Exact ground state of quantum spin systems

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Topics

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

Refs: J. Kurmann, H. Thomas, and G. Muller, Physica **112 A**, 235 (1982),

M. Rezai, A. Langari and J. Abouie, Phys. Rev. B. **81**, 060401 (R) (2010).

Lecture 2

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

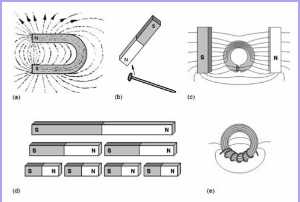
Refs: J. Abouie, A. Langari and M. Siahatgar, J. Phys. :Condens. Matter **22**, 216008 (2010).

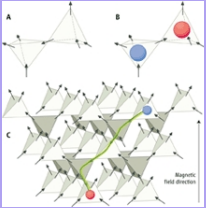
S. M. Giampaolo, G. Adesso, and F. Illuminati, Phys. Rev. Lett. **104**, 207202 (2010).

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





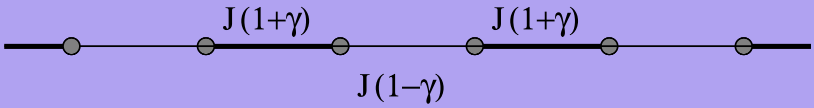
Some examples

Exotic effects in spin models

- Haldane's Conjecture: (for spin S Anti-Ferromagnetic Heisenberg (AFH) chain)

S	Spectrum	Correlation functions
Integer	Gapful	Exponential decay
Half integer	Gapless	Algebraic decay

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



Some examples

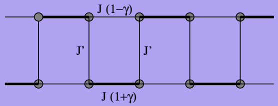
Exotic effects in spin models

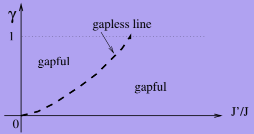
- Ladders (Coupled chains, Ex: spin-1/2 AFH n-leg ladder)

n	Spectrum	Correlation functions
Even	Gapful	Exponential decay
Odd	Gapless	Algebraic decay

- *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.

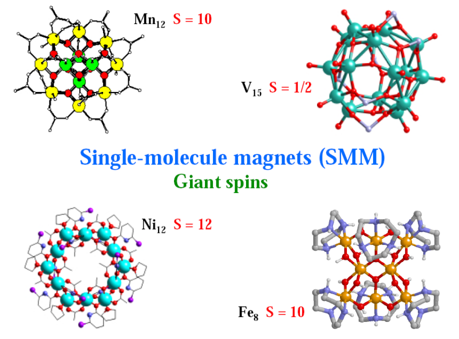




Some examples

Single Molecule Magnets (SMM)

- A giant moelcule composed of some tens of atoms



Mn_{12} : $4 \times Mn^{4+}$ each with $S = \frac{3}{2}$ and $8 \times Mn^{3+}$ with $S = 2$
Fe_8 : $8 \times Fe^{3+}$ 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, ...

$$\lim_{T\to 0}\langle A\rangle_T = \lim_{T\to 0}\frac{\sum_i \langle\psi_i|A|\psi_i\rangle e^{\frac{-E_i}{k_B T}}}{Z} =$$

$$\lim_{T\to 0}\frac{\langle\psi_0|A|\psi_0\rangle e^{\frac{-E_0}{k_B T}} + \sum_{i\neq 0}\langle\psi_i|A|\psi_i\rangle e^{\frac{-(E_i-E_0)}{k_B T}}}{e^{\frac{-E_0}{k_B T}} + \sum_{i\neq 0} e^{\frac{-(E_i-E_0)}{k_B T}}} = \langle\psi_0|A|\psi_0\rangle$$

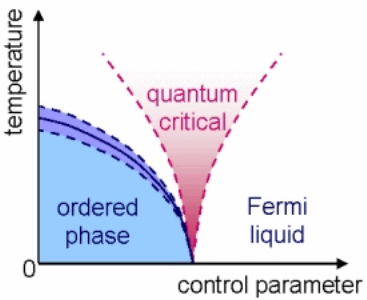
$|\psi_0\rangle \equiv$ ground state, $E_0 < E_1 < E_2 ...$

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

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

$J^\mu, \mu = x, y, z$ are the exchange couplings in different directions
h' is proportional to the magnetic field
σ and ρ are spin operators

Factorized eigenstate

We are looking for a factorized state which is satisfied by

$$|\psi\rangle = |\sigma\rangle|\rho\rangle \Longrightarrow H'|\psi\rangle = \epsilon|\psi\rangle \quad (2)$$

$|\rho\rangle$ and $|\sigma\rangle$ are the single particle states

The single particle kets

$\sigma = 1/2$, $\rho = 1$

$$|\sigma\rangle = a_+|+\frac{1}{2}\rangle + a_-|-\frac{1}{2}\rangle, \quad |\rho\rangle = b_+|+1\rangle + b_0|0\rangle + b_-|-1\rangle. \tag{3}$$

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 (θ,φ) and (β,α), respectively.

$$a_+ = \cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right) \quad , \quad a_- = \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right), \tag{4}$$

$$b_+ = \frac{1}{2}(1+\cos\beta)\exp(-i\alpha), b_0 = \frac{1}{\sqrt{2}}\sin\beta, b_- = \frac{1}{2}(1-\cos\beta)\exp(i\alpha).$$

Solution

Solving a set of linear coupled equations

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

$$|\psi\rangle = |\sigma\rangle|\rho\rangle \Longrightarrow H'|\psi\rangle = \epsilon|\psi\rangle$$

$$\begin{aligned} h' = h'_f &= \frac{\sqrt{4J^xJ^y + 5{J^z}^2 + J^zC_1}}{2\sqrt{2}}, \\ C_1 &\equiv \sqrt{8(2J^x + J^y)(J^x + 2J^y) + 9{J^z}^2}, \\ \epsilon &= \frac{J^xJ^y}{2J^z} - \frac{h_f'^2}{J^z}. \end{aligned} \quad (5)$$

Parameters of the factorized eigenstate

$$\theta = 2\tan^{-1}\sqrt{\left|\frac{A_1}{A_2}\right|} \quad , \quad \varphi = \arg A_1 + \frac{1}{2}\arg A_3,$$
$$\beta = \cos^{-1}\frac{|A_3|-1}{|A_3|+1} \quad , \quad \alpha = -\frac{1}{2}\arg A_3, \tag{6}$$

where

$$\begin{aligned}
A_1 &= \frac{(a_-)(b_0)}{(a_+)(b_-)} = \frac{\sqrt{2}\,(J^z + h'_f + 2\epsilon)}{J^x + J^y}, \\
A_2 &= \frac{(a_+)(b_0)}{(a_-)(b_-)} = \frac{\sqrt{2}\,(-J^z + 3h'_f + 2\epsilon)}{J^x - J^y}, \\
A_3 &= \frac{b_+}{b_-} = \frac{A_1(J^y - J^x)}{\sqrt{2}\left(J^z + 3h'_f - 2\epsilon\right)}.
\end{aligned}$$

Different choices

The above expressions justify that A_1 and A_3 are real values which imply that their arguments be either 0 or π. Thus, there are four possible choices for α and ϕ,

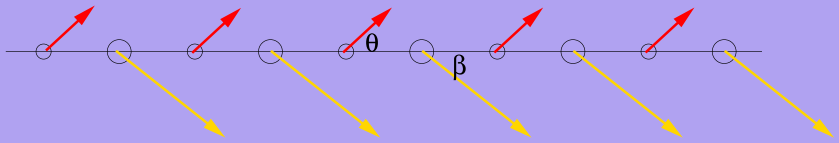
$$(I) \quad \alpha = 0, \quad \varphi = 0, \qquad (III) \; \alpha = \frac{\pi}{2}, \quad \varphi = -\frac{\pi}{2},$$
$$(II) \quad \alpha = 0, \quad \varphi = \pi, \qquad (IV) \; \alpha = \frac{\pi}{2}, \quad \varphi = \frac{\pi}{2}.$$

- 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

Ferrimagnetic chain



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

Is the factorized state a ground state?

The Hamiltonian is the sume 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 (σ,ρ) Hamiltonian on arbitrary lattice and interactions

$$H=\sum_{i,r}\left[\zeta_i\hat{\zeta}_{i+r}(J_r^x\sigma_i^x\rho_{i+r}^x+J_r^y\sigma_i^y\rho_{i+r}^y)+J_r^z\sigma_i^z\rho_{i+r}^z\right]+h\sum_i(\sigma_i^z+\rho_i^z),\quad (7)$$

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

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

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

$$D_y(\beta)=exp(\frac{-i\hat{J}_y^\rho\beta}{\hbar}),\qquad [\hat{J}_x^\rho,\hat{J}_y^\rho]=i\hbar\hat{J}_z^\rho,\ \text{(Angular momentums)}$$

General procedure

Asking for ferromagnetic eigenstate

$$
\begin{aligned}
D^{\dagger} H' D = \tilde{H}' = & (J^{z}\cos\beta\cos\theta + J^{x}\sin\beta\sin\theta)\sigma^{z'}\rho^{z''} \\
& + (J^{x}\cos\beta\cos\theta + J^{z}\sin\beta\sin\theta)\sigma^{x'}\rho^{x''} + J^{y}\sigma^{y'}\rho^{y''} \\
& + (-J^{z}\sin\beta\cos\theta + J^{x}\cos\beta\sin\theta)\sigma^{z'}\rho^{x''} \\
& + (J^{x}\sin\beta\cos\theta - J^{z}\cos\beta\sin\theta)\sigma^{x'}\rho^{z''} \\
& + h'(\cos\beta\rho^{z''} - \sin\beta\rho^{x''} + \cos\theta\sigma^{z'} - \sin\theta\sigma^{x'}),
\end{aligned} \tag{8}
$$

By defining the ladder operators:

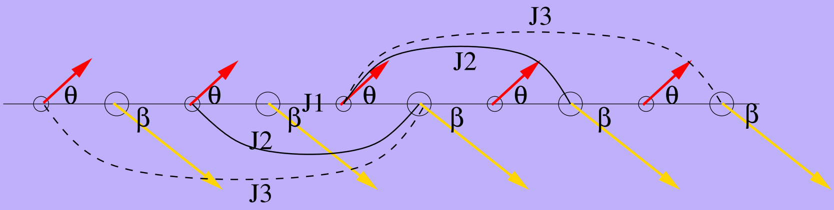
$$
\sigma^{\pm} = \frac{\sigma^{x'} \pm i\sigma^{y'}}{2}, \qquad \rho^{\pm} = \frac{\rho^{x'} \pm i\rho^{y'}}{2} \tag{9}
$$

General procedure

Solution

$$
\begin{aligned}
\cos\theta &= -\frac{h_f'^2 J^y + J^x(J^{z^2} - J^{y^2})\rho\sigma + h_f' J^z(J^y\rho + J^x\sigma)}{h_f'^2 J^x + J^y(J^{z^2} - J^{x^2})\rho\sigma + h_f' J^z(J^x\rho + J^y\sigma)},\\
\cos\beta &= -\frac{h_f'^2 J^y + J^x(J^{z^2} - J^{y^2})\rho\sigma + h_f' J^z(J^y\sigma + J^x\rho)}{h_f'^2 J^x + J^y(J^{z^2} - J^{x^2})\rho\sigma + h_f' J^z(J^x\sigma + J^y\rho)},\\
h_f' &= \sqrt{\frac{1}{2}\left(2J^xJ^y\rho\sigma + (\rho^2+\sigma^2)J^{z^2} + J^zC_2\right)},\\
C_2 &\equiv \sqrt{4\rho\sigma(\rho J^x + \sigma J^y)(\sigma J^x + \rho J^y) + (\rho^2-\sigma^2)^2 J^{z^2}},\\
\epsilon &= \frac{J^xJ^y}{J^z}\sigma\rho - \frac{h_f'^2}{J^z}.
\end{aligned}
\tag{10}
$$

Constraint on long range interaction



The same angle is necessary for each pair

$$J_r^\mu = \lambda(r) J^\mu, \quad \mu = x, y, z, \quad \lambda(r) > 0. \tag{11}$$

The above condition guarantees a unique pair of (θ, β) 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

  M. Rezai, A. Langari and J. Abouie, Phys. Rev. B. **81**, 060401 (R) (2010).

- A general proof is also given in

  R. Rossingnoli and N. Canosa and J. M. Matera, Phys. Rev. A. **80**, 062325 (2009).

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

Acknowledgment

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