b^\dagger b \quad S_B^+ = b^\dagger \left[s - \frac{b^\dagger b}{2} \right]^{1/2}$$

with

$$[a, a^\dagger] = 1 \qquad [b, b^\dagger] = 1 \qquad [a, b] = 0 \qquad [a, b^\dagger] = 0$$

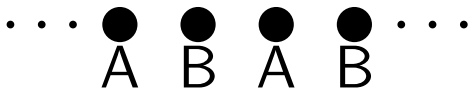


Figure: AB lattice, artificially doubling the unit cell. We put the distance between 2 A sub-lattices to be 1. Let length of the entire chain be L.

Classical limit in the AFM case

Expanding around a Neel state, using $1/s$ as a small parameter.

$$S_A^z = s - a^\dagger a \qquad S_A^- = \sqrt{s}\ a^\dagger$$
$$S_B^z = -s + b^\dagger b \qquad S_B^+ = \sqrt{s}\ b^\dagger$$

Using this and after Fourier transforming, dropping a constant term, and keeping only terms of order $O(s)$,

$$a_i = \sqrt{\frac{1}{L}} \sum_k e^{ikR_i} a_k \qquad b_i = \sqrt{\frac{1}{L}} \sum_k e^{ik(R_i+1/2)} b_k$$

$$H = 2Js \sum_k a_k^\dagger a_k + b_k^\dagger b_k + \cos(k/2) a_k b_{-k} + \cos(k/2) b_{-k}^\dagger a_k^\dagger$$

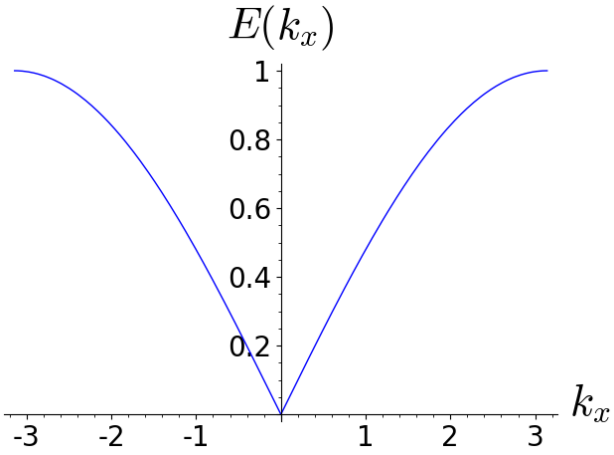
Bogoliubov transformation

The Bogoliubov transformation,

$$c_k = u_k a_k - v_k b^\dagger_{-k}$$
$$d_k = u_k b_k - v_k a^\dagger_{-k}$$
$$|u_k|^2 - |v_k|^2 = 1$$

diagonalize the Hamiltonian,

$$H = 2Js\left[1 - \cos(k/2)\right]^{1/2}\left(c_k^\dagger c_k + d_k^\dagger d_k\right)$$



Have we shown that the chain is gapless?

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This approximation only works if the ground state is close to the Neel state. The ground state defined as,

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This can be checked by comparing $\langle S^z \rangle$ in the ground state to that of the Neel state,

$$\langle \Psi_{\text{Neel}} | S_i^z | \Psi_{\text{Neel}} \rangle = \pm s$$

$$\langle \Psi_0 | S_i^z | \Psi_0 \rangle = \pm s + \int dk \frac{1}{2} \left[\frac{1}{|\sin(k)|} - 1 \right]$$

Remember,

$$S_A^- = a^\dagger \left[s - \frac{a^\dagger a}{2} \right]^{1/2}$$

The correction in infinite for any s.

Outline

LSM theory

Statement of the theorem:

Any half integer spin chain that is symmetric under parity is either gapless or has a degenerate ground state that breaks parity.

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Construct a state $|\Psi_1\rangle = \hat{\eta}\,|\Psi_0\rangle$ with,

$\hat{\eta} = R^z(\{\theta_i\}) = e^{i\sum_{i=-l}^{l}\theta_i S_i^z}$ (rotation about odd number of local z-axes)

$$\theta_i = \frac{R_i + l}{l}\pi$$

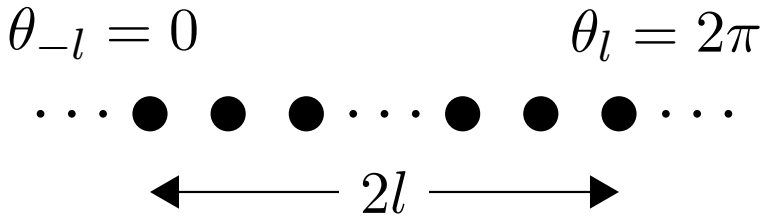


Figure: LSM unitary operator act on only on the part of the chian from $-l$ to l.

LSM theory

We need to show 2 things as $l \to \infty$ to show the system is gapless:

1. $\langle \Psi_1 | H - E_0 | \Psi_1 \rangle \to 0$ shows it's a low energy excitation. (E_0 is the ground state energy.)
2. $\langle \Psi_1 | \Psi_0 \rangle \to 0$ shows that $|\Psi_1\rangle \neq |\Psi_0\rangle$

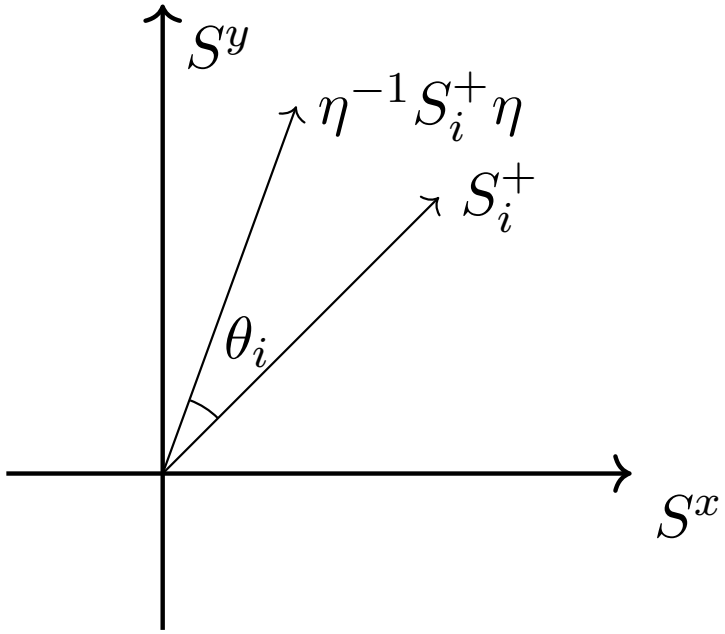
$\langle \Psi_1 | H - E_0 | \Psi_1 \rangle \to 0$

First we notice that,

$$R^{z-1}(\theta_i) S_i^{\pm} R^z(\theta_i) = e^{\pm i\theta_i} S^{\pm}.$$

Remember

$$H = J \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + S_i^z S_{i+1}^z$$



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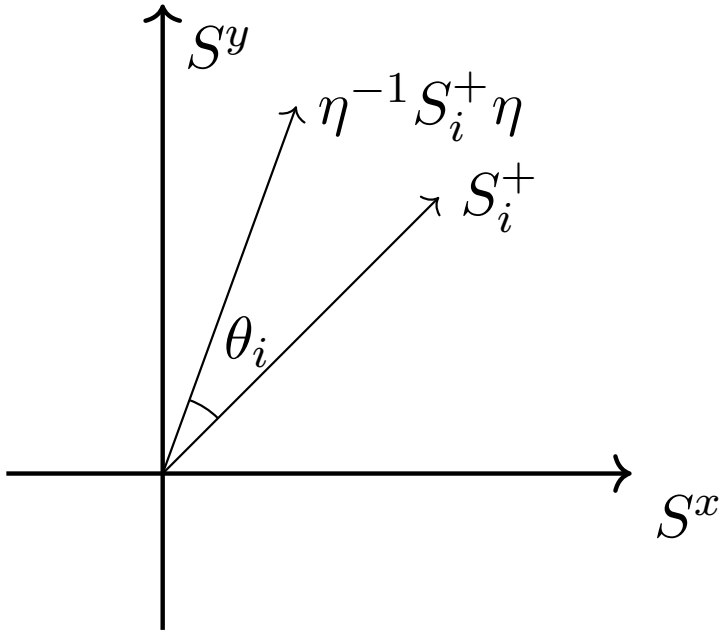

Remember

$$H = J \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + S_i^z S_{i+1}^z$$

$$\eta^{-1} H \eta = H + J \sum_{i=-l}^{l-1} \left[e^{\frac{-i\pi}{l}} - 1 \right] S_i^+ S_{i+1}^- + \left[e^{\frac{i\pi}{l}} - 1 \right] S_i^- S_{i+1}^+$$

$$\langle \Psi_1 | H - E_0 | \Psi_1 \rangle = \langle \Psi_0 | \eta^{-1} H \eta - E_0 | \Psi_0 \rangle$$

$$= 2J \left[\cos(\frac{\pi}{l}) - 1 \right] \sum_{i=0}^{l-1} \langle \Psi_0 | S_i^+ S_{i+1}^- + S_i^- S_{i-1}^+ | \Psi_0 \rangle$$

$$= 2\pi^2 J e_0 \frac{1}{l}$$ **Doesn't depend on spin.**

$\langle \Psi_1 | \Psi_0 \rangle \to 0$

We study the parity of the state $|\Psi_1\rangle$ as compared to the parity of the ground state $|\Psi_0\rangle$. Let the parity operator be $\mathcal{P}$.

$$\mathcal{P} H \mathcal{P}^{-1} = H$$
$$\mathcal{P} |\Psi_0\rangle = \pm |\Psi_0\rangle$$
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Using $\mathcal{P} S_i^z \mathcal{P}^{-1} = -S_{-i}^z$,

$$\mathcal{P} \eta \mathcal{P}^{-1} = e^{i2\pi \sum_{i=-l}^{l} S_i^z} \eta \ = \begin{cases} \eta & s \text{ integer} \\ -\eta & s \text{ half integer} \end{cases}$$

Outline

Majumdar-Gosh Model (a warm up)

For a spin-1/2 chain,

$$H = J\sum_i (\vec{S}_i + \vec{S}_{i+1} + \vec{S}_{i+2})^2 = J\sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{2}\vec{S}_i \cdot \vec{S}_{i+2}$$

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The ground state must have any adjacent 3 sites to have total spin of 1/2.
This can be achieved by paring adjacent spins into singlets.

$$\bullet\!-\!\bullet \quad \bullet\!-\!\bullet \quad \bullet\!-\!\bullet$$

$$|\Psi_0\rangle = |\phi_{\alpha_1}\phi_{\alpha_2}\phi_{\alpha_3}\phi_{\alpha_4}\ldots\rangle\, \epsilon^{\alpha_1\alpha_2}\epsilon^{\alpha_3\alpha_4}\ldots$$

(a)

$$-\!\bullet \quad \bullet\!-\!\bullet \quad \bullet\!-\!\bullet \quad \bullet\!-$$

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(b)

Figure: Two ways adjacent spins can be paired into singlets.

Majumdar-Gosh Model

Remarks about the ground sates:

- A contraction between 2 spin-1/2 into a spin singlet is called a valence bond. These ground states of the Majumadar-Gosh model are valence bond states with all the spins contracted.

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- This suggest the existence of a gap.

Valence bond states

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We need a way to generalize valence bond states to higher spins
For spin-1 we think of each spin site as being made of 2 spin-1/2s.
And always construct states that are symmetric in same site spin-1/2s.
The following can be used as a basis on each site,

$$|\phi_{\alpha_1\alpha_2}\rangle = |\phi_{\alpha_2\alpha_1}\rangle = \frac{1}{\sqrt{2}}(|\phi_{\alpha_1}\phi_{\alpha_2}\rangle + |\phi_{\alpha_2}\phi_{\alpha_1}\rangle)$$

$$\langle\phi_{\alpha_1\alpha_2}|\phi_{\beta_1\beta_2}\rangle = \delta_{\alpha_1\beta_1}\delta_{\alpha_2\beta_2} + \delta_{\alpha_1\beta_2}\delta_{\alpha_2\beta_1}$$

Valence bond states

Let's look at the possible valence bond states of spin-1 chain.

$$-\bullet-\bullet-\bullet-\bullet-\bullet-\bullet-$$

$$|\Psi^{\text{VBS}}_{\alpha_1\alpha_{2L}}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8}\ldots\rangle\,\epsilon^{\alpha_2\alpha_3}\epsilon^{\alpha_4\alpha_5}\ldots$$

(a)

$$\bullet\frown\bullet \quad \bullet\frown\bullet \quad \bullet\frown\bullet$$

$$|\Psi^{\text{VB1}}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8}\ldots\rangle\,\epsilon^{\alpha_1\alpha_3}\epsilon^{\alpha_2\alpha_4}\ldots$$

(b)

$$\smile\bullet \quad \bullet\frown\bullet \quad \bullet\frown\bullet \quad \bullet\smile$$

$$|\Psi^{\text{VB2}}_{\alpha_1\alpha_2\alpha_{2L-1}\alpha_{2L}}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8}\ldots\rangle\,\epsilon^{\alpha_3\alpha_5}\epsilon^{\alpha_4\alpha_6}\ldots$$

(c)

Figure: 3 possible valence bond states. (a) is the VBS partially dimerized state. (b) and (c) are the fully dimerized states.

AKLT model

The AKLT model is a spin-1 chian model with the VBS state being the ground state,

$$
\begin{aligned}
H &= 2J \sum_i P^{(2)}(\vec{S}_i + \vec{S}_{i+1}) \\
&= J \sum_i \frac{1}{12}(\vec{S}_i + \vec{S}_{i+1})^2((\vec{S}_i + \vec{S}_{i+1})^2 - 2) \\
&= J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 + \text{const.}
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This Hamiltonian is positive definite, the ground state will have $E_0 = 0$.
The VBS state has for every 2 adjacent spin sites 2 of the 4 spin-1/2s to be contracted into a spin singlet.
Hence the total spin of any 2 adjacent spin sites cannot be 2 with only 2 spin-1/2s left. This shows the VBS state to be a ground state.

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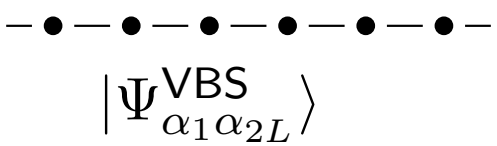
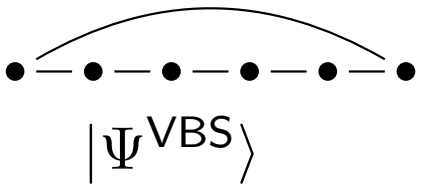
What is more subtle is to show that this is the only ground state! It is the unique ground state up to some boundary modification.



One can get around this by considering an infinite system, or to be more concrete, study the system under periodic boundary conditions.



Correlation length of the VBS state

$$\vec{S}\,|\phi_{\alpha_1\alpha_2}\rangle = \frac{1}{2}(\vec{\sigma}_{\beta\alpha_1}\,|\phi_{\beta\alpha_2}\rangle + \vec{\sigma}_{\beta\alpha_2}\,|\phi_{\alpha_1\beta}\rangle)$$

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Trivia

Looking on the more general Hamiltonian,

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} - \beta (\vec{S}_i \cdot \vec{S}_{i+1})^2$$

there is another solvable point at $\beta = 1$, which is gapless.

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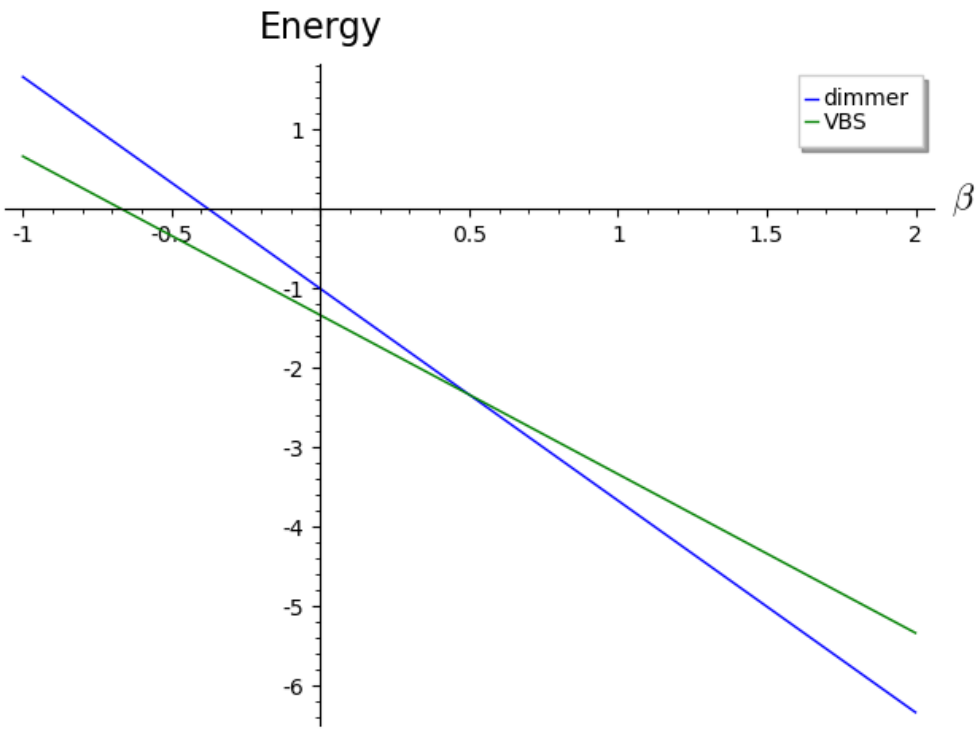
A phase transition occur at $\beta = 1$. The graphs suggests that the phase transition occur between the VBS and the dimerized state.



Outline

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Such along range correlation between the ends of the chain can only happen if the bulk closes a gap.