Exact ground state of quantum spin systems

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Lecture 1

- Some General introduction to spin systems
- Exact factorized ground state for a pair of spins
- Generalization of factorized state to arbitrary spins, lattices and interactions
- Proof of the factorized state to be the ground state


Lecture 2

- The factorized ground state for frustrated spin models
- The spin wave theory
- Application of spin wave theory close to factorized state

**Motivation**

**Why spin models are important?**

- They are basic models in quantum magnetism, Ex: Ising model and Heisenberg model, ...
- Many novel phenomena and exotic phases, Ex: connection to High $T_c$ superconductivity, magnetic monopoles
- Important for quantum information science and computation models
- Spin models are incorporated in many other disciplines, Biophysics, ...
- Fundamental theory for magnetic models, Ex: Marshal theorem
Some examples

Exotic effects in spin models

- **Haldane’s Conjecture**: (for spin $S$ Anti-Ferromagnetic Heisenberg (AFH) chain)

<table>
<thead>
<tr>
<th>$S$</th>
<th>Spectrum</th>
<th>Correlation functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Integer</td>
<td>Gapful</td>
<td>Exponential decay</td>
</tr>
<tr>
<td>Half integer</td>
<td>Gapless</td>
<td>Algebraic decay</td>
</tr>
</tbody>
</table>

- **Bond Alternation** (Affleck, et.al PRB36 (1987))
  Spin-1/2 dimerized ($\gamma \neq 0$) AFH is **gapful**.

  \[ J(1+\gamma) \quad J(1+\gamma) \quad J(1-\gamma) \]
Some examples

Exotic effects in spin models

- **Ladders** (Coupled chains, Ex: spin-1/2 AFH \( n \)-leg ladder)

<table>
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<tr>
<th>( n )</th>
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</tr>
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<tbody>
<tr>
<td>Even</td>
<td>Gapful</td>
<td>Exponential decay</td>
</tr>
<tr>
<td>Odd</td>
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</tr>
</tbody>
</table>

- **Bond Alternation** *(Martin-Delgado, et.al PRL77, (1996))*

The staggered bond-alternation \( s=1/2 \) AFH ladder has two gapful phases which are separated by a **gapless line** and depends on the bond-alternation parameter.

![Diagram](image)
Some examples

Single Molecule Magnets (SMM)

- A giant molecule composed of some tens of atoms

\[ \text{Mn}_{12} : 4 \times \text{Mn}^{4+} \text{ each with } S = \frac{3}{2} \text{ and } 8 \times \text{Mn}^{3+} \text{ with } S = 2 \]

\[ \text{Fe}_8 : 8 \times \text{Fe}^{3+} \text{ each with } S = \frac{5}{2} \]
Why ground state is important?

Quantum phase transitions (QPT)

It is a phase transition at $T = 0$ due quantum fluctuations by change of a parameter in Hamiltonian, like pressure, magnetic field, impurity concentration, ...

\[
\lim_{T \to 0} \langle A \rangle_T = \lim_{T \to 0} \frac{\sum_i \langle \psi_i | A | \psi_i \rangle e^{-E_i}}{Z} = \frac{\langle \psi_0 | A | \psi_0 \rangle e^{-E_0}}{e^{-E_0} + \sum_{i \neq 0} \langle \psi_i | A | \psi_i \rangle e^{-(E_i - E_0)}} = \langle \psi_0 | A | \psi_0 \rangle
\]

$|\psi_0\rangle \equiv$ ground state, $E_0 < E_1 < E_2...$
Why ground state is important?

Fermi temperature is typically, \( T_f = 10^4 \)

Most of properties can be captured via the ground state.

Low temperature behaviours are affected by the nature of ground state.
Two spins model

Fully anisotropic Heisenberg model in a magnetic field

\[ H' = J^x \sigma^x \rho^x + J^y \sigma^y \rho^y + J^z \sigma^z \rho^z + h' (\sigma^z + \rho^z), \]  
(1)

\( J^\mu, \mu = x, y, z \) are the exchange couplings in different directions
\( h' \) is proportional to the magnetic field
\( \sigma \) and \( \rho \) are spin operators

Factorized eigenstate

We are looking for a factorized state which is satisfied by

\[ |\psi\rangle = |\sigma\rangle |\rho\rangle \implies H'|\psi\rangle = \epsilon |\psi\rangle \]  
(2)

\( |\rho\rangle \) and \( |\sigma\rangle \) are the single particle states
The single particle kets

\[ \sigma = \frac{1}{2}, \quad \rho = 1 \]

\[
|\sigma\rangle = a_+|+\rangle + \frac{1}{2} + a_-|-\frac{1}{2}\rangle, \quad |\rho\rangle = b_+|+1\rangle + b_0|0\rangle + b_-|-1\rangle.
\]

(3)

Parametrization of the coefficients

The coefficients \(a_{\pm}\) and \(b_{\pm,0}\) are defined such that the single particle states \(|\sigma\rangle\) and \(|\rho\rangle\) are the eigenstates of \(\vec{\sigma} \cdot \hat{n}'\) and \(\vec{\rho} \cdot \hat{n}''\) with eigenvalues \(+\frac{1}{2}\) and \(+1\); respectively. The unit vectors \(\hat{n}'\) and \(\hat{n}''\) are defined by spherical angles \((\theta, \varphi)\) and \((\beta, \alpha)\), respectively.

\[
a_+ = \cos \frac{\theta}{2} \exp \left(-i \frac{\varphi}{2}\right), \quad a_- = \sin \frac{\theta}{2} \exp \left(i \frac{\varphi}{2}\right),
\]

(4)

\[
b_+ = \frac{1}{2} (1 + \cos \beta) \exp (-i \alpha), \quad b_0 = \frac{1}{\sqrt{2}} \sin \beta, \quad b_- = \frac{1}{2} (1 - \cos \beta) \exp (i \alpha).
\]
Solving a set of linear coupled equations

\[ H' = J^x \sigma^x \rho^x + J^y \sigma^y \rho^y + J^z \sigma^z \rho^z + h'(\sigma^z + \rho^z), \]

\[ |\psi\rangle = |\sigma\rangle |\rho\rangle \implies H'|\psi\rangle = \epsilon |\psi\rangle \]

\[ h' = h'_f = \frac{\sqrt{4J^x J^y + 5J^z J^z + J^z C_1}}{2\sqrt{2}}, \]

\[ C_1 \equiv \sqrt{8(2J^x + J^y)(J^x + 2J^y) + 9J^z J^z}, \]

\[ \epsilon = \frac{J^x J^y}{2J^z} - \frac{h'^2}{J^z}. \]

(5)
Parameters of the factorized eigenstate

\[ \theta = 2 \tan^{-1} \sqrt{\frac{|A_1|}{|A_2|}}, \quad \phi = \arg A_1 + \frac{1}{2} \arg A_3, \]

\[ \beta = \cos^{-1} \frac{|A_3| - 1}{|A_3| + 1}, \quad \alpha = -\frac{1}{2} \arg A_3, \quad (6) \]

where

\[ A_1 = \frac{(a_-)(b_0)}{(a_+)(b_-)} = \frac{\sqrt{2} (J^z + h'_f + 2\epsilon)}{J^x + J^y}, \]

\[ A_2 = \frac{(a_+)(b_0)}{(a_-)(b_-)} = \frac{\sqrt{2} (-J^z + 3h'_f + 2\epsilon)}{J^x - J^y}, \]

\[ A_3 = \frac{b_+}{b_-} = \frac{A_1 (J^y - J^x)}{\sqrt{2} (J^z + 3h'_f - 2\epsilon)}. \]
Different choices

The above expressions justify that $A_1$ and $A_3$ are real values which imply that their arguments be either 0 or $\pi$. Thus, there are four possible choices for $\alpha$ and $\phi$,

(I) $\alpha = 0, \ \varphi = 0$

(II) $\alpha = 0, \ \varphi = \pi$

(III) $\alpha = \frac{\pi}{2}, \ \varphi = -\frac{\pi}{2}$

(IV) $\alpha = \frac{\pi}{2}, \ \varphi = \frac{\pi}{2}$

• Spins are located in the xz-plane for choices I and II
• Spins are located in the yz-plane for III and IV
• yz-plane spins are mapped to xz-plane by interchange of $J^x \leftrightarrow J^y$.
• $(\theta, \varphi = 0) \equiv (-\theta, \varphi = \pi)$

Therefore, we only consider (I): $\alpha = 0, \varphi = 0$, as a general case.
Extension to \((1/2, 1)\) ferrimagnetic chain

The factorized state is: 
\[
|\psi\rangle = \bigotimes_{i=1}^{N_c} |\sigma_i(\theta)\rangle |\rho_i(\beta)\rangle.
\]

Is the factorized state a ground state?

The Hamiltonian is the sum of two-body terms, each term is in its minimum energy, thus the sum is in its minimum energy.

\[
H_i' = J^x \sigma_i^x \rho_i^x + J^y \sigma_i^y \rho_i^y + J^z \sigma_i^z \rho_i^z + h'(\sigma_i^z + \rho_i^z),
\]

\[
H = \sum_{i}^{N_c} H_i'
\]
Generalization to arbitrary spin model

General \((\sigma, \rho)\) Hamiltonian on arbitrary lattice and interactions

\[
H = \sum_{i, r} \left[ \zeta_i \hat{\zeta}_{i+r} (J^x_r \sigma^x_i \rho^x_{i+r} + J^y_r \sigma^y_i \rho^y_{i+r} + J^z_r \sigma^z_i \rho^z_{i+r}) \right] + h \sum_i (\sigma^z_i + \rho^z_i), \quad (7)
\]

The Hamiltonian is again a sum of bond terms: \(H = \sum_{i, r} H'_{i, r}\)

General procedure

- Rotation on different spins to get a ferromagnetic state

The rotation operator is \(D = D^\sigma(0, \theta, 0)D^\rho(0, \beta, 0)\) where

\[
D^\rho(0, \beta, 0) = D(\alpha = 0, \beta, \gamma = 0) = D_z(\alpha)D_y(\beta)D_z(\gamma),
\]

\[
D_y(\beta) = \exp\left(\frac{-i \hat{J}^y_\beta}{\hbar}\right), \quad [\hat{J}^x_\rho, \hat{J}^y_\rho] = i\hbar \hat{J}^z_\rho, \quad \text{(Angular momentums)}
\]
General procedure

Asking for ferromagnetic eigenstate

\[ D^\dagger H' D = \tilde{H}' = (J^z \cos \beta \cos \theta + J^x \sin \beta \sin \theta)\sigma^{z'}\rho^{z''} + (J^x \cos \beta \cos \theta + J^z \sin \beta \sin \theta)\sigma^{x'}\rho^{x''} + J^y \sigma^y \rho^y + (-J^z \sin \beta \cos \theta + J^x \cos \beta \sin \theta)\sigma^{z'}\rho^{x''} \\
+ (J^x \sin \beta \cos \theta - J^z \cos \beta \sin \theta)\sigma^{x'}\rho^{z''} + h'(\cos \beta \rho^{z''} - \sin \beta \rho^{x''} + \cos \theta \sigma^{z'} - \sin \theta \sigma^{x'}) \]  

(8)

By defining the ladder operators:

\[ \sigma^\pm = \frac{\sigma^{x'} \pm i\sigma^{y'}}{2}, \quad \rho^\pm = \frac{\rho^{x'} \pm i\rho^{y'}}{2} \]  

(9)
General procedure

Solution

\[ \cos \theta = - \frac{h'_f J^y + J^x (J^z^2 - J^y^2) \rho \sigma + h'_f J^z (J^y \rho + J^x \sigma)}{h'_f J^x + J^y (J^z^2 - J^x^2) \rho \sigma + h'_f J^z (J^x \rho + J^y \sigma)} , \]

\[ \cos \beta = - \frac{h'_f J^y + J^x (J^z^2 - J^y^2) \rho \sigma + h'_f J^z (J^y \sigma + J^x \rho)}{h'_f J^x + J^y (J^z^2 - J^x^2) \rho \sigma + h'_f J^z (J^x \sigma + J^y \rho)} , \]

\[ h'_f = \sqrt{\frac{1}{2} (2 J^x J^y \rho \sigma + (\rho^2 + \sigma^2) J^z^2 + J^z C_2)} , \]

\[ C_2 \equiv \sqrt{4 \rho \sigma (\rho J^x + \sigma J^y)(\sigma J^x + \rho J^y) + (\rho^2 - \sigma^2)^2 J^z^2} , \]

\[ \epsilon = \frac{J^x J^y}{J^z} \sigma \rho - \frac{h'_f^2}{J^z} . \]
The same angle is necessary for each pair

\[ J_\mu^\mu = \lambda(r)J_\mu^\mu, \quad \mu = x, y, z, \quad \lambda(r) > 0. \]  \hspace{1cm} (11)

The above condition guarantees a unique pair of \((\theta, \beta)\) as a solution of Eq.(10).
Proof

Simple proof for each spin magnitude

Check out if the energy of the factorized state is the ground state energy of each pairs of spins. **Note: Managable for small spins.**

General proof

- Implementing the spin wave theory where nonzero gap validates the minimum energy of the factorized state, see lecture 2 and

- A general proof is also given in

An extended version is available in persian by Masoud Mardani (pdf).
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