A discussion on possible spin liquid state in the spin $\frac{1}{2}$ $J_1 - J_2$ Heisenberg AFM on square lattice

arxiv : 1112.2241, 1112.3331

March 20, 2012

Outline

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1. Spin 1/2 $J_1 - J_2$ Heisenberg AFM on a square lattice
2. Some recent results on the ground state phase diagram
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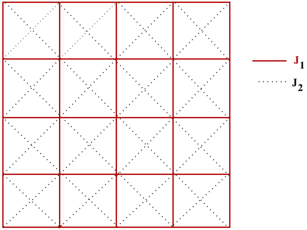
$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S_i}.\mathbf{S_j} + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S_i}.\mathbf{S_j}$$

- A simple model used to study the interplay of frustration effects and quantum fluctuations as well as quantum phase transitions driven by frustration.
- It is of interest as it realizes several interesting phenomenon which are relevant to a large class of 2D frustated quantum magnets.



- An unit square cell with J_1, J_2 antiferromagnetic (AFM) coupling

- Ground state phases:

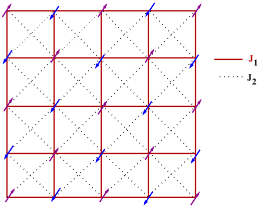


Figure: Néel Order

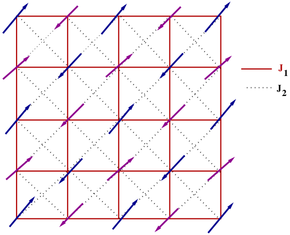
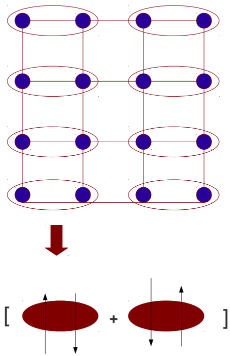


Figure: Striped AFM

- Small values of $J_2 \Rightarrow$ Néel order
- Large values of $J_2 \Rightarrow$ Striped AFM
- Competing $\mathbf{J_1}$ and $\mathbf{J_2}$ couplings $\Rightarrow$ Frustrations $\Rightarrow$ Magnetically disordered phases !

- The most probable candidate for the intermediate state:



- Spins are paired into $S = 0$ valence bonds which breaks the lattice symmetry as they crystallize into a preffered arrangement

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- Recent predictions :
  A spin liquid state in the intermediate region :
- X.G Wen and his co-workers (arxiv: 1112.3331) Uses Tensor Product States ansatz for the ground state of the wave function.
- L. Balents and his co-workers (arxiv: 1112.2241) Uses DMRG ; $0.41 \leq J_2/J_1 \leq 0.62$

- What are Spin liquids ?
  - The spin liquid is an ordered spin state destabilized by quantum fluctuations and geometric frustrations leading to liquid-like properties.
  - There are no long range order even down to the lowest temperatures and the spectrum is gaped.

- Ground state energy, magnetization, dimer order, plaquette order parameter of finite lattice with PBC ($L = 4, 6, 8, 12, 16$)

- Tensor product states (TPS).
- Imaginary time evolution method to evolve from a random TPS to the ground state of $\mathcal{H}$.
- For numerical evaluation, bond dimension used is upto D=9.

- Ground state (GS) energy:
  - Decrease in the GS energy as the bond dimension is increased.

$$E(J_2, L, D) = E(J_2, L) + c_{J_2}/D^3$$

  - A finite size scaling (FSS) formula is then employed to extrapolate the ground state energy in the thermodynamic limit,

$$E(J_2, L) = E(J_2) + d_{J_2}/L^3$$

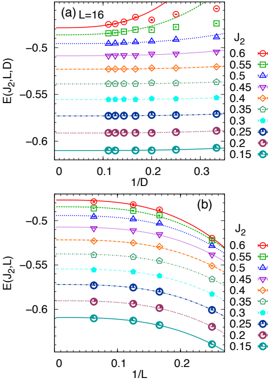

Figure: (a) The finite size ($L = 16$) ground state energies at different bond dimensions $D = 3, 4, 5, 6, 7, 8, 9$, and their extrapolation (from ground energies at bond dimensions $D = 6, 7, 8, 9$) to $D \to \infty$ limit. (b) The finite size scaling of $E(J_2, L)$ obtained from (a) to the thermodynamic limit.

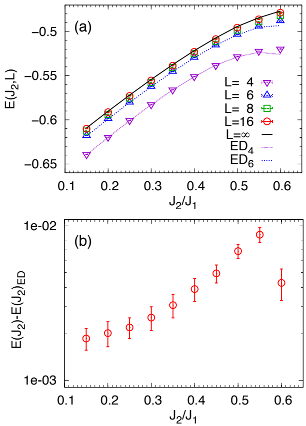

Figure: Finite size energies $E(J_2, L)$ (a) and their thermodynamic limits $E(J_2)$ from the FSS . The purple and blue dashed lines are the ED energies for lattice sizes $L = 4, 6$ respectively. (b) Energy differences between $E(J_2)$ from this study and those extrapolated from an ED study upto 40 spins

- Exact Diagonalization calculation: J. Richter and J. Schulenberg, Euro. Phys. J B, 73,117 (2010)

- Magnetization:
  - Staggered magnetization:

$$M^2 = \frac{1}{4L^2} \sum_{x_i, y_i = 1}^{2} \sum_{x_j, y_j = 1}^{L} (-1)^{\phi} \mathbf{S}_{(x_i, y_i)} \cdot \mathbf{S}_{(x_j, y_j)}$$

    where $\phi = x_i - x_j + y_i - y_j$.
  - A FSS scaling formula is then employed to extrapolate M^2 in the thermodynamic limit,

$$M^2(J_2, L) = M^2(J_2) + e^1_{J_2}/L + e^2_{J_2}/L^2$$

- Continuous phase transition between the AF phase and the paramagnetic phase.

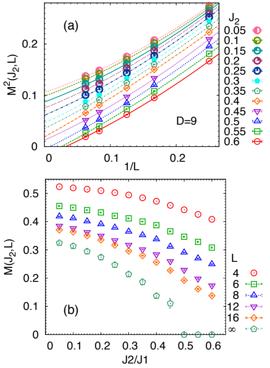

Figure: (a) The FSS of the magnetization square to their thermodynamic limits. (b) The finite size magnetization $M(J_2, L)$ and their thermodynamic limits $M(J_2)$ obtained from (a) as a function of J_2/J_1.

- Order parameters:
  - Columnar order:

$$D_X = \frac{1}{L^2} \sum_{x,y=1}^{L} (-1)^x \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x+1,y)},$$

$$D_Y = \frac{1}{L^2} \sum_{x,y=1}^{L} (-1)^y \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x,y+1)}$$

  - Staggered dimer order:

$$D_X^s = \frac{1}{L^2} \sum_{x,y=1}^{L} (-1)^{x+y} \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x+1,y)}$$

$$D_Y^s = \frac{1}{L^2} \sum_{x,y=1}^{L} (-1)^{x+y} \mathbf{S}_{(x,y)} \cdot \mathbf{S}_{(x,y+1)}$$

- Plaquette order:

$$Q_\alpha = \frac{2}{L^2} \sum_{p_\alpha \in \alpha} \left(P_{\square, p_\alpha} + P^{-1}_{\square, p_\alpha} \right)$$

- $P_{\square, p_\alpha}$ is the cyclic exchange operator of the four spins on a given plaquette p_α, and p_α belongs to the α^{th} of the total 4 distinguished plaquettes.
- for a bond dimension $D < 5$ the paramagnetic ground state has mixed columnar and staggered VBS orders of a magnitude 10^{-2}.

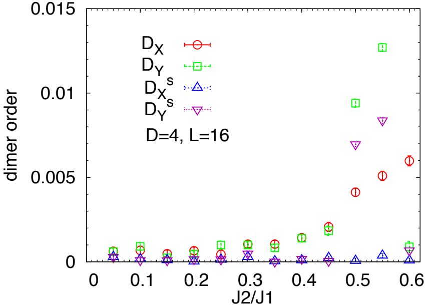

Figure: The columnar dimer order D_X, D_Y and staggered dimer order D^s_X, D^s_Y as a function of J_2/J_1 at bond dimension $D = 4$ for system size $L = 16$.

- after $D \geq 5$, the dimer orders disappear when ground state energy further decreases implying the local minimal effects of these ordered states.
- At the largest bond dimension $D = 9$, the plaquette order parameter Q_α at 4 distinguished plaquettes are the same, which means the plaquette valence bond state is not favored either.
- Hence so far, the most possible state of the paramagnetic phase is a spin liquid state with topological order.

- Rényi Entanglement Entropy S_2

- γ is the universal constant term of S_2
- In the AF phase, γ is very close to zero, while in the paramagnetic phase, γ reaches a conspicuously large value between to 0.6 and 1. However, due to the presence of corners on the boundary of subset A, it is not clear if the observed γ is entirely due to the topological entanglement entropy or not.
- A non-zero γ is a strong indication for a topological quantum spin liquid.

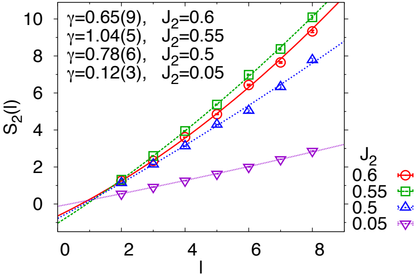

Figure: The Renyi entropy S_2 of a square subset A of length l in a $L \times L$ ($L = 16$) system evaluated from a TPS of bond dimension $D = 9$.

- Some results from Balent and his co-workers (1112.2241):
  - Order parameters

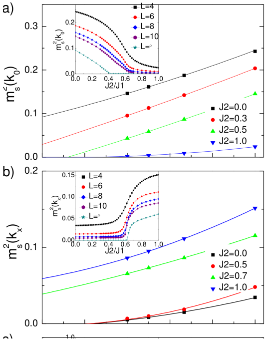

Figure: Finite-size extrapolations of the magnetic order parameters and spin excitation gaps. (a) The Néel AFM order parameter $m_s^2(\mathbf{k})$ at wavevector $\mathbf{k}_0 = (\pi, \pi)$ and (b) stripe AFM order parameter $m_s^2(\mathbf{k})$ at wavevector $\mathbf{k}_x = (\pi, 0)$ or $\mathbf{k}_y = (0, \pi)$, for various values of J_2, fitted using second-order polynomials in $1/L$. Néel AFM order disappears for $J_2 > 0.41$, while stripe AFM order develops for $J_2 > 0.62$, as seen in the corresponding insets.

- Phase diagram

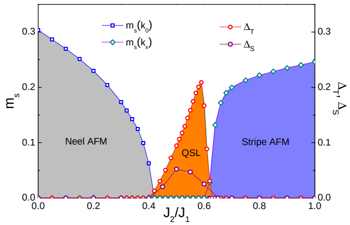

Figure: The ground state phase diagram for the spin-$\frac{1}{2}$ AFM Heisenberg J_1-J_2 model on the square lattice, as determined by accurate DMRG calculations on long cylinders with L_y up to 10.

- Three different phases are found: Néel antiferromagnet (AFM), topological quantum spin liquid (QSL), and stripe AFM phase. $m_s(\mathbf{k}_0 = (\pi, \pi))$ [$m_s(\mathbf{k}_x = (\pi, 0))$] denotes the staggered magnetization in the Néel AFM phase [stripe AFM phase].
- Δ_S and Δ_T denote the spin singlet gap and spin triplet gap, respectively.

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- Through a finite D scaling and finite size scaling (FSS), the ground state energies in the thermodynamic limit are in good agreement with the results from a state of art ED study with a difference at an order of $10^{-3}J_1$ per site.
- Through FSS, the staggered magnetization diminishes to zero in a window of $J_2^{c_1} \in (0.45 : 0.5)$, suggesting a continuous quantum phase transition at a critical point $J_2^{c_1} \approx 0.47$.
- The nature of the paramagnetic phase are probed using 3 sets of order parameters: the columnar dimer order D_X and D_Y, the staggered dimer order D_X^s and D_Y^s, and the plaquette order Q_α. At larger bond dimension D ($D \geq 5$), it is found that both $D^s_{X,Y}$, $D_{X,Y} \approx 0$ and ruled out the columnar and staggered dimer orders.
- The plaquette order parameter on 4 distinguished plaquettes are found to be the same and also ruled ous the PVBS order.
- The constant part of the Renyi entanglement entropy for the paramagnetic phase and found strong evidence to support the possibility of being a spin liquid.
- A probable phase diagram of the ground state of the $J_1 - J_2$ model is given by Balents and his co-workers.