Exact ground state of quantum spin systems

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Outline

Lecture 2

- Frustration and obstacle in the minimization of energy
- The factorized ground state for frustrated spin models
- The spin wave theory
- Application of spin wave theory close to factorized state

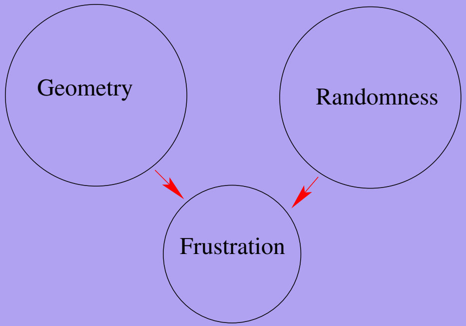
References:
G. Müller and R. E. Shrock, Phys. Rev. B. 32, 5845 (1985).
J. Abouie, A. Langari and M. Siahatgar, J. Phys. :Condens. Matter **22**, 216008 (2010).
S. M. Giampaolo, G. Adesso, and F. Illuminati, Phys. Rev. Lett. **104**, 207202 (2010).

Notice

Whitin lecture-2 we consider a homogenous spin model, namely $\sigma = \rho = 1/2$.

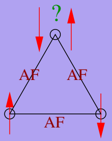
Frustration

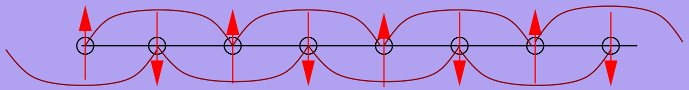
Two sources of frustration



Frustration

Antiferromagnetic (AF) interaction





Is there any way to minimize all bonds simultaneously?

Problem in the algorithm of exact factorized state, lecture-1

The addition of frustration prohibits to minimize all bonds simultaneously.
The factorized state is not necessarily the ground state, could it be?

Yes, under certain constraint and conditions.

Frustration and exact ground state

Anisotropic spin-1/2 Heisenberg chain with NN and NNN interaction

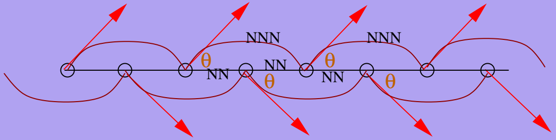
$$H = \sum_{r=NN,NNN} \sum_i \left[(J_r^x s_i^x s_{i+r}^x + J_r^y s_i^y s_{i+r}^y) + J_r^z s_i^z s_{i+r}^z + h s_i^z \right] \qquad (1)$$

Let define f to be the ratio of NNN to NN interactions, $f = \frac{J_{NNN}^{\alpha}}{J_{NN}^{\alpha}}$.

- The factorized state is the ground state for $f = 0$.
- Is the factorized state the ground state for $f \neq 0$?

Constraints

Anisotropic spin-1/2 Heisenberg chain with NN and NNN interaction



The angle θ which comes from NN or NNN bond should be the same.

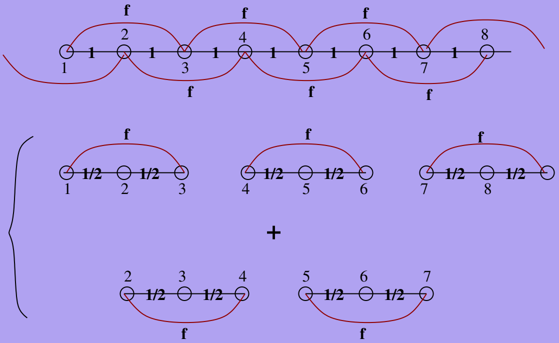
The homogenous spin chain, $\sigma = \rho = s$

$$\cos(\theta_{NN}^{AF}) = \sqrt{\frac{J^y + J^z}{J^x + J^z}} = \cos(\theta_{NNN}^{F}) = \sqrt{\frac{f(J^y - J^z)}{f(J^x - J^z)}} \Longrightarrow J^z = 0.$$

The solution $J^x = J^y$ which gives the trivial state $\theta = 0$ is not considered.

Conditions

Is the factorized state the ground state?

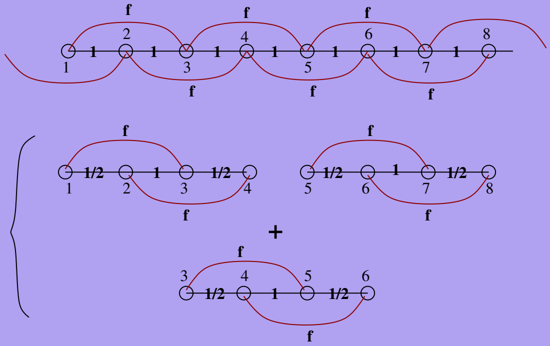


Imposing the factorized state be the ground state of the 3-sites block

$$f < f_c = \frac{1}{2}\left(\frac{J^x + J^y - \sqrt{J^x J^y}}{J^x + J^y}\right) \tag{2}$$

Improvement of the condition

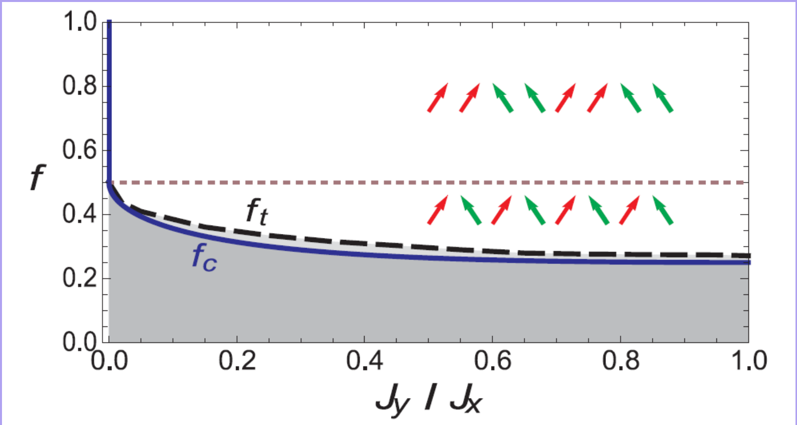
Decomposition to 4-sites block



Only numerical solution exists.

Conditions for the spin 1/2 chain with NN and NNN interactions

Decomposition up to around 10-sites



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

Spin wave theory (SWT)

Anisotropic spin-1/2 chain in a transverse magnetic field

$$H = J\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + hS_i^x), \tag{3}$$

$$\cos(\theta) = -\sqrt{\frac{1+\Delta}{2}}, \qquad h_f = \sqrt{2(1+\Delta)} \tag{4}$$

Spin wave approach

- Selecting a background as the vacuum of the bosonized theory
- Expressing the Hamiltonian in terms of bosonic quasi-particles
- Analysing the model in terms of bosonic quasi-particles

SWT close to the factorizing point

Exact factorized ground state as the vacuum of SWT

$$\tilde{H} = \tilde{D}^\dagger H \tilde{D}, \qquad \tilde{D} = \bigotimes_{i\in A, j\in B} \mathcal{D}_i(-\theta)\mathcal{D}_j(\theta), \qquad \mathcal{D}_i(\theta) = exp(-i\theta S_i^y/\hbar).$$

Label of spins $A = 1, 3, 5, \ldots, B = 2, 4, 6, \ldots$
After rotation the factorized state is the polarized state.

Holstein-Primakoff bosonic operators, $a, a^\dagger, b, b^\dagger$

$$\begin{aligned} \tilde{S}^+_{Ai} &= (2S - a_i^\dagger a_i)^{1/2} a_i, \qquad & \tilde{S}^x_{Ai} = S - a_i^\dagger a_i, \\ \tilde{S}^+_{Bj} &= (2S - b_j^\dagger b_j)^{1/2} b_j, \qquad & \tilde{S}^x_{Bj} = S - b_j^\dagger b_j, \end{aligned}$$

Linear SWT approximation

$$\tilde{S}^+_{Ai} \simeq \sqrt{2S} a_i, \qquad \tilde{S}^+_{Bi} \simeq \sqrt{2S} b_i.$$

SWT close to the factorizing point

Fourier transformation

$$a_l = \frac{1}{\sqrt{N}} \sum_k e^{-ikl} a_k, \qquad b_l = \frac{1}{\sqrt{N}} \sum_k e^{-i(kl+\frac{k}{2})} b_k,$$

Rotation to diagonalizing bosonic quasi-particles

$$\psi_k = \cos\eta_k a_k - \sin\eta_k b_k, \qquad \chi_k = \sin\eta_k a_k + \cos\eta_k b_k,$$

$$\tilde{\mathcal{H}} = E_0 + \sum_k (\omega_k^+ \chi_k^\dagger \chi_k + \omega_k^- \psi_k^\dagger \psi_k),$$

$$\omega_k^\pm = \frac{h}{h_f}(1+\Delta) - \Delta \pm \Delta \cos\frac{k}{2},$$

$$E_0 = \frac{N}{2}(\Delta - h h_f) + \omega_0^+ (t^+)^2 + \sqrt{2N(1-\Delta^2)}(\frac{h}{h_f} - 1) t^+,$$

$$t^+ = (\sqrt{\frac{N}{2}(1-\Delta^2)} \times (1 - \frac{h}{h_f}))/\omega_0^+. \tag{5}$$

Thermodynamic properties

Specific heat implementing SWT

$$\tilde{n}_k^{\pm} = \sum_{n^-,n^+} n_k^{\pm} P_k(n^+, n^-), \quad n_k^+ = \chi_k^\dagger \chi_k, \quad n_k^- = \psi_k^\dagger \psi_k,$$

$$\sum_{n^+,n^-} P_k(n^+, n^-) = 1,$$

$P_k(n^+, n^-) \equiv$ probability of prallel n^+ and antiparallel n^- modes.

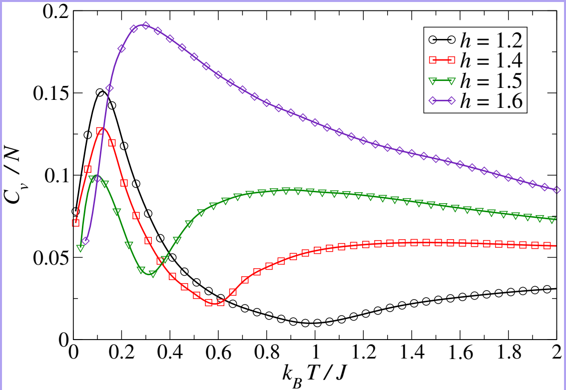
$$F = E_0 + \sum_k (\omega_k^+ \tilde{n}_k^+ + \omega_k^- \tilde{n}_k^-) + T \sum_k \sum_{n^+,n^-} P_k(n^-, n^+) \ln P_k(n^-, n^+).$$

The number of bosons are controlled by the following constraint which is the magnetization in x-direction,

$$M_x = s - \frac{1}{2N} \sum_k (\tilde{n}_k^+ + \tilde{n}_k^-) - \frac{(t^+)^2}{2N}.$$

Thermodynamic properties

Specific heat close to the factorizing field



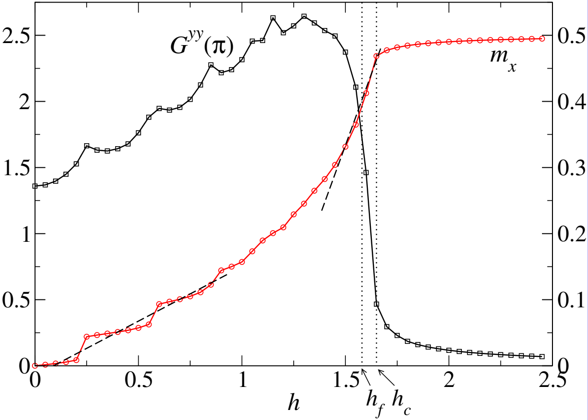
$$h_f \simeq 1.58$$

Two energy scale $(\omega_k^{\pm}) \Longrightarrow$ Two dynamics.

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

Phase diagram

Staggered magnetization (y) and magnetization (x)



Open problems

Exact factorized ground state

- Dimerized, trimerized,... spin chains
- Two dimensioanl models
- Approximation close to the exact factorized state of the above models
- Frustrated spin chain with arbitrary spin
- Two dimensional frustrated models

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http://spin.cscm.ir/

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