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

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

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

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Ferromagnetism: $J < 0$

$$|\Psi_{\mathsf{FM}}\rangle = |{+s} \ \ {+s} \ \ {+s} \ldots\rangle$$

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Anti-ferromagnetism: $J < 0$

$$\begin{aligned} |\Psi_{\mathsf{Neel}}\rangle &= |+s \;\; -s \;\; +s \ldots\rangle \\ H\,|\Psi_{\mathsf{Neel}}\rangle &\neq E_0\,|\Psi_{\mathsf{Neel}}\rangle \\ |\Psi_0\rangle &\neq |\Psi_{\mathsf{Neel}}\rangle \end{aligned}$$

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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

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

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

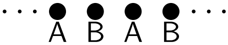


Figure: AB lattice, artificially doubling the unit cell. We put the distance between 2 A sub-lattices to be 1. Let length of the entire chain be L.

with

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

Classical limit in the AFM case

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

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

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

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

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

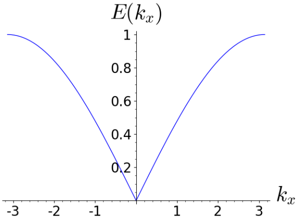
Bogoliubov transformation

The Bogoliubov transformation,

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

diagonalize the Hamiltonian,

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



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,

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

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

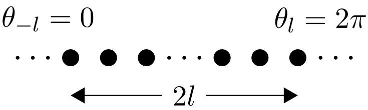


Figure: LSM unitary operator act on only on the part of the chian from $-l$ to l.

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 $|\Psi_1\rangle \neq |\Psi_0\rangle$

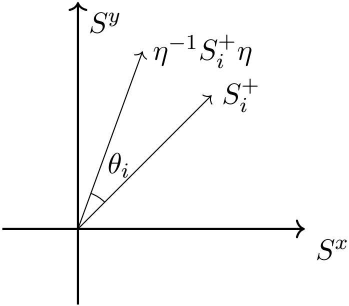
$\langle \Psi_1 | H - E_0 | \Psi_1 \rangle \to 0$

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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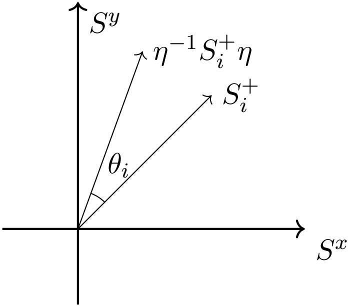

Remember

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

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

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

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

$$= 2\pi^2 J e_0 \frac{1}{l}$$ **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 $\mathcal{P} S_i^z \mathcal{P}^{-1} = -S_{-i}^z$,

$$\mathcal{P} \eta \mathcal{P}^{-1} = e^{i 2\pi \sum_{i=-l}^{l} S_i^z} \eta \; = \begin{cases} \eta & s \text{ integer} \\ -\eta & s \text{ half integer} \end{cases}$$

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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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)

—•   •—•   •—•   •—

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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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$$\langle \vec{S}_i \cdot \vec{S}_j \rangle = 0 \ \text{ for } |R_i - R_j| > 1$$

- This suggest the existence of a gap.

Valence bond states

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And always construct states that are symmetric in same site spin-1/2s.

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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.

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

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

(a)

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

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

(b)

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

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

(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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$$\left|\Psi^{\mathsf{VBS}}_{\alpha_1\alpha_{2L}}\right\rangle$$

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

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

$$\left|\Psi^{\mathsf{VBS}}\right\rangle$$

Correlation length of the VBS state

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

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

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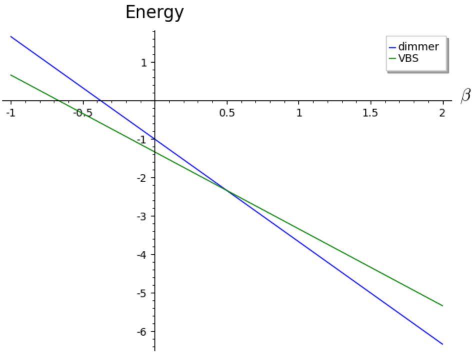
A phase transition occur at $\beta = 1$. The graphs suggests that the phase transition occur between the VBS and the dimerized state.



Outline

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Such a weird situation at the boundaries can only be changed by a transformations that mixes the boundaries.
Such along range correlation between the ends of the chain can only happen if the bulk closes a gap.