Frustrated magnets: triangular and kagome lattices

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Entanglement in Strongly Correlated Systems

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[W.J. Hu (now at Rice) and R. Thomale (Wurzburg)]

Searching for non-magnetic ground states

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)

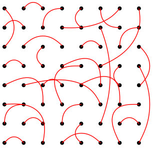
  "Resonating valence-bond" (quantum spin liquid) states

  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

$RVB =$



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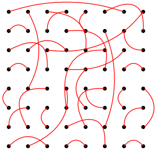

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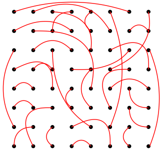


$+ \dots$

The Heisenberg model on the kagome lattice

- In the 1990s, several studies (classical and quantum models)

Macroscopic degeneracy of the classical ground state
order by disorder at low temperatures: $T \approx 0.005J$ nematic, octupolar?

Chalker, Holdsworth, and Shender, Phys. Rev. Lett. **68**, 855 (1992)

Harris, Kallin, and Berlinsky, Phys. Rev. B **45**, 2899 (1992)

Huse and Rutenberg, Phys. Rev. B **45**, 7536 (1992)

Reimers and Berlinsky, Phys. Rev. B **48**, 9539 (1993)

Zhitomirsky, Phys. Rev. B **78**, 094423 (2008)

ED: Extremely unusual low-energy spectrum of the $S = 1/2$ quantum model
finite (?) triplet gap, i.e., $\Delta E \approx J/20$
exponentially (?) large number of singlets states below the first triplet

Lecheminant *et al.*, Phys. Rev. B **56**, 2521 (1997)

Sindzingre and Lhuillier, EPL **88**, 27009 (2009)

A quantum spin liquid?

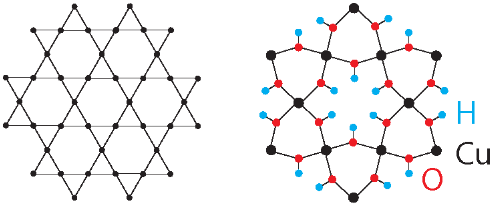
Spin waves and ED: Zeng and Elser, Phys. Rev. B **42**, 8436 (1990)

SU(N), large-N: Sachdev, Phys. Rev. B **45**, 12377 (1992)

Series expansions: Singh and Huse, Phys. Rev. Lett. **68**, 1766 (1992)

High-temperature expansions and ED: Elstner and Young, Phys. Rev. B **50**, 6871 (1994)

Herbertsmithite
$ZnCu_3(OH)_6Cl_2$
Best $S = 1/2$ Heisenberg model on the kagome lattice:
small 3D coupling,
small DM interactions,
few impurities



$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \mathrm{DM} + \mathrm{Impurities} + \mathrm{3D\ couplings} + \dots$$

- No magnetic order down to 50mK (despite $T_{CW} \simeq 200$K)
- Spin susceptibility rises with $T \to 0$ but then saturates below 0.5K
- Specific heat $C_v \propto T$ below 0.5K
- No sign of spin gap in dynamical Neutron scattering measurements

Mendels *et al.*, Phys. Rev. Lett. **98**, 077204 (2007)
Helton *et al.*, Phys. Rev. Lett. **98**, 107204 (2007)
Olariu *et al.*, Phys. Rev. Lett. **100**, 087202 (2008)
de Vries *et al.*, Phys. Rev. Lett. **100**, 157205 (2008)

- Recently, some evidence for a gap in NMR experiments

Fu, Imai, Han, and Lee, Science **350**, 655 (2015)

The Heisenberg model on the kagome lattice

- Today, the Heisenberg model on the kagome lattice has a second childhood

A gapped Z_2 spin liquid? Density-matrix renormalization group and descendants

Yan, Huse, and White, Science **332**, 1173 (2011)

Depenbrock, McCulloch, and Schollwock, Phys. Rev. Lett. **109**, 067201 (2012)

Jiang, Wang, and Balents, Nat. Phys. **8**, 902 (2012)

Nishimoto, Shibata, and Hotta, Nat. Commun. **4**, 2287 (2013)

Xie *et al.*, Phys. Rev. X **4**, 011025 (2014)

A gapless spin liquid? Fermionic variational wave functions

Ran, Hermele, Lee, and Wen, Phys. Rev. Lett. **98**, 117205 (2007)

Hermele, Ran, Lee, and Wen, Phys. Rev. B **77**, 224413 (2008)

Iqbal, Becca, and Poilblanc, Phys. Rev. B **84**, 020407 (2011)

Iqbal, Becca, Sorella, and Poilblanc, Phys. Rev. B **87**, 060405 (2013)

A chiral topological spin liquid? Schwinger boson mean-field

Messio, Bernu, Lhuillier, Phys. Rev. Lett. **108**, 207204 (2012)

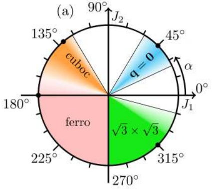
First suggested by Yang, Warman, and Girvin, Phys. Rev. Lett. **70**, 2641 (1993) [Kalmeyer and Laughlin, Phys. Rev. Lett. **59**, 2095 (1987)]

A valence-bond solid? Quantum dimer models or Series expansions

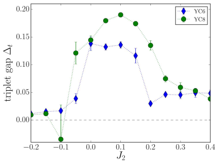
Singh and Huse, Phys. Rev. B **76**, 180407 (2007)

Poilblanc, Mambrini, and Schwandt, Phys. Rev. B **81**, 180402 (2010)

- The quantum case: $J_1 - J_2$ model

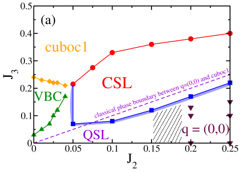


Suttner *et al.*, Phys. Rev. B **89**, 020408 (2014)

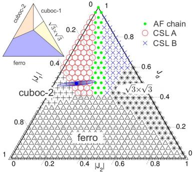


Kolley *et al.*, Phys. Rev. B **91**, 104418 (2015)

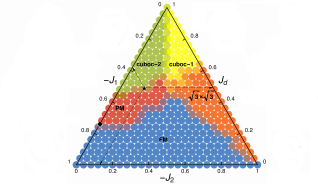
- The quantum case: $J_1 - J_2 - J_3$ model (also for J_1, $J_2 < 0$ for Kapellasite)



Gong *et al.*, Phys. Rev. B **91**, 075112 (2015)



Bieri *et al.*, Phys. Rev. B **92**, 060407 (2015)



Iqbal *et al.*, arXiv:1506.03436

The J_1-J_2 Heisenberg model on the triangular lattice

- The Heisenberg model on the triangular lattice is magnetically ordered

  Huse and Elser, Phys. Rev. Lett. **60**, 2531 (1988)

  Capriotti, Trumper, and Sorella, Phys. Rev. Lett. **82**, 3899 (1999)

  White and Chernyshev, Phys. Rev. Lett. **99**, 127004 (2007)

- Recently people become interested in the J_1-J_2 model

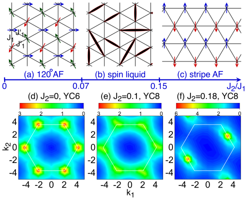
  A gapped Z_2 spin liquid (with nematic order)? Density-matrix renormalization group

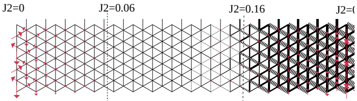
  Zhu and White, Phys. Rev. B **92**, 041105 (2015)

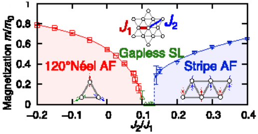
  Hu, Gong, Zhu, and Sheng, arXiv:1505.06276

  A gapless spin liquid? Fermionic variational wave functions

  Kaneko, Morita, and Imada, J. Phys. Soc. Jpn. **83** 093707 (2014)







Fermionic representation of a spin-1/2

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

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

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

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

$c_{i,\uparrow}^\dagger$ (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:

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

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

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

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

Mean-field approximation

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

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

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

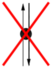
Beyond the mean-field approach

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

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

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

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



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

The Gutzwiller projector may have a strong effect on the mean-field state

- Develop magnetic order? Yes, projecting free fermions

  Li, EPL **103**, 57002 (2013)

- Develop dimer order? Yes, on odd legs with a gapped spectrum

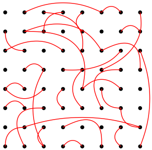
  Sorella, Capriotti, Becca, and Parola, Phys. Rev. Lett. **91**, 257005 (2003)

- Turn gapless spin liquids into gapped ones or vice-versa?

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

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

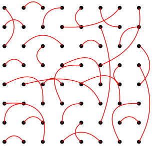
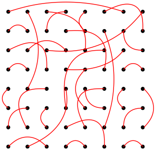
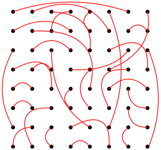
It is a linear superposition of all singlet configurations (that may overlap)



$+ \ldots$

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

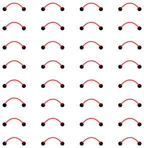
Anderson, Science **235**, 1196 (1987)

 $+$  $+$  $+ \ldots$

Valence-bond states: liquids and solids

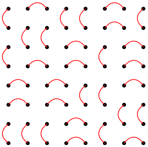
- Different pairing functions give different states...

Valence-bond solid



breaks translational/rotational symmetries

Short-range RVB



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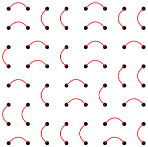

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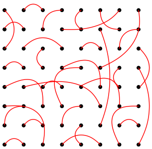
Long-range RVB



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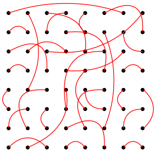


+ ...

Going to the excitation spectrum

If a variational approach works also low-energy excitations must be described

$$\mathcal{H}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu\delta_{ij}) c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{i,j} (\eta_{ij} + \zeta\delta_{ij})(c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + c^{\dagger}_{j,\uparrow} c^{\dagger}_{i,\downarrow}) + h.c.$$

After a Bogoliubov transformation:

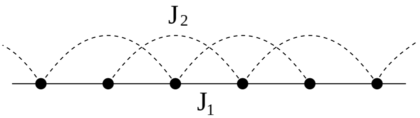
$$\mathcal{H}_{\mathrm{MF}} = \sum_{k} (E_k \psi^{\dagger}_k \psi_k - E_k \phi^{\dagger}_k \phi_k)$$

The ground state is:

$$|\Phi^0_{\mathrm{MF}}\rangle = \prod_k \phi^{\dagger}_k |0\rangle$$

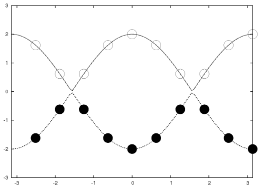
Excited states are obtained by:

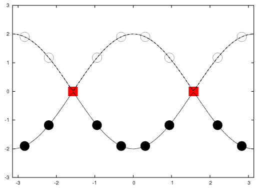
$$\phi_{q_1} \dots \phi_{q_n} \psi^{\dagger}_{p_1} \dots \psi^{\dagger}_{p_m} |\Phi^0_{\mathrm{MF}}\rangle$$



Unfrustrated case $J_2 = 0$ (gapless): the best variational state has a gapless E_k

- Periodic/antiperiodic boundary conditions can be used in the MF Hamiltonian
  $N = 4n + 2$ has no zero-energy modes $k = \pm\pi/2$ with PBC
  $N = 4n$ has no zero-energy modes $k = \pm\pi/2$ with APBC



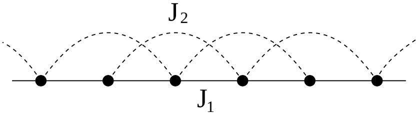


For $N = 30$

$E_{var}^{PBC,S=0} = -0.44393$ $\quad E_{ex}^{gs} = -0.44406$ $\quad \langle \Psi_{var}^{PBC,S=0} | \Psi_{ex}^{gs} \rangle = 0.999$

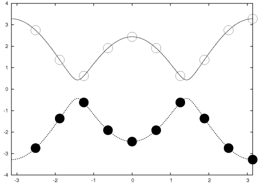
$E_{var}^{APBC,S=1} = -0.43893$ $\quad E_{ex}^{S=1} = -0.43916$ $\quad \langle \Psi_{var}^{APBC,S=1} | \Psi_{ex}^{S=1} \rangle = 0.998$

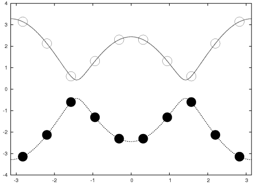
$E_{var}^{APBC,S=0} = -0.43578$ $\quad E_{ex}^{S=0} = -0.43652$ $\quad \langle \Psi_{var}^{APBC,S=0} | \Psi_{ex}^{S=0} \rangle = 0.993$



Frustrated case $J_2 = 0.4$ (dimerized): the best variational state has a gapped E_k

- Periodic/antiperiodic boundary conditions can be used in the MF Hamiltonian
  Both $N = 4n$ and $N = 4n + 2$ have no zero-energy modes





For $N = 30$

$E_{var}^{PBC,S=0} = -0.38048$ $\quad E_{ex}^{gs} = -0.38073$ $\quad \langle \Psi_{var}^{PBC,S=0} | \Psi_{ex}^{gs} \rangle = 0.998$

$E_{var}^{APBC,S=0} = -0.37958$ $\quad E_{ex}^{S=0} = -0.37983$ $\quad \langle \Psi_{var}^{APBC,S=0} | \Psi_{ex}^{S=0} \rangle = 0.997$

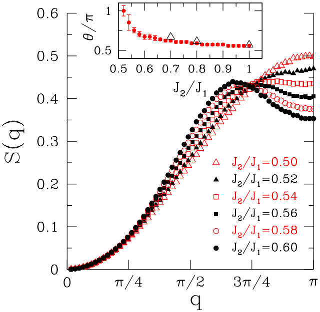
- Spin-spin correlations:

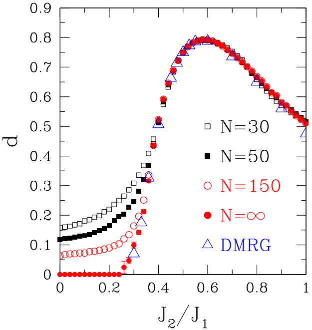
$$S(q) = \frac{1}{N} \sum_{R,R'} e^{iq(R-R')} \langle S^z_R S^z_{R'} \rangle$$

- Dimer-dimer correlations:

$$\Theta(R - R') = \langle S^z_R S^z_{R+x} S^z_{R'} S^z_{R'+x} \rangle - \langle S^z_R S^z_{R+x} \rangle \langle S^z_{R'} S^z_{R'+x} \rangle$$

$$d^2 = 9 \lim_{|R|\to\infty} |(\Theta(R - x) - 2\Theta(R) + \Theta(R + x)|$$





Becca, Capriotti, Parola, and Sorella, arXiv:0905.4854

Towards the exact ground state

How can we improve the variational state?
By the application of a few Lanczos steps!

$$|\Psi_{p-LS}\rangle = \left(1 + \sum_{m=1,\ldots,p} \alpha_m \mathcal{H}^m\right) |\Psi_{VMC}\rangle$$

- For $p \to \infty$, $|\Psi_{p-LS}\rangle$ converges to the exact ground state, provided $\langle \Psi_0 | \Psi_{VMC} \rangle \neq 0$
- On large systems, only FEW Lanczos steps are affordable: We can do up to $p = 2$

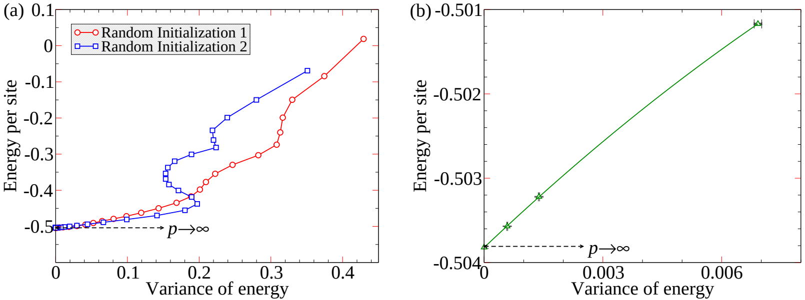
- A zero-variance extrapolation can be done

Whenever $|\Psi_{VMC}\rangle$ is sufficiently close to the ground state:

$$E \simeq E_0 + \text{const} \times \sigma^2$$

$$E = \langle \mathcal{H} \rangle / N$$
$$\sigma^2 = (\langle \mathcal{H}^2 \rangle - E^2)/N$$

How does it work?

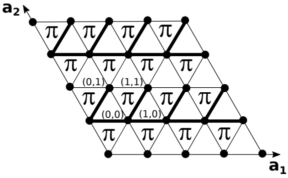


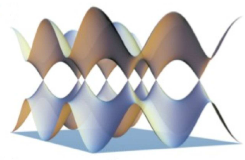
- As for the kagome lattice, one can define an ansatz with non-trivial fluxes ($\chi_{ij} = \pm 1$)

$$\mathcal{H}_{\mathrm{MF}} = \sum_{i,j,\alpha} \chi_{ij} c^{\dagger}_{i,\alpha} c_{j,\alpha}$$

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

U(1) Dirac state
Very good energy per site ($J_2/J_1 = 0.125$)
$E/J_1 = -0.5020$
$E_{DMRG}/J_1 = -0.5126$





- The uniform RVB state with $\chi_{ij} = 1$ has a much worse variational energy

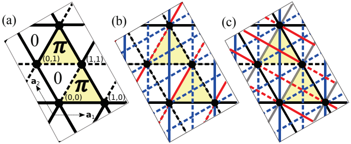
Can we have Z_2 gapped spin liquid or nematic states (DMRG)?

Projective symmetry-group analysis

Zheng, Mei, and Qi, arXiv:1505.05351

Lu, arXiv:1505.06495

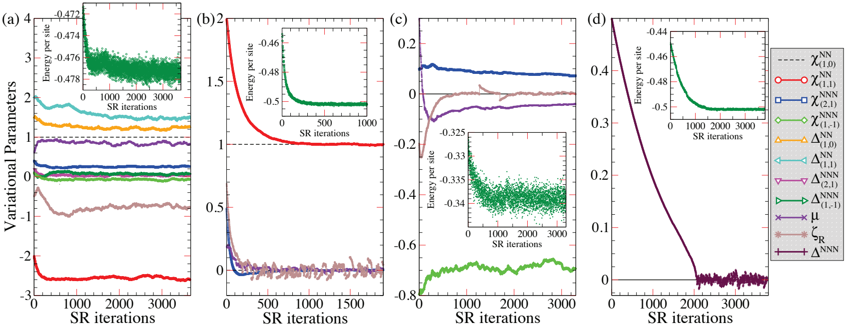
$$u_{ij} = \begin{pmatrix} \chi_{ij}^* & \Delta_{ij} \\ \Delta_{ij}^* & -\chi_{ij} \end{pmatrix}$$



Symmetric Abrikosov-fermion states							Nematic states: mean-field amplitudes				Schwinger-boson states
Label	η_{12}	g_σ	g_{C_6}	onsite $[0,0]$	NN $[1,1]$	NNN $[2,1]$	NN $[1,0]$	NN $[1,1]$	NNN $[2,1]$	NNN $[1,-1]$	(p_1, p_2, p_3)
#1	1	τ^0	τ^0	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	(1,1,0)
#2	-1	τ^0	τ^0	$\tau^{1,3}$	0	0	0	0	0	0	(0,1,0)
#3	1	τ^0	$i\tau^2$	0	0	0	0	0	0	0	
#4	-1	τ^0	$i\tau^2$	0	0	$\tau^{1,3}$	$\tau^{1,3}$	0	$\tau^{1,3}$	$\tau^{1,3}$	
#5	1	τ^0	$i\tau^3$	τ^3	τ^3	τ^3	τ^3	τ^3	τ^3	τ^3	(1,1,1)
#6	-1	τ^0	$i\tau^3$	τ^3	0	τ^1	τ^1	0	τ^1	τ^1	(0,1,1)
#7	1	$i\tau^2$	τ^0	0	0	0	$\tau^{1,3}$	0	$\tau^{1,3}$	0	
#8	-1	$i\tau^2$	τ^0	0	0	0	0	0	0	0	
#9	1	$i\tau^2$	$i\tau^2$	0	0	0	0	0	0	0	
#10	-1	$i\tau^2$	$i\tau^2$	0	$\tau^{1,3}$	0	$\tau^{1,3}$	$\tau^{1,3}$	$\tau^{1,3}$	0	
#11	1	$i\tau^2$	$i\tau^3$	0	0	0	τ^3	0	τ^3	0	
#12	-1	$i\tau^2$	$i\tau^3$	0	τ^1	0	τ^1	τ^1	τ^1	0	
#13	1	$i\tau^3$	τ^0	τ^3	τ^3	τ^3	$\tau^{1,3}$	τ^3	$\tau^{1,3}$	τ^3	(1,0,0)
#14	-1	$i\tau^3$	τ^0	τ^3	0	0	0	0	0	0	(0,0,0)
#15	1	$i\tau^3$	$i\tau^1$	0	0	0	τ^1	0	τ^1	0	
#16	-1	$i\tau^3$	$i\tau^1$	0	0	τ^3	τ^3	0	τ^3	τ^3	
#17	1	$i\tau^3$	$i\tau^2$	0	0	0	0	0	0	0	
#18	-1	$i\tau^3$	$i\tau^2$	0	τ^1	τ^3	$\tau^{1,3}$	τ^1	$\tau^{1,3}$	τ^3	
#19	1	$i\tau^3$	$i\tau^3$	τ^3	τ^3	τ^3	τ^3	τ^3	τ^3	τ^3	(1,0,1)
#20	-1	$i\tau^3$	$i\tau^3$	τ^3	τ^1	0	τ^1	τ^1	τ^1	0	(0,0,1)

- Only one gapped SL connected with the U(1) Dirac state, Number 20
- Three gapped nematic states (Number 1, 6, and 20)

Can we have Z_2 gapped spin liquid or nematic states (DMRG)?

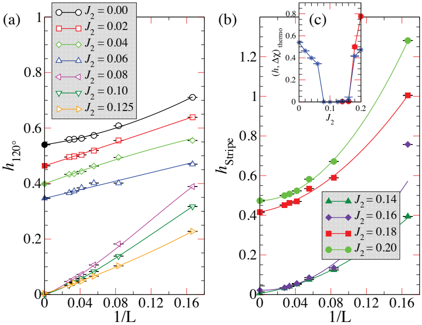


- (a) Nematic instability of the uniform U(1) RVB (Number 1)
- (b) Nematic instability of the U(1) Dirac state (Number 20)
- (c) Number 6
- (d) Gapless Z_2 spin liquid (Number 18)

$$\mathcal{H}_{\mathrm{AF}} = \sum_{ij} \chi_{ij} (c^\dagger_{j,\uparrow} c_{i,\uparrow} + c^\dagger_{j,\downarrow} c_{i,\downarrow}) + h \sum_j e^{i\mathbf{Q}\cdot\mathbf{R}_j} S^x_j$$

Non-trivial hopping amplitudes of (a) and (b)

$$|\Psi_{\mathrm{AF}}\rangle = \exp\left\{ \frac{1}{2} \sum_{i,j} v_{i,j} S^z_i S^z_j \right\} \mathcal{P}_G |\Phi_{\mathrm{AF}}\rangle$$



For $J_2 = 0$:

The thermodynamic energy is

$E/J_1 = -0.54532(1)$

$E_{DMRG}/J_1 \simeq -0.551(2)$

Gong and Hu (private communication)

Difficult extrapolation

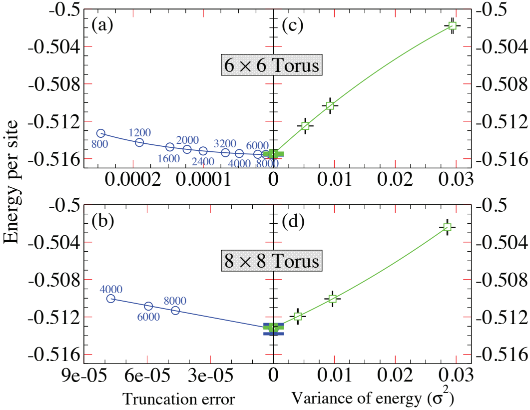
$E_{GFMCSR}/J_1 = -0.5458(1)$

Capriotti, Trumper, and and Sorella, Phys. Rev. Lett. **82**, 3899 (1999)

Calculations on 6×6 and 8×8 clusters

Our zero-variance extrapolation gives for $J_2/J_1 = 0.125$:

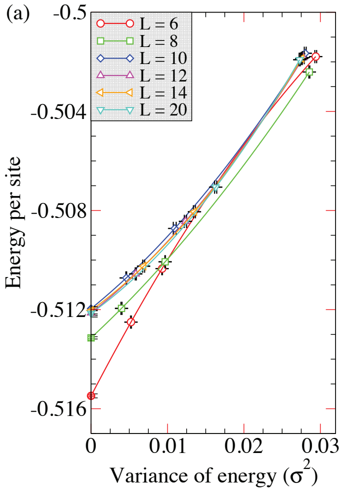
- For the 6×6: $E/J_1 = -0.51548(8)$
- For the 8×8: $E/J_1 = -0.51314(4)$



DMRG gives:

- For the 6×6: $E/J_1 = -0.51557(5)$
- For the 8×8: $E/J_1 = -0.5133(5)$

The Lanczos step extrapolations for $J_2/J_1 = 0.125$

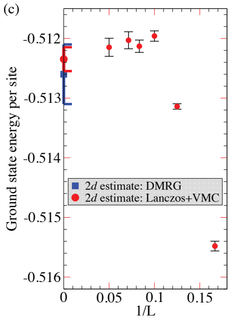


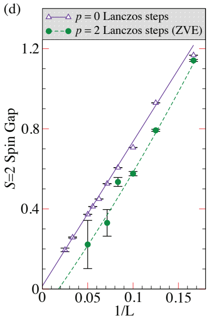
- We separately extrapolate both $S = 0$ and $S = 2$ energies
- Then the gap (zero-variance) gap is computed

The $S = 2$ gap for $J_2/J_1 = 0.125$

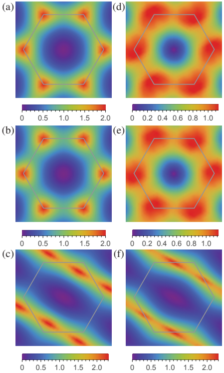
- The ground-state energy is better than previous variational calculations $E/J_1 = -0.5028(1)$

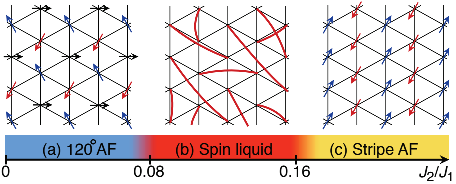
Kaneko, Morita, and Imada, J. Phys. Soc. Jpn. **83** 093707 (2014)





- The final result is $\Delta_2 = -0.17(21)$
- The "upper" bound is given by $\Delta_2 \simeq 0.02$
- The variational gap is $\Delta_2 = 0.015(24)$





- The VMC calculations indicate a gapless spin liquid
- No evidences for gapped/nematic states in the frustrated regime
- A complete comparison among VMC, DMRG, and fRG can be found in:

Y. Iqbal, W.-J. Hu, R. Thomale, D. Poilblanc, and F. Becca, arXiv:1601.06018

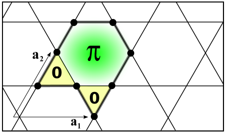
- A variational ansatz with only hopping but non-trivial fluxes has been proposed $(\chi_{ij} = \pm 1)$

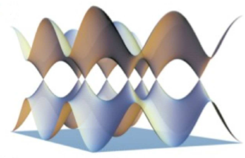
$$\mathcal{H}_{\rm MF} = \sum_{i,j,\alpha} \chi_{ij} c^{\dagger}_{i,\alpha} c_{j,\alpha}$$

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

U(1) Dirac state
Very good energy per site
$E/J_1 = -0.4286$
$E_{DMRG}/J_1 = -0.4385$

Ran, Hermele, Lee, and Wen, Phys. Rev. Lett. **98**, 117205 (2007)





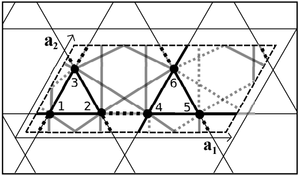
- The uniform RVB state with $\chi_{ij} = 1$ has a much worse variational energy

Can we have a Z_2 gapped spin liquid (DMRG)?

Projective symmetry-group analysis

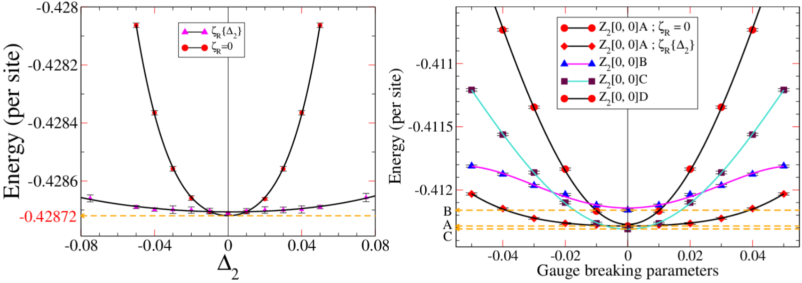
Lu, Ran, and Lee, Phys. Rev. B **83**, 224413 (2011)

$$u_{ij} = \begin{pmatrix} \chi_{ij}^* & \Delta_{ij} \\ \Delta_{ij}^* & -\chi_{ij} \end{pmatrix}$$



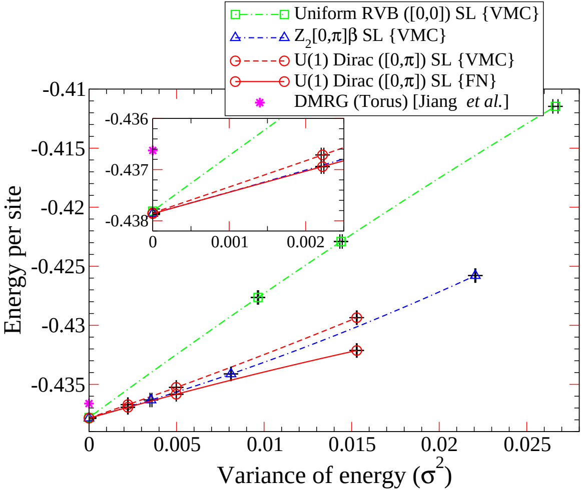
No.	η_{12}	Λ_s	u_α	u_β	u_γ	$\tilde{u}_\gamma$	Label	Gapped?
1	$+1$	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	$Z_2[0,0]A$	Yes
2	-1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	0	$\mathbb{Z}_2[0,\pi]\beta$	**Yes**
3	$+1$	0	τ^2,τ^3	0	0	0	$Z_2[\pi,\pi]A$	No
4	-1	0	τ^2,τ^3	0	0	τ^2,τ^3	$Z_2[\pi,0]A$	No
5	$+1$	τ^3	τ^2,τ^3	τ^3	τ^3	τ^3	$Z_2[0,0]B$	Yes
6	-1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^2	$Z_2[0,\pi]\alpha$	No
7	$+1$	0	0	τ^2,τ^3	0	0	–	–
8	-1	0	0	τ^2,τ^3	0	0	–	–
9	$+1$	0	0	0	τ^2,τ^3	0	–	–
10	-1	0	0	0	τ^2,τ^3	0	–	–
11	$+1$	0	0	τ^2	τ^2	0	–	–
12	-1	0	0	τ^2	τ^2	0	–	–
13	$+1$	τ^3	τ^3	τ^2,τ^3	τ^3	τ^3	$Z_2[0,0]D$	Yes
14	-1	τ^3	τ^3	τ^2,τ^3	τ^3	0	$Z_2[0,\pi]\gamma$	No
15	$+1$	τ^3	τ^3	τ^3	τ^2,τ^3	τ^3	$Z_2[0,0]C$	Yes
16	-1	τ^3	τ^3	τ^3	τ^2,τ^3	0	$Z_2[0,\pi]\delta$	No
17	$+1$	0	τ^2	τ^3	0	0	$Z_2[\pi,\pi]B$	No
18	-1	0	τ^2	τ^3	0	τ^3	$Z_2[\pi,0]B$	No
19	$+1$	0	τ^2	0	τ^2	0	$Z_2[\pi,\pi]C$	No
20	-1	0	τ^2	0	τ^2	τ^3	$Z_2[\pi,0]C$	No

- Only one gapped SL connected with the U(1) Dirac state, called $Z_2[0,\pi]\beta$
- Four gapped SL connected with the Uniform RVB



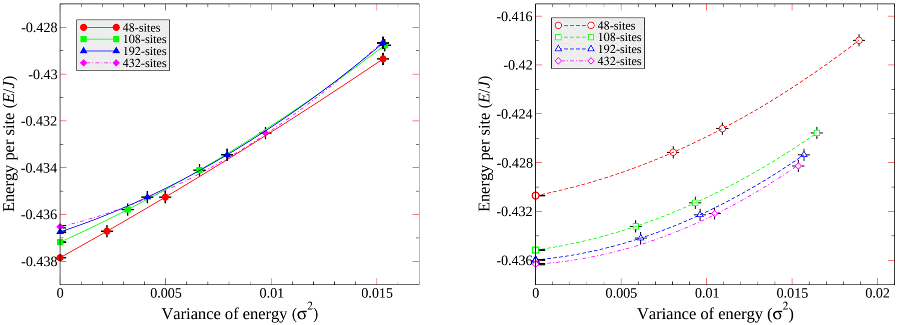
- Both the Uniform RVB and the U(1) Dirac states are stable against opening a gap

Our zero-variance extrapolation gives: $E/J_1 \simeq -0.4378$



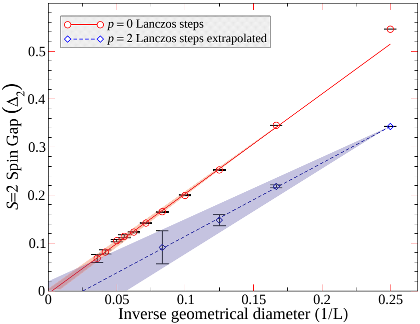
$E/J_1 \simeq -0.4387$ by ED, A. Lauchli (never published)
$E/J_1 \simeq -0.4381$ by DMRG, S. White (private communication)

The Lanczos step extrapolations



- We separately extrapolate both $S = 0$ and $S = 2$ energies
- Then the gap (zero-variance) gap is computed

The $S = 2$ gap



- The final result is $\Delta_2 = -0.04 \pm 0.06$
- The "upper" bound is given by $\Delta_2 \simeq 0.02$
- The $S = 1$ gap should be $\Delta_1 \lesssim 0.01$

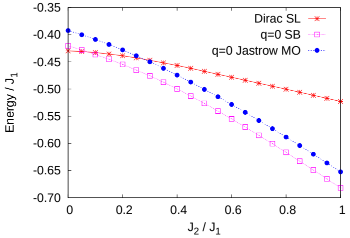
Much smaller than previous DMRG estimations

More similar to recent calculations by Nishimoto *et al.* $\Delta_1 = 0.05 \pm 0.02$

Nishimoto, Shibata, and Hotta, Nat. Commun. **4**, 2287 (2013)

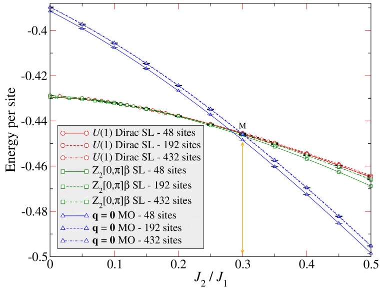
$$|\Psi_{\mathrm{AF}}\rangle = \exp\left\{\frac{1}{2}\sum_{i,j} v_{i,j} S_i^z S_j^z\right\} |\mathrm{AF;XY}\rangle$$

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



Small size calculations (6×6)

Tay and Motrunich, Phys. Rev. B **84**, 020404 (2011)

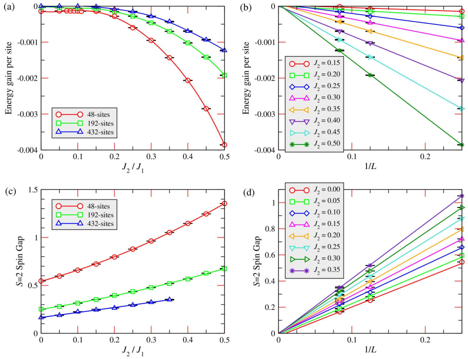


- Onset of $q = 0$ magnetic order for $J_2/J_1 > 0.3$
- Finite (tiny) energy gain of the $Z_2[0,\pi]\beta$ state over the U(1) Dirac state

Size scaling of energy and spin gap for $J_2 > 0$

In the thermodynamic limit:

- The energy gain of the $Z_2[0,\pi]\beta$ state over the U(1) Dirac state goes to zero
- The $S = 2$ gap goes to zero



- Recently, a claim for the stability of the $Z_2[0,\pi]\beta$ has been done (???)

Tao Li, arXiv:1601.02165

Conclusions

- Also for the kagome lattice, the VMC finds a gapless spin liquid

Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Physical Review B **87**, 060405 (2013)

Y. Iqbal, D. Poilblanc, and F. Becca, Physical Review B **89**, 020407 (2014)

- No evidences for gapped states, also for $J_2/J_1 > 0$
  For $J_2 = 0$ the energy gain is not larger than $\approx 10^{-6} J_1$

  For $J_2 > 0$ the energy gain is finite in finite sizes

Tao Li, arXiv:1601.02165

  For $J_2/J_1 = 0.2$ the energy gain is $\approx 5 \times 10^{-5}$ for $L = 12$

  Is it going to zero in the thermodynamic limit?