Dirac spin liquids in frustrated Heisenberg models: kagome and triangular lattices

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

S · S Matter, October 2015

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W.-J. Hu (CSU, Northridge → Rice), S. Gong, D. N. Sheng (CSU, Northridge)

New Entry (?): R. Thomale (Wurzburg): will he be converted by Yasir?

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)

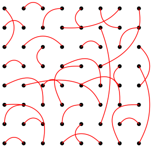
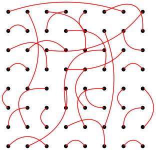
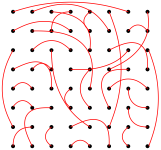
Fazekas and Anderson, Phil. Mag. **30**, 423 (1974)

"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

$RVB =$  $+$  $+$  $+ \ldots$

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)

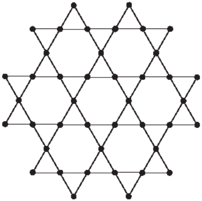
SU(N), large-N: Sachdev, Phys. Rev. B **45**, 12377 (1992)

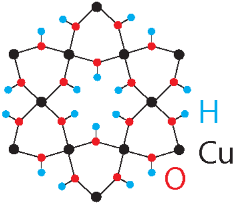
Series expansions: Singh and Huse, Phys. Rev. Lett. **68**, 1766 (1992)

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

The Heisenberg model on the kagome lattice

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





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

- 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)
Imai *et al.*, Phys. Rev. Lett. **100**, 077203 (2008)
de Vries *et al.*, Phys. Rev. Lett. **103**, 237201 (2009)
Jeong *et al.*, Phys. Rev. Lett. **107**, 237201 (2011)
Han *et al.*, Nature **492**, 407 (2012)

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 (algebraic) 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)

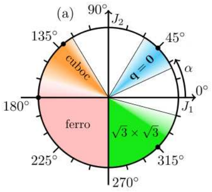
First suggested by Yang, Warman, and Girvin, Phys. Rev. Lett. **70**, 2641 (1993) [Kalmeyer and Laughlin, Phys. Rev. Lett. **59**, 2095 (1987)]

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

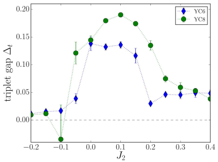
Singh and Huse, Phys. Rev. B **76**, 180407 (2007)

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

- The quantum case: $J_1 - J_2$ model

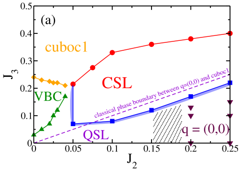


Suttner *et al.*, Phys. Rev. B **89**, 020408 (2014)

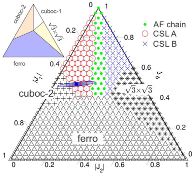


Kolley *et al.*, Phys. Rev. B **91**, 104418 (2015)

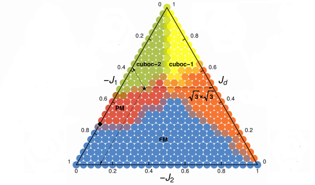
- The quantum case: $J_1 - J_2 - J_3$ model (also for J_1, $J_2 < 0$ for Kapellasite)



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

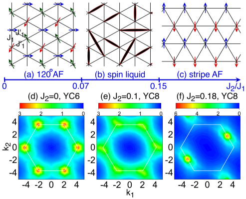
  A gapped Z_2 spin liquid (with nematic order)? Density-matrix renormalization group

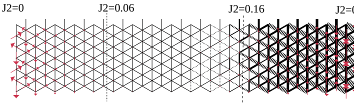
  Zhu and White, Phys. Rev. B **92**, 041105 (2015)

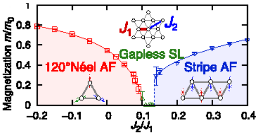
  Hu, Gong, Zhu, and Sheng, arXiv:1505.06276

  A gapless spin liquid? Fermionic variational wave functions

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







Numerical approaches

There are very few cases where exact solutions of microscopic spin models can be obtained

- Exact diagonalizations are limited to relatively small lattices
- Quantum Monte Carlo suffers from the sign problem for generic models
- Series expansions may have a slow convergence and problematic extrapolations
- Functional renormalization group is based upon uncontrolled truncations
- (Cluster) Dynamical mean-field theory is not suited for frustrated systems

Two kinds of variational approaches have shown to be particularly effective and accurate

- Density-matrix renormalization group (DMRG) or tensor network approaches
  Brute force methods based upon a blind "optimization"
  Many variational parameters

- Projected fermionic/bosonic (partonic) wave functions
  Educated guess based upon suitably constructed quantum states
  Few variational parameters

Accuracy of variational methods

- ALL variational approaches contain a bias (also DMRG)
- In the thermodynamic limit, the variational energy differ from the exact one
  by an INFINITE amount (accuracy on the energy per site)
  The overlap between the ground state and any variational ansatz goes to zero

We can always construct wrong variational states with a high accuracy

See for example, Balents, Phys. Rev. B **90**, 245116 (2014)

- Sure, this is especially true for gapless systems
- Also numerically exact methods may suffer from similar problems:
  Quantum Monte Carlo because of errorbars
  Exact diagonalizations because of small clusters

So, should we give up and throw away numerical methods?

No, because we can still obtain the correct answer in many cases

It works in cases where a local order parameter is present

More difficult for models with topological order or gapless excitations

Accuracy of variational methods

- Construct your wave function starting from a LOCAL Hamiltonian
  (e.g., Gutzwiller projected mean-field states of short-range Hamiltonians)
- A "brute force" many-parameter optimization may be dangerous
  (e.g., even Gutzwiller projected states that have not a short-range parent Hamiltonian)
- A variational wave function depending upon a parameter $|\Psi(\alpha)\rangle$

$$\frac{\delta}{\delta\alpha}|\Psi(\alpha)\rangle = \Theta_\alpha|\Psi(\alpha)\rangle$$

e.g., the Gutzwiller WF

Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963)

$$|\Psi(\alpha)\rangle = \exp(\alpha D)|FS\rangle$$

$$\frac{\delta}{\delta\alpha}|\Psi(\alpha)\rangle = D|\Psi(\alpha)\rangle$$

$$\frac{\delta E(\alpha)}{\delta\alpha} = 0 \Longrightarrow \langle\mathcal{H}\Theta_\alpha\rangle - \langle\mathcal{H}\rangle\langle\Theta_\alpha\rangle = 0$$

The same as the exact result $\Longrightarrow$ accuracy on the operator Θ_α

- 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:

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

$$c_{i,\uparrow} c_{i,\downarrow} = 0$$

- 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

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

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 → gapped spin liquid
- Gapless energy spectrum → gapless spin liquid

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

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

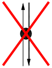
- Finite h → magnetic order

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

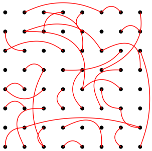
  Sorella, Capriotti, Becca, and Parola, Phys. Rev. Lett. **91**, 257005 (2003)

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

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

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

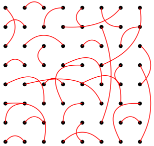
It is a linear superposition of all singlet configurations (that may overlap)



$+ \ldots$

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

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



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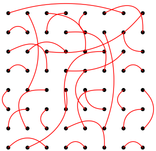

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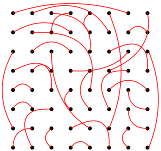


$+ \ldots$

Going to the excitation spectrum

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

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

After a Bogoliubov transformation:

$$\mathcal{H}_{\rm MF} = \sum_k (E_k \psi^\dagger_k \psi_k - E_k \phi^\dagger_k \phi_k)$$

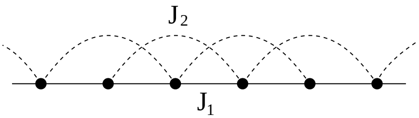
The ground state is:

$$|\Phi^0_{\rm MF}\rangle = \prod_k \phi^\dagger_k |0\rangle$$

Excited states are obtained by:

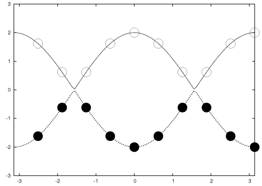
$$\phi_{q_1} \dots \phi_{q_n} \psi^\dagger_{p_1} \dots \psi^\dagger_{p_m} |\Phi^0_{\rm MF}\rangle$$

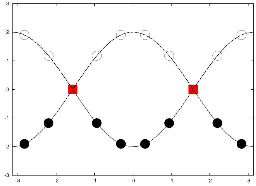
Gapless and gapped states in one dimension



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





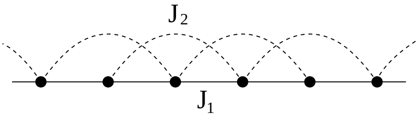
For $N = 30$

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

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

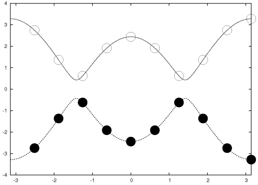
$E_{var}^{APBC,S=0} = -0.43578$ $\quad E_{ex}^{S=0} = -0.43652$ $\quad \langle \Psi_{var}^{APBC,S=0} | \Psi_{ex}^{S=0} \rangle = 0.993$

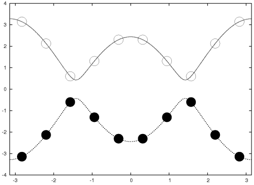
Gapless and gapped states in one dimension



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 $N = 30$

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

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

Gapless and gapped states in one dimension

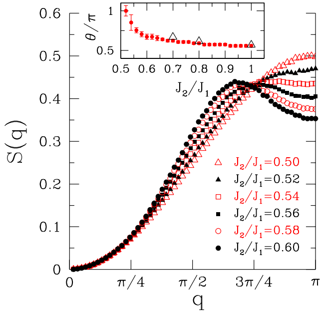
- Spin-spin correlations:

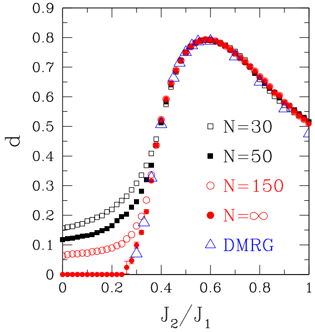
$$S(q) = \frac{1}{N} \sum_{R,R'} e^{iq(R-R')} \langle S^z_R S^z_{R'} \rangle$$

- 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 $p = 2$

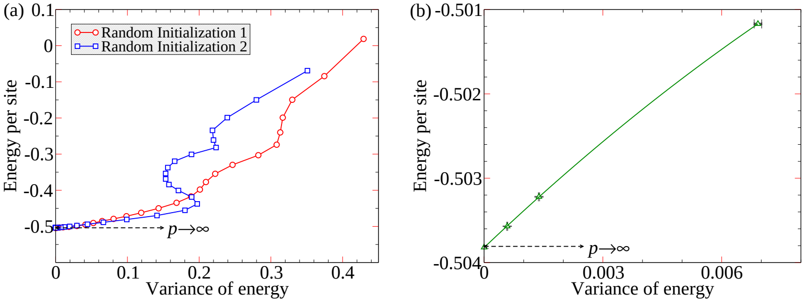
- A zero-variance extrapolation can be done

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?



The Heisenberg model with only J_1

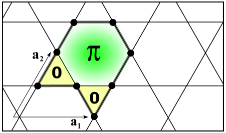
- A variational ansatz with only hopping but non-trivial fluxes has been proposed ($\chi_{ij} = \pm 1$)

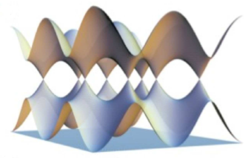
$$\mathcal{H}_{\rm MF} = \sum_{i,j,\alpha} \chi_{ij} c^{\dagger}_{i,\alpha} c_{j,\alpha}$$

- 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)



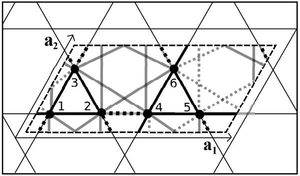


- The uniform RVB state with $\chi_{ij} = 1$ has a much worse variational energy

Projective symmetry-group analysis

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

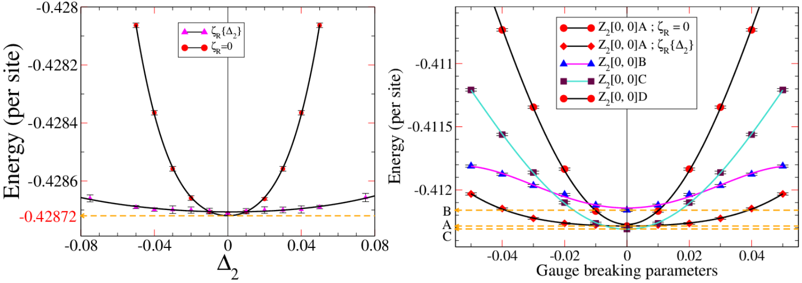
$$u_{ij} = \begin{pmatrix} \chi^*_{ij} & \Delta_{ij} \\ \Delta^*_{ij} & -\chi_{ij} \end{pmatrix}$$



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

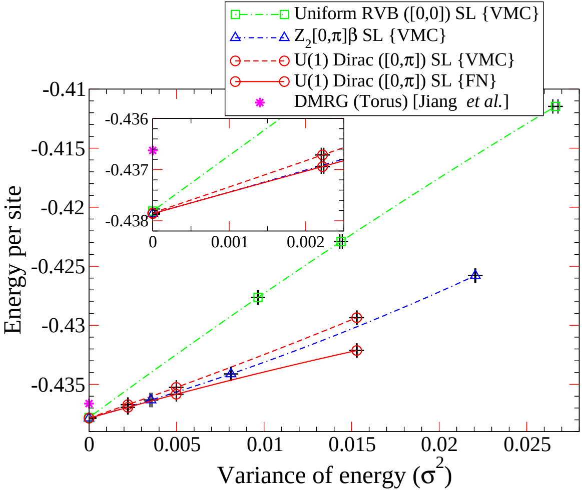
- Only one gapped SL connected with the U(1) Dirac state, called $Z_2[0,\pi]\beta$
- Four gapped SL connected with the Uniform RVB

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



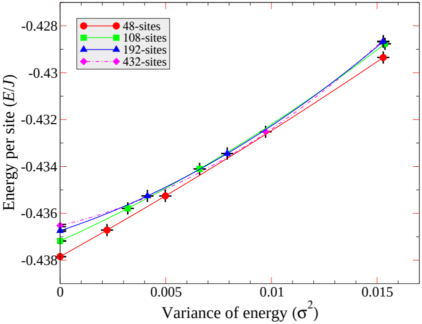
- Both the Uniform RVB and the U(1) Dirac states are stable against opening a gap

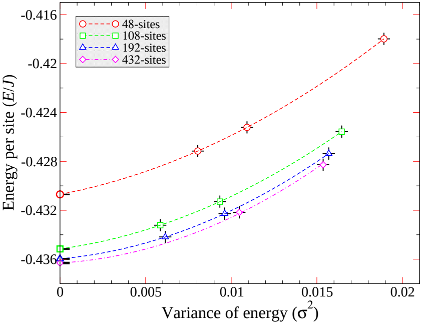
Our zero-variance extrapolation gives: $E/J_1 \simeq -0.4378$



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

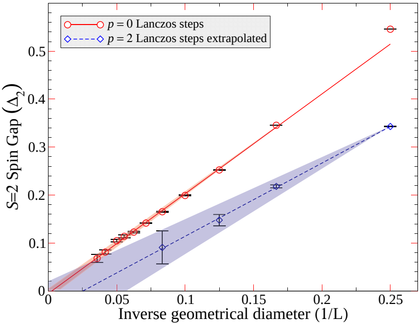
The Lanczos step extrapolations





- 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

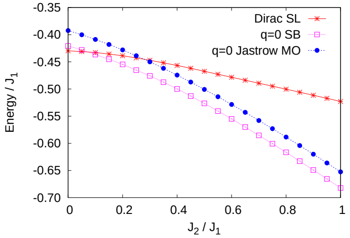
More similar to recent calculations by Nishimoto *et al.* $\Delta_1 = 0.05 \pm 0.02$

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

Energies for $J_2 > 0$: comparison with the $q = 0$ magnetic state

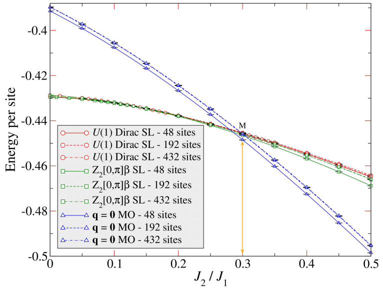
$$|\Psi_{\rm AF}\rangle = \exp\left\{\frac{1}{2}\sum_{i,j} v_{i,j} S_i^z S_j^z\right\}|{\rm AF;XY}\rangle$$

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



Small size calculations (6×6)

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

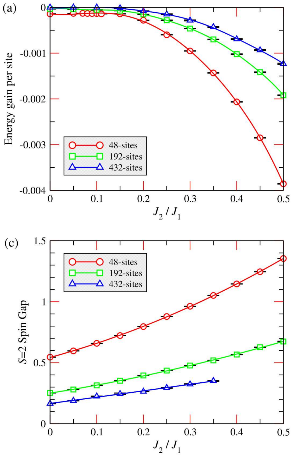


- Onset of $q = 0$ magnetic order for $J_2/J_1 > 0.3$
- Finite (tiny) energy gain of the $Z_2[0,\pi]\beta$ state over the U(1) Dirac state

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



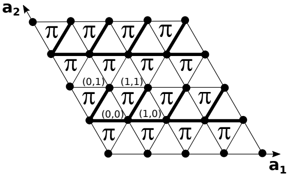
The $J_1 - J_2$ Heisenberg model

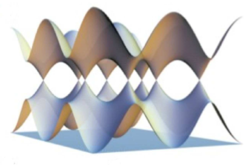
- As for the kagome lattice, one can define an ansatz with non-trivial fluxes ($\chi_{ij} = \pm 1$)

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

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

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





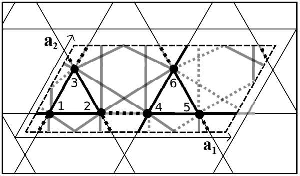
- The uniform RVB state with $\chi_{ij} = 1$ has a much worse variational energy

Projective symmetry-group analysis

Zheng, Mei, and Qi, arXiv:1505.05351

Lu, arXiv:1505.06495

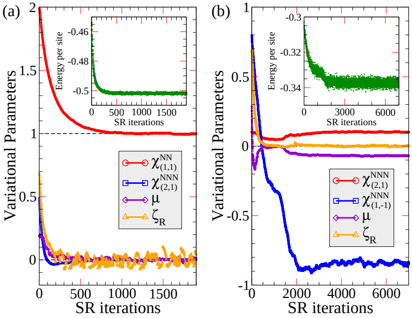
$$u_{ij} = \begin{pmatrix} \chi_{ij}^* & \Delta_{ij} \\ \Delta_{ij}^* & -\chi_{ij} \end{pmatrix}$$



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)?

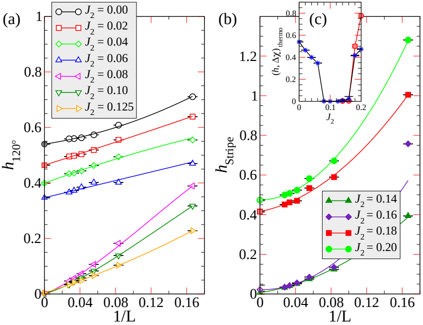


- The Number 20 is unstable and flows back to the U(1) Dirac state
- The Number 6 is stable but has a much higher energy
- Also Number 1 has a much higher energy

Magnetic states

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

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



For $J_2 = 0$:

The thermodynamic energy is (best variational ever!)

$E/J_1 = -0.54534(1)$

$E_{DMRG}/J_1 \simeq -0.544$

Gong and Hu (private communication)

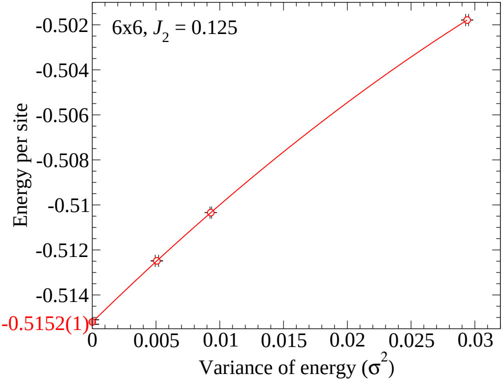
Difficult extrapolation

$E_{GFMCSR}/J_1 = -0.545(1)$

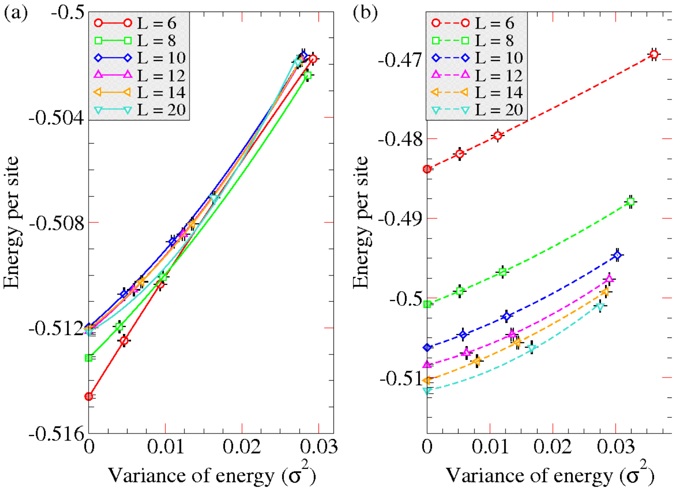
Yunoki and Sorella, Phys. Rev. B **74**, 014408 (2006)

Calculations on the 36-site cluster

Our zero-variance extrapolation gives for $J_2/J_1 = 0.125$: $E/J_1 \simeq -0.5152$



$E/J_1 \simeq -0.51556$ by ED

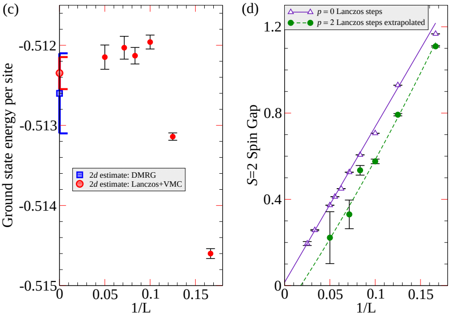


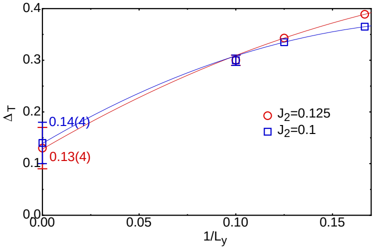
- We separately extrapolate both $S = 0$ and $S = 2$ energies
- Then the gap (zero-variance) gap is computed

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

- The ground-state energy is better than previous variational calculations $E/J_1 = -0.5031(1)$

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





Gong and Hu (private communication)

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

Conclusions?

- Good news:

  1) Some evidence of spin liquids in "realistic" spin models
  2) Discrepancies between DMRG and variational states decrease with time

- Bad news:

  1) Disagreement about the spin gap
  2) Why is the "spin liquid" region always so small?

- Future steps?

  From the DMRG side:

  Improve calculations for different topological sectors
  Improve the extrapolations with L_y

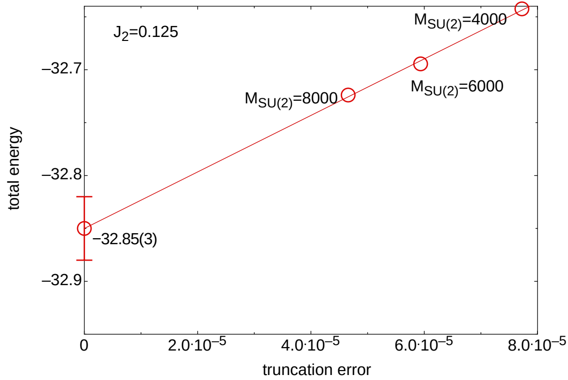
  From the VMC side:

  More Lanczos steps
  Improve the variational state (Backflow correlations)

  Tocchio, Becca, Parola, and Sorella, Phys. Rev. B **78**, 041101 (2008)

  Tocchio, Becca, and Gros, Phys. Rev. B **83**, 195138 (2011)

- Calculations on the 8×8 torus

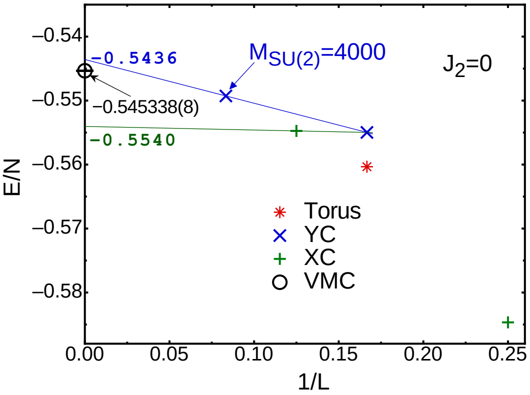


$$E_{DMRG}/J_1 = -0.5133(5)$$

Gong and Hu (private communication)

$$E_{ZVE}/J_1 = -0.5131(2)$$

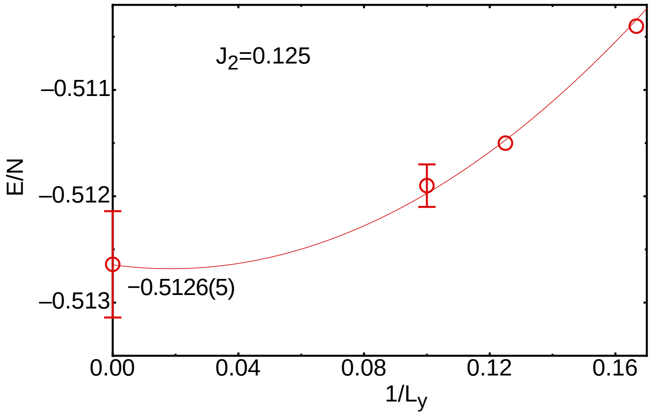
- Extrapolation for $J_2 = 0$



Gong and Hu (private communication)

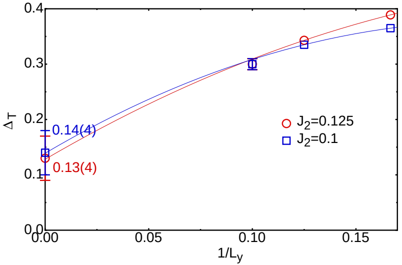
Some DMRG results on the triangular lattice

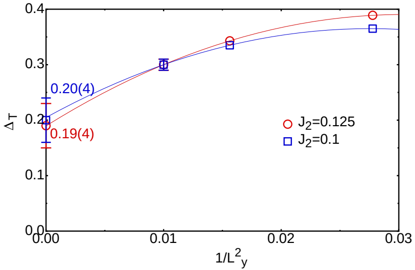
- Extrapolations for $J_2/J_1 = 0.125$



Gong and Hu (private communication)

- Extrapolations for the $S = 1$ spin gap





Gong and Hu (private communication)