The frustrated Heisenberg model on the honeycomb lattice

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CNR IOM-DEMOCRITOS and International School for Advanced Studies (SISSA)

Entanglement in Strongly Correlated Systems

F. Ferrari (SISSA)

[A. di Ciolo (now in Salerno) and J. Carrasquilla (now at d-wave)]

Can quantum fluctuations prevent magnetic order down to $T = 0$?

- Many theoretical suggestions since P.W. Anderson (1973)

Anderson, Mater. Res. Bull. **8**, 153 (1973)

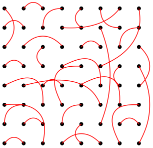
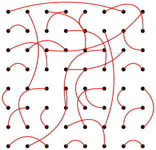
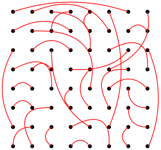
Fazekas and Anderson, Phil. Mag. **30**, 423 (1974)

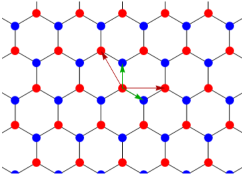
"Resonating valence-bond" (quantum spin liquid) states

Idea: the best state for two spin-1/2 spins is a valence bond (a spin singlet):

$$|VB\rangle_{\mathbf{R},\mathbf{R}'} = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{\mathbf{R}} |\downarrow\rangle_{\mathbf{R}'} - |\downarrow\rangle_{\mathbf{R}} |\uparrow\rangle_{\mathbf{R}'} \right)$$

Every spin of the lattice is coupled to a partner
Then, take a superposition of different valence bond configurations

$RVB =$  $+$  $+$  $+ \dots$



Bravais vectors: $\mathbf{a} = (1, 0)$ and $\mathbf{b} = (-1/2, \sqrt{3}/2)$

$$\mathcal{H} = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,k \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_k$$

Classical and semi-classical approaches

E. Rastelli, A. Tassi, and L. Reatto, Physica B **97**, 1 (1979)

J.B. Fouet, P. Sindzingre, and C. Lhuillier, Eur. Phys. J. B **20**, 241 (2001)

A. Mulder *et al.*, Phys. Rev. B **81**, 214419 (2010)

Quantum spin liquid (gapped) or dimer/plaquette order?

ED: A.F. Albuquerque *et al.*, Phys. Rev. B **84**, 024406 (2011)

VMC: B.K. Clark, D.A. Abanin, and S.L. Sondhi, Phys. Rev. Lett. **107**, 087204 (2011)

CC and ED: D.J.J. Farnell *et al.* Phys. Rev. B **84**, 012403 (2011)

fRG: J. Reuther, D.A. Abanin, and R. Thomale, Phys. Rev. B **84**, 014417 (2011)

Series exp: J. Oitmaa and R.R.P. Singh, Phys. Rev. B **84**, 094424 (2011)

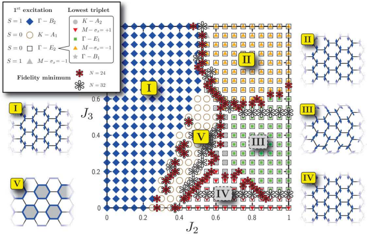
More recent DMRG calculations suggested a plaquette order

Z. Zhu, D.A. Huse, and S.R. White, Phys. Rev. Lett. **110**, 127205 (2013)

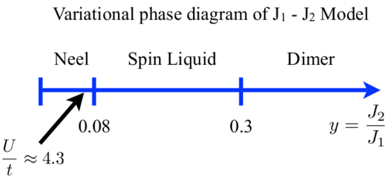
R. Ganesh, J. van den Brink, and S. Nishimoto, Phys. Rev. Lett. **110**, 127203 (2013)

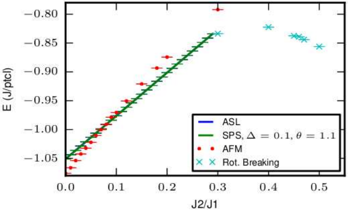
S.-S. Gong *et al.*, Phys. Rev. B **88**, 165138 (2013)

Previous ED and VMC results



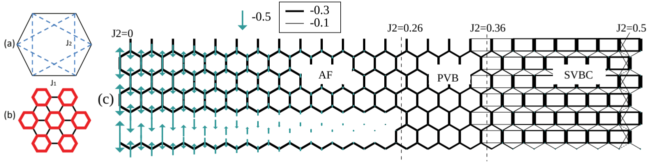
A.F. Albuquerque *et al.*, Phys. Rev. B **84**, 024406 (2011)



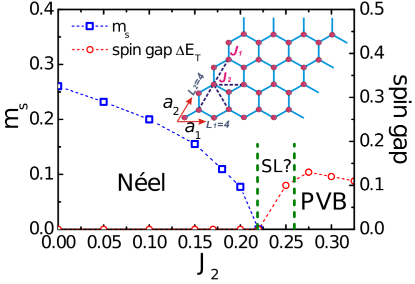


B.K. Clark, D.A. Abanin, and S.L. Sondhi, Phys. Rev. Lett. **107**, 087204 (2011)

Previous DMRG results

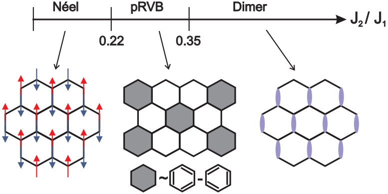


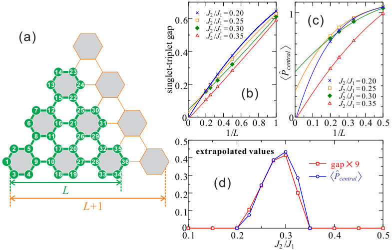
Z. Zhu, D.A. Huse, and S.R. White, Phys. Rev. Lett. **110**, 127205 (2013)

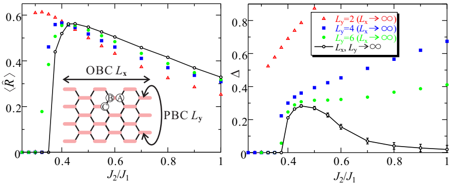


S.-S. Gong *et al.*, Phys. Rev. B **88**, 165138 (2013)

Previous DMRG results







R. Ganesh, J. van den Brink, and S. Nishimoto, Phys. Rev. Lett. **110**, 127203 (2013)

The classical phase diagram (I)

On sublattice $\mathcal{A}$: $\mathbf{S}_i = S\Big[\cos(\mathbf{Q}\cdot\mathbf{R}_i), \sin(\mathbf{Q}\cdot\mathbf{R}_i), 0\Big]$

On sublattice $\mathcal{B}$: $\mathbf{S}_i = -S\Big[\cos(\mathbf{Q}\cdot\mathbf{R}_i+\eta), \sin(\mathbf{Q}\cdot\mathbf{R}_i+\eta), 0\Big]$

- The Classical energy (per spin) for a generic coplanar spin wave is given by:

$$E_{\rm cl} = -\frac{J_1 S^2}{2}\Big[\cos\eta+\cos(\eta-Q_b)+\cos(\eta-Q_a-Q_b)\Big]+J_2 S^2\Big[\cos Q_a+\cos Q_b+\cos(Q_a+Q_b)\Big]$$

where $Q_a = \mathbf{Q}\cdot\mathbf{a} = Q_x$ and $Q_b = \mathbf{Q}\cdot\mathbf{b} = -Q_x/2+\sqrt{3}Q_y/2$

- The minimization of $E_{\rm cl}$ gives:

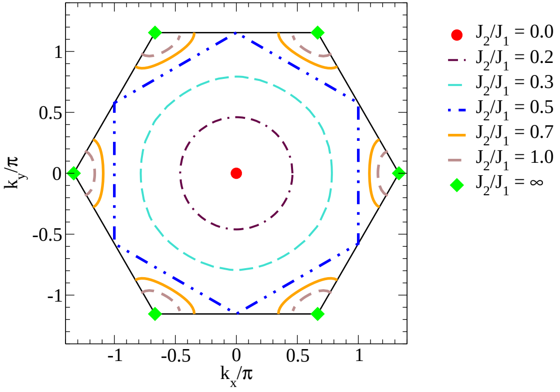
$$\cos Q_a^* + \cos Q_b^* + \cos(Q_a^*+Q_b^*) = \frac{1}{2}\left[\left(\frac{J_1}{2J_2}\right)^2 - 3\right]$$

$$\sin\eta^* = \frac{2J_2}{J_1}\left[\sin Q_b^* + \sin(Q_a^*+Q_b^*)\right]$$

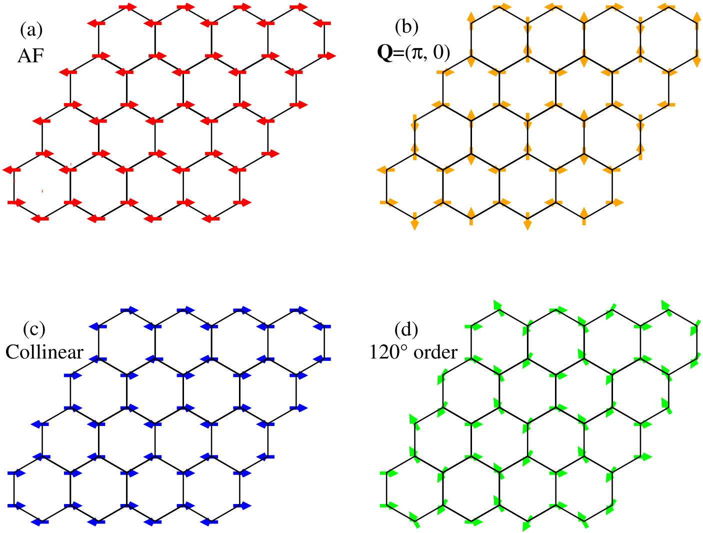
$$\cos\eta^* = \frac{2J_2}{J_1}\left[1+\cos Q_b^* + \cos(Q_a^*+Q_b^*)\right]$$

The classical phase diagram (II)

- The AF $\mathbf{Q} = (0,0)$ Néel state is stable for $J_2/J_1 < 1/6$
- Degenerate spiral (type I) states for $1/6 < J_2/J_1 < 1/2$
- (For $J_2/J_1 = 1/2$, collinear states are present)
- Degenerate spiral (type II) states for $J_2/J_1 > 1/2$

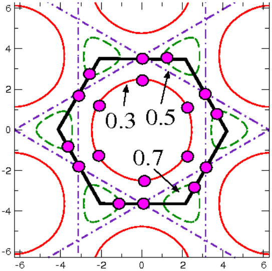


Examples of important magnetic orderings



Holstein-Primakoff spin wave theory at the leading order in $1/S$

- Order by disorder selection: six spiral wave-vectors lying along the classical manifold (wave-vectors along particular high-symmetry directions)



- Quantum fluctuations can melt the spiral order in a wide range of J_2/J_1

A. Mulder *et al.*, Phys. Rev. B **81**, 214419 (2010)

- The variational states containing quantum fluctuations are defined by:

$$|\Psi\rangle = \mathcal{J}_z \mathcal{P}_{S^z_{\rm tot}=0} |{\rm Cl}\rangle$$

- $|{\rm Cl}\rangle$ is a classical state where each spin points in a given direction in the XY plane
  It is described by a wave vector $\mathbf{Q}$ and a phase shift η:

$$|{\rm Cl}\rangle = \prod_i \left(|\downarrow\rangle_i + e^{\imath(\mathbf{Q}\cdot\mathbf{R}_i+\eta_i)} |\uparrow\rangle_i \right) = \prod_i e^{\imath(\mathbf{Q}\cdot\mathbf{R}_i+\eta_i)(S^z_i+1/2)} \left(|\downarrow\rangle_i + |\uparrow\rangle_i \right)$$

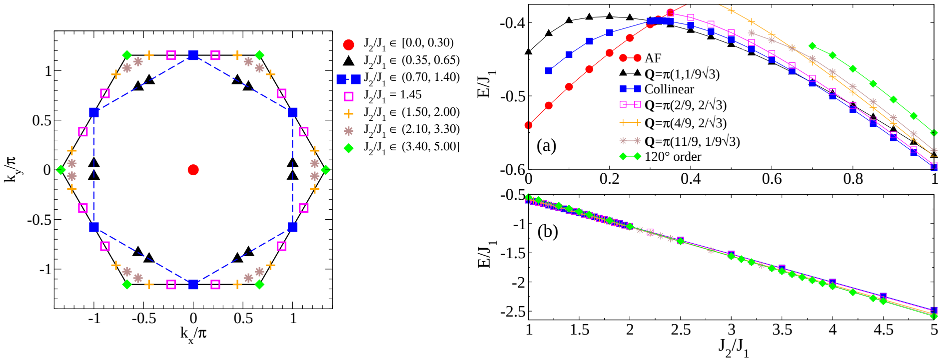
- Quantum fluctuations are generated by the Jastrow factor
  $\mathcal{J}_z$ describes out-of-plane fluctuations

$$\mathcal{J}_z = \exp\left(\frac{1}{2} \sum_{ij} v_{ij} S^z_i S^z_j \right)$$

E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991)

- Results for the 18×18 cluster

  (Only a finite number of **Q** vectors are available)



A. Di Ciolo, J. Carrasquilla, F. Becca, M. Rigol, and V. Galitski, Phys. Rev. B **89**, 094413 (2014)

Fermionic representation of a spin-1/2

- A faithful representation of spin-1/2 is given by:

$$S_i^z = \frac{1}{2}\left(c_{i,\uparrow}^\dagger c_{i,\uparrow} - c_{i,\downarrow}^\dagger c_{i,\downarrow}\right)$$
$$S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow}$$
$$S_i^- = c_{i,\downarrow}^\dagger c_{i,\uparrow}$$

$\{c_{i,\alpha}, c_{j,\beta}^\dagger\} = \delta_{ij}\delta_{\alpha\beta}$

$\{c_{i,\alpha}, c_{j,\beta}\} = 0$

$c_{i,\uparrow}^\dagger$ (or $c_{i,\downarrow}^\dagger$) changes S_i^z by 1/2 (or −1/2) and creates a "spinon"

- For a model with one spin per site, we must impose the constraints:

$$c_{i,\uparrow}^\dagger c_{i,\uparrow} + c_{i,\downarrow}^\dagger c_{i,\downarrow} = 1 \qquad\qquad c_{i,\uparrow} c_{i,\downarrow} = 0$$

- There is a huge redundancy, $SU(2)$ local "gauge" transformations:

$$c_{j,\uparrow} \to a_{11} c_{j,\uparrow} + a_{21} c_{j,\downarrow}^\dagger$$
$$c_{j,\downarrow}^\dagger \to a_{12} c_{j,\uparrow} + a_{22} c_{j,\downarrow}^\dagger$$

Affleck, Zou, Hsu, and Anderson, Phys. Rev. B **38**, 745 (1988)

Whitout breaking the SU(2) spin symmetry, the mean-field Hamiltonian is

$$\mathcal{H}_{\rm MF} = \sum_{ij} \chi_{ij} (c^\dagger_{j,\uparrow} c_{i,\uparrow} + c^\dagger_{j,\downarrow} c_{i,\downarrow}) + \Delta_{ij} (c^\dagger_{j,\uparrow} c^\dagger_{i,\downarrow} + c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}) + h.c.$$

Magnetic order can be included breaking the SU(2) symmetry

$$\mathcal{H}_{\rm MF} \Longrightarrow \mathcal{H}_{\rm AF} = \mathcal{H}_{\rm MF} + h \sum_j e^{i\mathbf{Q}\cdot\mathbf{R}_j} S^x_j$$

At the mean-field level, the constraint is only valid in average (global constraint)

$$\mathcal{H}_{\rm MF} \to \mathcal{H}_{\rm MF} - \mu \sum_i (c^\dagger_{i,\uparrow} c_{i,\uparrow} + c^\dagger_{i,\downarrow} c_{i,\downarrow} - 1) + \zeta \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} + h.c.$$

- Gapped energy spectrum $\to$ gapped spin liquid
- Gapless energy spectrum $\to$ gapless spin liquid

  Both gapped and gapless phases of the Kitaev compass model are reproduced

  Burnell and Nayak, Phys. Rev. B **84**, 125125 (2011)

- Finite h $\to$ magnetic order

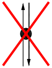
Beyond the mean-field approach

For $h = 0$, the ground state has the form of a BCS wave function:

$$|\Phi_{\rm MF}\rangle = \exp\left\{\sum_{i,j} f_{i,j}(c^\dagger_{i,\uparrow}c^\dagger_{j,\downarrow} + c^\dagger_{j,\uparrow}c^\dagger_{i,\downarrow})\right\}$$

The exact local constraint can be enforced but a Monte Carlo sampling is necessary

$$|RVB\rangle = \mathcal{P}_G|\Phi_{\rm MF}\rangle \qquad \mathcal{P}_G = \prod_i (1 - n_{i,\uparrow}n_{i,\downarrow})$$

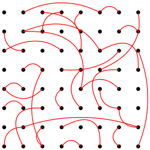


A Monte Carlo sampling implies calculations of determinants, which can be computed in a polynomial time

- The mean-field wave function has a BCS-like form

$$|\Phi_{MF}\rangle = \exp\left\{ \frac{1}{2} \sum_{i,j} f_{i,j} c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} \right\} |0\rangle$$

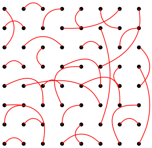
It is a linear superposition of all singlet configurations (that may overlap)



$+ \ldots$

- After projection, only non-overlapping singlets survive: the resonating valence-bond (RVB) wave function

Anderson, Science **235**, 1196 (1987)



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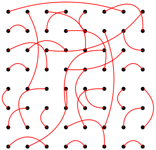

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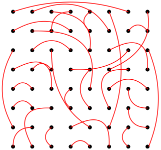
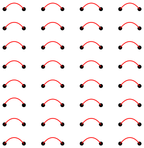


$+ \ldots$

Valence-bond states: liquids and solids

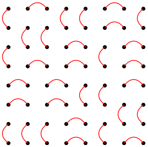
- Different pairing functions give different states...

Valence-bond solid



breaks translational/rotational symmetries

Short-range RVB



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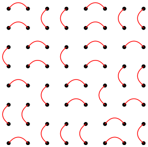
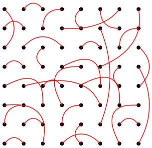


+ ...

Long-range RVB



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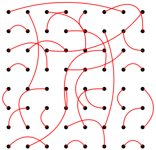


+ ...

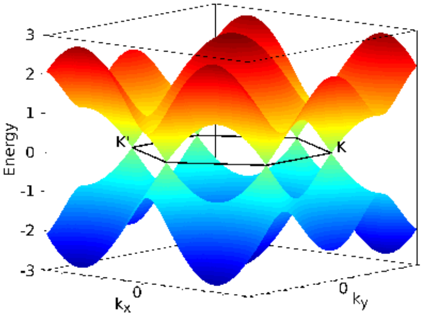
The "mother" of all wave functions

- The simplest wave function can be defined with $\chi_{ij} = t$ and no pairing $\Delta_{ij} = 0$

$$\mathcal{H}_{\rm MF} = t \sum_{\langle i,j \rangle,\alpha} c^\dagger_{i,\alpha} c_{j,\alpha} + \text{h.c.}$$

- Dirac points in the spinon spectrum
- U(1) gauge structure
- Power-law spin-spin correlations

U(1) Dirac state
Very good energy per site
especially for $J_2/J_1 \approx 0.2$



The AF state for small J_2/J_1

$$|\Psi\rangle = \mathcal{J}_z \mathcal{P}_{S^z_{\rm tot}=0} \mathcal{P}_G |\Phi_{\rm MF}\rangle$$

where $|\Psi_{\rm MF}\rangle$ is the ground state of:

$$\mathcal{H}_{\rm MF} = t \sum_{\langle i,j \rangle,\alpha} c^\dagger_{i,\alpha} c_{j,\alpha} + \text{h.c.} + h \sum_j e^{i\mathbf{Q}\cdot\mathbf{R}_j + \eta_j} S^x_j$$

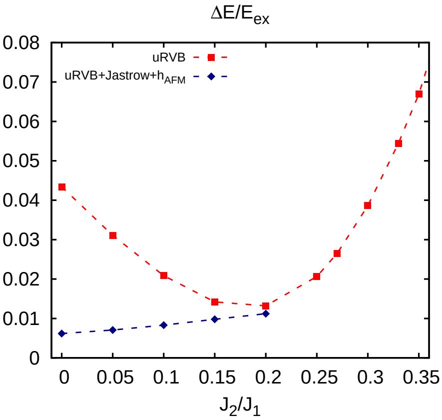
with $\mathbf{Q} = (0,0)$ and $\eta_j = 0$ (π) on $\mathcal{A}$ $(\mathcal{B})$ sublattices.

- For $t = 0$, $|\Psi_{\rm MF}\rangle \to |\text{Cl}\rangle$ (localized, i.e., “bosonic, state)
- Remarkably (and mysteriously), there is a finite energy gain with $t \neq 0$
- Quantum fluctuations are generated by the Jastrow factor

$$\mathcal{J}_z = \exp\left(\frac{1}{2} \sum_{ij} v_{ij} S^z_i S^z_j \right)$$

Accuracy of the AF state

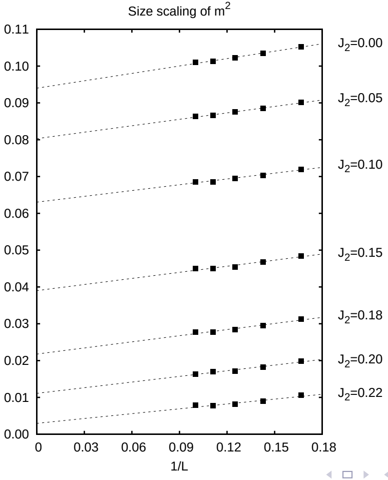
- Results for the accuracy on the 24-site cluster



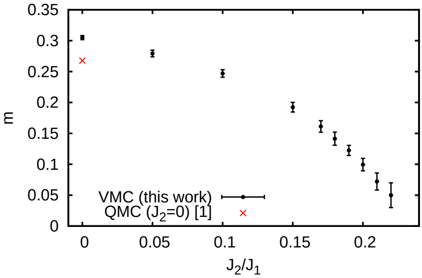
Size scaling of the AF order parameter for small J_2/J_1

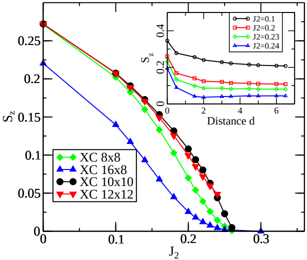
- We compute the isotropic spin-spin correlations at the largest distance

$$m^2 = \lim_{r\to\infty} \langle \mathbf{S}_0 \cdot \mathbf{S}_r \rangle$$



The AF state for small J_2/J_1





Z. Zhu *et al.*, Phys. Rev. Lett. **110**, 127205 (2013)

The magnetically disordered phase for intermediate J_2/J_1

- Is it a gapped or gapless spin liquid?

Based on a wrong prejudice
(the Hubbard model sustains a gapped SL phase for moderate U/t)
people were interested in gapped SL in the $J_1 - J_2$ model

Projective symmetry-group (PSG) analysis

Y.-M. Lu and Y. Ran, Phys. Rev. B **84**, 024420 (2011)

Only one gapped SL with short-range couplings
Number 19, called sublattice pairing state (SPS)

All the other states are gapless

TABLE I. A summary of all 24 different PSGs with IGG = $\{\pm\tau^0\}$ around the u-RVB ansatz. They correspond to 24 different Z_2 SLs near the u-RVB state.

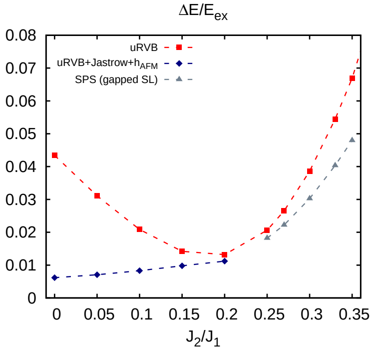
No.	g_T	g_σ	g_{C_6}	g_1	g_2
1	τ^0	τ^0	τ^0	τ^0	τ^0
2	τ^0	τ^0	$i\tau^3$	τ^0	τ^0
3	τ^0	τ^0	$i\tau^3$	$e^{i2\pi/3\tau^1}$	$e^{-i2\pi/3\tau^1}$
4	τ^0	$i\tau^3$	$i\tau^3$	τ^0	τ^0
5	τ^0	$i\tau^3$	$i\tau^3$	τ^0	τ^0
6	τ^0	$i\tau^3$	$i\tau^1$	τ^0	τ^0
7	τ^0	$i\tau^3$	$e^{i\pi/6\tau^1}$	τ^0	τ^0
8	τ^0	$i\tau^3$	$e^{i\pi/3\tau^1}$	τ^0	τ^0
9	τ^0	$i\tau^3$	$i\tau^1$	$e^{i2\pi/3\tau^3}$	$e^{-i2\pi/3\tau^3}$
10	τ^0	$i\tau^3$	$e^{i2\pi/3\tau^1}$	$i\left(\frac{\tau^1}{\sqrt{3}} - \sqrt{\frac{2}{3}}\tau^2\right)$	$i\left(\frac{\tau^3}{\sqrt{2}} - \frac{\tau^2}{\sqrt{6}} - \frac{\tau^1}{\sqrt{3}}\right)$
11	$i\tau^3$	τ^0	τ^0	τ^0	τ^0
12	$i\tau^3$	τ^0	$i\tau^3$	τ^0	τ^0
13	$i\tau^3$	τ^0	$i\tau^1$	τ^0	τ^0
14	$i\tau^3$	τ^0	$i\tau^1$	$e^{i2\pi/3\tau^3}$	$e^{-i2\pi/3\tau^3}$
15	$i\tau^3$	$i\tau^3$	τ^0	τ^0	τ^0
16	$i\tau^3$	$i\tau^3$	$i\tau^3$	τ^0	τ^0
17	$i\tau^3$	$i\tau^3$	$i\tau^1$	τ^0	τ^0
18	$i\tau^3$	$i\tau^3$	$i\tau^1$	$e^{i2\pi/3\tau^3}$	$e^{-i2\pi/3\tau^3}$
19	$i\tau^3$	$i\tau^1$	$i\tau^1$	τ^0	τ^0
20	$i\tau^3$	$i\tau^1$	$i\tau^2$	τ^0	τ^0
21	$i\tau^3$	$i\tau^1$	τ^0	τ^0	τ^0
22	$i\tau^3$	$i\tau^1$	$i\tau^3$	τ^0	τ^0
23	$i\tau^3$	$i\tau^1$	$e^{i\pi/6\tau^3}$	τ^0	τ^0
24	$i\tau^3$	$i\tau^1$	$e^{i\pi/3\tau^3}$	τ^0	τ^0

The SPS gapped spin liquid

- The SPS state has NN hopping and NNN pairing
  (with opposite phases on the two sublattices)

$$\mathcal{H}_{\rm MF} = t \sum_{\langle i,j \rangle,\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} + \Delta e^{\imath\theta} \sum_{\langle\langle i,k \rangle\rangle \in \mathcal{A}} c^{\dagger}_{i,\uparrow} c^{\dagger}_{k,\downarrow} + \Delta e^{-\imath\theta} \sum_{\langle\langle i,k \rangle\rangle \in \mathcal{B}} c^{\dagger}_{i,\uparrow} c^{\dagger}_{k,\downarrow} + {\rm h.c.}$$

- Results for the accuracy on the 24-site cluster



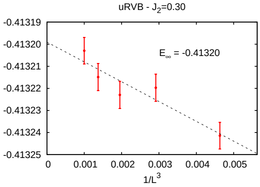
The SPS gapped spin liquid

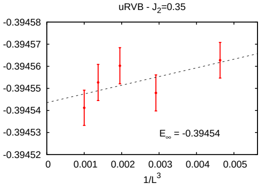
- The variational energy is (almost) insensitive on θ
- The "best" energy is obtained with $\theta = 0$ (corresponding to a $U(1)$ SL)
- Previous VMC calculations by B. Clark were affected by a mistake

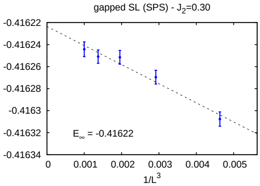
B.K. Clark, D.A. Abanin, and S.L. Sondhi, Phys. Rev. Lett. **107**, 087204 (2011)

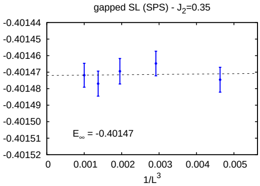
More reliable calculations by O. Motrunich

S.-S. Gong *et al.*, Phys. Rev. B **88**, 165138 (2013)





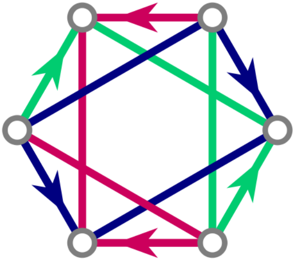




A gapless Z_2 spin liquid

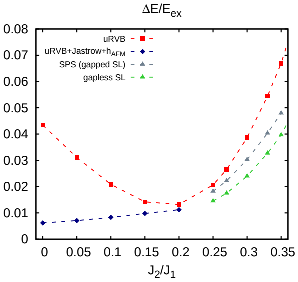
- There is a gapless state with NN hopping and NNN pairing

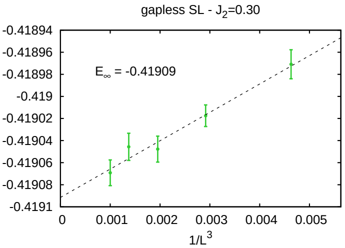
$$\mathcal{H}_{\mathrm{MF}} = \sum_{\langle i,j \rangle, \alpha} t e^{\imath \theta_{ij}} c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{\langle\langle i,k \rangle\rangle} \Delta e^{-\imath \theta_{ik}} c^{\dagger}_{i,\uparrow} c^{\dagger}_{k,\downarrow} + \mathrm{h.c.}$$

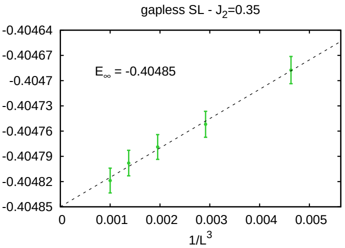


BLUE: $\theta_{ij} = 0$
RED: $\theta_{ij} = 2\pi/3$
GREEN: $\theta_{ij} = 4\pi/3$

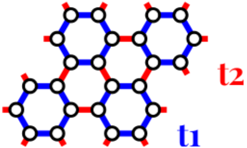
A gapless Z_2 spin liquid



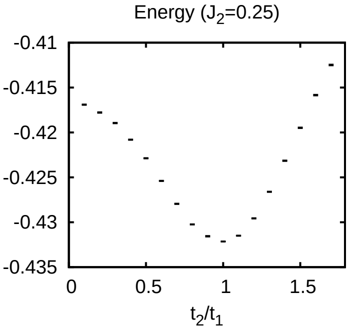


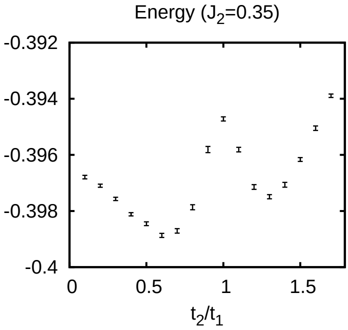


- Is it a valence-bond solid (VBS), with plaquette order?

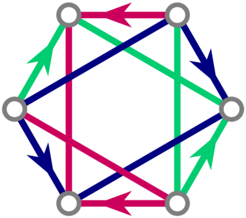


- On the $4 \times 4 \times 6$ cluster, the energy landscape:

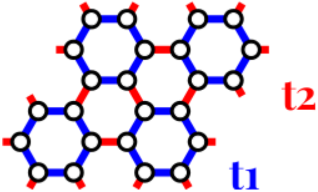




Is the gapless SL stable against VBS order?



+



- On the $10 \times 10 \times 6$ cluster:

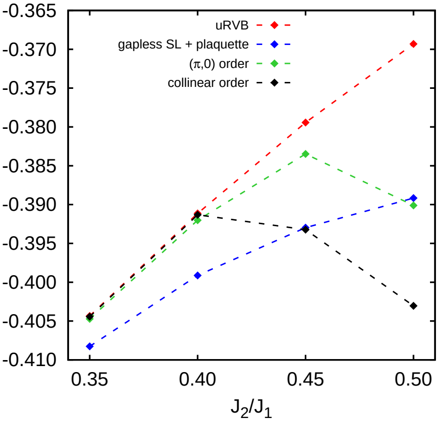
For $J_2/J_1 = 0.30$ $E_{\rm SL} = -0.41907(1) \longrightarrow E_{\rm SL+VBS} = -0.41950(1)$

For $J_2/J_1 = 0.35$ $E_{\rm SL} = -0.40482(1) \longrightarrow E_{\rm SL+VBS} = -0.40675(2)$

- No sign of dimer order is found (at most anti-plaquette)

The collinear state becomes energetically favorable for $J_2/J_1 > 0.45$

- On the $4 \times 4 \times 6$ cluster:



Conclusions

By using Jastrow-Slater variational wave functions

- $\mathbf{Q} = (0, 0)$ up to $J_2/J_1 \approx 0.25$

  (in agreement with DMRG results!)

- The SPS gapped SL is a local minimum
  but other states compete with it in the highly-frustrated regime

- A 6-site plaquette state is stabilized up to $J_2/J_1 \approx 0.45$
  (in agreement with DMRG results!)

- A collinear AF state with $\mathbf{Q} = (0, \frac{2\pi}{\sqrt{3}})$ is found for $0.45 < J_2/J_1 < 0.55$

- Chiral phases (with J_3?)

- Deconfined criticality?
  (yesterday: $\eta_s \approx 0.75$ and $\nu_s \approx 0.67$???)