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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4. Symmetry of the VBS state
Heisenberg model

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

\[
H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}
\]

\[
= J \sum_i S^+_i S^-_{i+1} + S^-_i S^+_i + S^z_i S^z_{i+1},
\]

with

\[
S^+ = \frac{1}{\sqrt{2}} (S^x + iS^y) \quad S^- = \frac{1}{\sqrt{2}} (S^x - iS^y),
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\[
[S^i, S^j] = i\epsilon^{ijk} S^k \quad [S^+, S^-] = S^z
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Ferromagnetism: \(J < 0\)

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|\Psi_{FM}\rangle = |+s + s + s \ldots\rangle
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Anti-ferromagnetism: \( J < 0 \)

\[ |\Psi_{Neel}\rangle = |+s \ - s + s \ldots\rangle \]

\[ H |\Psi_{Neel}\rangle \neq E_0 |\Psi_{Neel}\rangle \]

\[ |\Psi_0\rangle \neq |\Psi_{Neel}\rangle \]
Classical limit in the AFM case

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We notice that,

\[ \langle \Psi_{\text{Neel}} | S_i^+ S_{i+1}^- | \Psi_{\text{Neel}} \rangle \propto s \]

\[ \langle \Psi_{\text{Neel}} | S_i^z S_{i+1}^z | \Psi_{\text{Neel}} \rangle \propto s^2. \]

Hence in the classical limit, \( s \to \infty \), one might expect the Neel state to approaches the ground state.
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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

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

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

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 \( L \).

with

\[ [a, a^\dagger] = 1 \quad [b, b^\dagger] = 1 \quad [a, b] = 0 \quad [a, b^\dagger] = 0 \]
Classical limit in the AFM case

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

$$S_A^z = s - a\dagger a$$

$$S_B^z = -s + b\dagger b$$

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

$$a_i = \sqrt{\frac{1}{L}} \sum_k e^{ikR_i} a_k$$

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

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

The Bogoliubov transformation,

\[ c_k = u_k a_k - v_k b_k^\dagger \]
\[ d_k = u_k b_k - v_k a_k^\dagger \]
\[ |u_k|^2 - |v_k|^2 = 1 \]

diagonalize the Hamiltonian,

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

Have we shown that the chain is gapless?
What goes wrong?

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

\[ c_k |\Psi_0\rangle = 0 \]
\[ d_k |\Psi_0\rangle = 0 \]

This can be checked by comparing \( \langle S_z \rangle \) in the ground state to that of the Neel state,

\[ \langle \Psi_{\text{Neel}} | S_z | \Psi_{\text{Neel}} \rangle = \pm s \]

Remember, \( S^- A = a \dagger [s - a \dagger a]^2 ]^{1/2} \)

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

The correction in infinite for any s.
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\[ \langle \Psi_{\text{Neel}} | S^z_i | \Psi_{\text{Neel}} \rangle = \pm s \]
\[ \langle \Psi_0 | S^z_i | \Psi_0 \rangle = \pm s + \int dk \frac{1}{2} \left[ \frac{1}{|\sin(k)|} - 1 \right] \]

Remember,

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

The correction in infinite for any \( s \).
1. Spin-waves for 1D AFM

2. Lieb-Shultz-Mattis theorem

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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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Any half integer spin chain that is symmetric under parity is either gapless or has a degenerate ground state that breaks parity.
Construct a state $|\Psi_1\rangle = \hat{\eta} |\Psi_0\rangle$ with,

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

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

$$\theta_{-l} = 0 \quad \theta_l = 2\pi$$

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

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

Remember

\[ H = J \sum_i S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + S_i^z S_{i+1}^z \]
\[ \langle \Psi_1 | H - E_0 | \Psi_1 \rangle \rightarrow 0 \]

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\[ H = J \sum_i S^+_i S^-_{i+1} + S^-_i S^+_{i+1} + S^z_i S^z_{i+1} \]

\[ \eta^{-1} H \eta = H + J \sum_{i=-l}^{l-1} \left[ e^{-i\pi i l} - 1 \right] S^+_i S^-_{i+1} + \left[ e^{i\pi i l} - 1 \right] S^-_i S^+_{i+1} \]

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

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

\[ = 2\pi^2 J e_0 \frac{1}{l} \text{ Doesn't depend on spin.} \]
\[ \langle \Psi_1 | \Psi_0 \rangle \to 0 \]

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 \\
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Using $\mathcal{P} S_i^z \mathcal{P}^{-1} = -S_{-i}^z$,

$$\mathcal{P} \eta \mathcal{P}^{-1} = e^{i2\pi \sum_{i=-l}^{l} S_i^z \eta} = \begin{cases} \eta & \text{s integer} \\ -\eta & \text{s half integer} \end{cases}$$
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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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Adding 3 spin-1/2 gives either spin-3/2 or spin-1/2. 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.

\[
|\Psi_0\rangle = |\phi_{\alpha_1} \phi_{\alpha_2} \phi_{\alpha_3} \phi_{\alpha_4} \ldots \rangle \epsilon_{\alpha_1 \alpha_2} \epsilon_{\alpha_3 \alpha_4} \ldots \\
(a)
\]

\[
|\Psi_0\rangle = |\phi_{\alpha_1} \phi_{\alpha_2} \phi_{\alpha_3} \phi_{\alpha_4} \phi_{\alpha_5} \ldots \rangle \epsilon_{\alpha_2 \alpha_3} \epsilon_{\alpha_4 \alpha_5} \ldots \\
(b)
\]

**Figure:** Two ways adjacent spins can be paired into singlets.
Majumdar-Gosh Model

Remarks about the ground states:

- A contraction between 2 spin-1/2 into a spin singlet is called a valence bond. These ground states of the Majumdar-Gosh model are valence bond states with all the spins contracted.
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- These states has a very short correlation length,

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\langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 \quad \text{for} \quad |R_i - R_j| > 1
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- This suggest the existence of a gap.
Valence bond states

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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.

\[
|\Psi^{\text{VBS}}_{\alpha_1\alpha_2L}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8} \cdots \rangle \epsilon^{\alpha_2\alpha_3}\epsilon^{\alpha_4\alpha_5} \cdots
\]

(a)

\[
|\Psi^{\text{VB1}}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8} \cdots \rangle \epsilon^{\alpha_1\alpha_3}\epsilon^{\alpha_2\alpha_4} \cdots
\]

(b)

\[
|\Psi^{\text{VB2}}_{\alpha_1\alpha_2\alpha_2L-1\alpha_2L}\rangle = |\phi_{\alpha_1\alpha_2}\phi_{\alpha_3\alpha_4}\phi_{\alpha_5\alpha_6}\phi_{\alpha_7\alpha_8} \cdots \rangle \epsilon^{\alpha_3\alpha_5}\epsilon^{\alpha_4\alpha_6} \cdots
\]

(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 chain model with the VBS state being the ground state,

\[ H = 2J \sum_i P^{(2)}(\vec{S}_i + \vec{S}_{i+1}) \]

\[ = J \sum_i \frac{1}{12}(\vec{S}_i + \vec{S}_{i+1})^2 ((\vec{S}_i + \vec{S}_{i+1})^2 - 2) \]

\[ = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3} (\vec{S}_i \cdot \vec{S}_{i+1})^2 + \text{const.} \]
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This Hamiltonian is positive definite, the ground state will have \(E_0 = 0\).
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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.
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.

\[ H \ket{\Psi_{VBS}} = 0 \]
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Correlation length of the VBS state

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

\[ \langle \vec{S}_i \cdot \vec{S}_j \rangle = 4(-1)^{R_j-R_i} 3^{-|R_j-R_i|} \]

\[ \xi = \frac{1}{\log 3} = 0.9 \]
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Finite length correlation function suggests the existence of a gap.
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\[ \xi = \frac{1}{\log 3} = 0.9 \]

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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

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
Symmetry of VBS state

No local order parameter characterizes the transition to the VBS state.

The periodic VBS chain preserve all local symmetries of the Hamiltonian like rotation, inversion, translation, and time reversal symmetry. This here is an example of a symmetry protected topology. Let's study the VBS state with open boundary condition.

The state has 2 "free" spin-1/2, one at each end of the chain, that transforms differently as compared to the bulk. Such a weird situation at the boundaries can only be changed by a transformation that mixes the boundaries. Such a long-range correlation between the ends of the chain can only happen if the bulk closes a gap.
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