A variational Monte Carlo approach for triplet and singlet low-energy states in frustrated magnets

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Entanglement in Strongly Correlated Systems, February 2020

UNIVERSITÀ
DEGLI STUDI DI TRIESTE

F. Ferrari, A. Parola, S. Sorella, and FB, Phys. Rev. B **97**, 235103 (2018)

F. Ferrari and FB, Phys. Rev. B **98**, 100405 (2018)

F. Ferrari and FB, unpublished

1. Motivations

2. Variational wave functions for spin models
   - "Old" approach for the ground state
   - "New" approach for excited states

3. Results
   - One-dimensional $J_1 - J_2$ model
   - Two-dimensional $J_1 - J_2$ Heisenberg model
   - The Heisenberg model on the kagome lattice (very preliminary)

4. Conclusions

Feynman construction for sound-waves and rotons in liquid Helium
single-mode approximation (SMA)

$$|\Psi_k\rangle = n_k |\Upsilon_0\rangle \qquad n_k = \frac{1}{\sqrt{L}} \sum_R e^{ikR} n_R$$

R.P. Feynman, *Statistical Mechanics*

A low-energy state is approximated by acting on the ground state with a simple operator

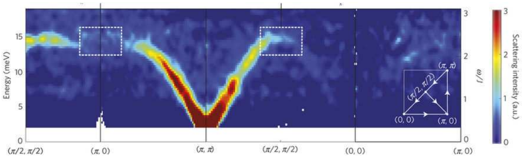
- Here, we focus on spin (Heisenberg) models on frustrated 1D and 2D lattices
- We want to do more than the SMA and assess the dynamical structure factor

$$S^a(q,\omega) = \sum_\alpha |\langle \Upsilon^q_\alpha | S^a_q | \Upsilon_0 \rangle|^2 \delta(\omega - E^q_\alpha + E_0),$$

$$S^a_q = \frac{1}{\sqrt{L}} \sum_R e^{iqR} S^a_R$$

- 2D Heisenberg model on the square lattice and $Cu(DCOO)_2{\cdot}4D_2O$

B. Dalla Piazza *et al.*, Nat. Phys. **11**, 62, (2015)



- QMC: Coexistence of magnons (low energy) and spinons (high energy)?

H.S., Y.Q. Qin, S. Capponi, S. Chesi, Z.Y. Meng, and A.W. Sandvik, Phys. Rev. X **7**, 041072 (2017)

- CST: attractive interaction between the spin waves

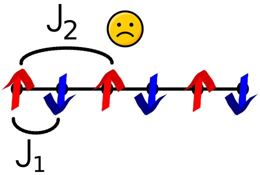
M. Powalski, K.P. Schmidt, and G.S. Uhrig, SciPost **4**, 001 (2018)

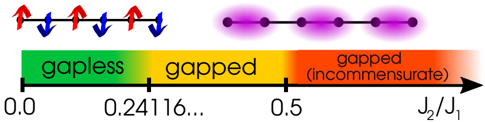
- iPEPS: proof-of-principle for the magnon dispesion

L. Vanderstraeten, J. Haegeman, and F. Verstraete, arXiv:1809.06747

- The simplest model with spin frustration in one dimension

$$\mathcal{H} = J_1 \sum_R \mathbf{S}_R \cdot \mathbf{S}_{R+1} + J_2 \sum_R \mathbf{S}_R \cdot \mathbf{S}_{R+2}$$





- Gapless phase for $J_2/J_1 < 0.241167(5)$
- Gapped (dimerized) phase for $J_2/J_1 > 0.241167(5)$
- Incommensurate spin-spin correlations for $J_2/J_1 \gtrsim 0.5$

H. Bethe, Z. Phys. **71**, 205 (1931)

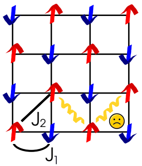
C.K. Majumdar and D.K. Ghosh, J. Math. Phys. **10**, 1388 (1969)

S.R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996)

S. Eggert, Phys. Rev. B **54**, 9612 (1996)

- The simplest model on the square lattice

$$\mathcal{H} = J_1 \sum_{\langle R,R' \rangle} \mathbf{S}_R \cdot \mathbf{S}_{R'} + J_2 \sum_{\langle\langle R,R' \rangle\rangle} \mathbf{S}_R \cdot \mathbf{S}_{R'}$$



- Infinitely many papers with partially contradictory results

S.-S. Gong *et al.*, Phys. Rev. Lett. **113**, 027201 (2014)

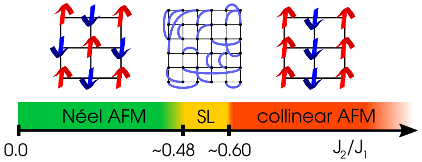
L. Wang *et al.*, Phys. Rev. B **94**, 075143 (2016)

D. Poilblanc and M. Mambrini, Phys. Rev. B **96**, 014414 (2017)

R. Haghshenas and D.N. Sheng, Phys. Rev. B **97**, 174408 (2018)

L. Wang and A.W. Sandvik, Phys. Rev. Lett. **121**, 107202 (2018)

- Possibly, a gapless spin liquid (SL) emerges between two AF phases



W.-J. Hu *et al.*, Phys. Rev. B **88**, 060402 (2013)

- **In 1D, the transition is located by looking at the singlet-triplet crossing**

K. Okamoto and K. Nomura, Phys. Lett. A **169**, 443 (1992)

G. Castilla, S. Chakravarty, and V.J. Emery, Phys. Rev. Lett. **75**, 1823 (1995)

- In the gapless region, the lowest-energy state is a triplet
- In the gapped region, the lowest-energy state is a singlet
- A the transition, the umklapp scattering vanishes and they are degenerate

The transition can be precisely located by exact calculations on small sizes ($L \approx 20$). Here, $\alpha = J_2/J_1$

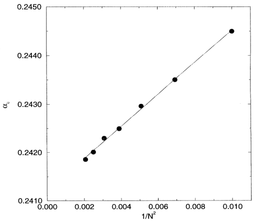


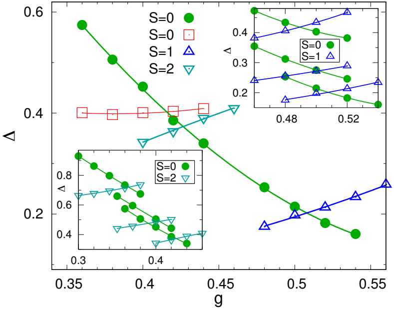
FIG. 1. $\alpha_c(N)$ vs $1/N^2$. The linear fit gives the intercept $\alpha_c = 0.2412$.

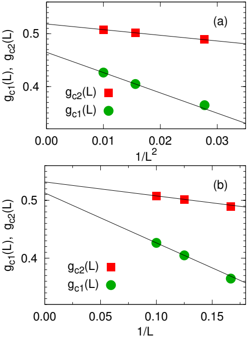
- **The best calculation gives $J_2/J_1 = 0.241167(5)$**

S. Eggert, Phys. Rev. B **54**, 9612 (1996)

- **In 2D, recent DMRG calculations highlighted a couple of level crossings**
  (on a cylinder geometry $2L \times L$ with $L = 6$, 8, and 10. Here $g = J_2/J_1$)

L. Wang and A.W. Sandvik, Phys. Rev. Lett. **121**, 107202 (2018)





- The singlet-quintuplet crossing corresponds to Néel to SL transition (?)
- The singlet-triplet crossing corresponds to the SL to valence-bond solid (?)

From spins to electrons...

- Consider the spin-1/2 Heisenberg model on a generic lattice

$$\mathcal{H} = \sum_{R,R'} J_{R,R'} \mathbf{S}_R \cdot \mathbf{S}_{R'}$$

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

$$S_R^a = \frac{1}{2} c_{R,\alpha}^\dagger \sigma_{\alpha,\beta}^a c_{R,\beta}$$

SU(2) gauge redundancy
e.g., $c_{R,\beta} \to e^{i\theta_R} c_{R,\beta}$

- The spin model is transformed into a purely interacting electronic system

$$\mathcal{H} = \sum_{R,R'} J_{R,R'} \sum_{\sigma,\sigma'} \left(\sigma\sigma' c_{R,\sigma}^\dagger c_{R,\sigma} c_{R',\sigma'}^\dagger c_{R',\sigma'} + \frac{1}{2} \delta_{\sigma',\bar{\sigma}} c_{R,\sigma}^\dagger c_{R,\sigma'} c_{R',\sigma'}^\dagger c_{R',\sigma} \right)$$

- One spin per site $\to$ we must impose the constraint

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

- The SU(2) symmetric mean-field approximation gives a BCS-like form

$$\mathcal{H}_0 = \sum_{R,R',\sigma} t_{R,R'} c^\dagger_{R,\sigma} c_{R',\sigma} + \sum_{R,R'} \Delta_{R,R'} c^\dagger_{R,\uparrow} c^\dagger_{R',\downarrow} + h.c.$$

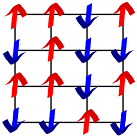
$\{t_{R,R'}\}$ and $\{\Delta_{R,R'}\}$ define the mean-field Ansatz $\longrightarrow$ BCS spectrum $\{\epsilon_\alpha\}$

The constraint is no longer satisfied locally (only on average)

- The constraint can be inserted by the Gutzwiller projector $\rightarrow$ **RVB**

$$|\Psi_0\rangle = \mathcal{P}_G |\Phi_0\rangle$$

$$\mathcal{P}_G = \prod_R (n_{R,\uparrow} - n_{R,\downarrow})^2$$



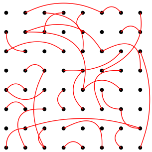
- The exact projection can be treated within the variational Monte Carlo approach

F. Becca and S. Sorella, *Quantum Monte Carlo Approaches for Correlated Systems*

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

$$|\Phi_0\rangle = \exp\left\{\sum_{i,j} f_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}\right\} |0\rangle = \left[1 + \sum_{i,j} f_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + \frac{1}{2}\left(\sum_{i,j} f_{i,j} c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow}\right)^2 + \dots\right] |0\rangle$$

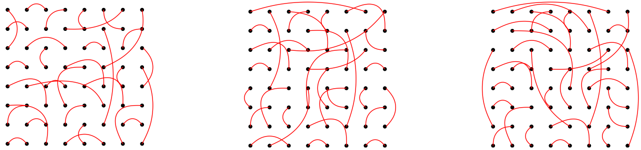
It is a linear superposition of all singlet configurations (that may overlap)



$+ \dots$

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

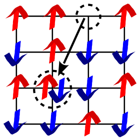
P.W. Anderson, Science **235**, 1196 (1987)



$+ \dots$

- For each momentum q a set of (two-spinon) states is defined

$$|q,R,\mathrm{trip}\rangle = \mathcal{P}_G \frac{1}{\sqrt{L}} \sum_{R'} e^{iqR'} (c^\dagger_{R+R',\uparrow} c_{R',\uparrow} - c^\dagger_{R+R',\downarrow} c_{R',\downarrow}) |\Phi_0\rangle$$



$$|q,R,\mathrm{sing}\rangle = \mathcal{P}_G \frac{1}{\sqrt{L}} \sum_{R'} e^{iqR'} (c^\dagger_{R+R',\uparrow} c_{R',\uparrow} + c^\dagger_{R+R',\downarrow} c_{R',\downarrow}) |\Phi_0\rangle$$

- The spin Hamiltonian is diagonalized within this (non-orthogonal) basis set

$$\sum_{R'} H^q_{R,R'} A^{n,q}_{R'} = E^q_n \sum_{R'} O^q_{R,R'} A^{n,q}_{R'}$$

$$H^q_{R,R'} = \langle q,R,\mathrm{trip}|\mathcal{H}|q,R',\mathrm{trip}\rangle \qquad O^q_{R,R'} = \langle q,R,\mathrm{trip}|q,R',\mathrm{trip}\rangle$$

or

$$H^q_{R,R'} = \langle q,R,\mathrm{sing}|\mathcal{H}|q,R',\mathrm{sing}\rangle \qquad O^q_{R,R'} = \langle q,R,\mathrm{sing}|q,R',\mathrm{sing}\rangle$$

Dynamical variational Monte Carlo

- The Matrix elements are computed within standard variational Monte Carlo

  T. Li and F. Yang, Phys. Rev. B **81**, 214509 (2010)

  (Slightly different because states have $S^z = 0$)

- The generic "eigenstate" of the Hamiltonian is

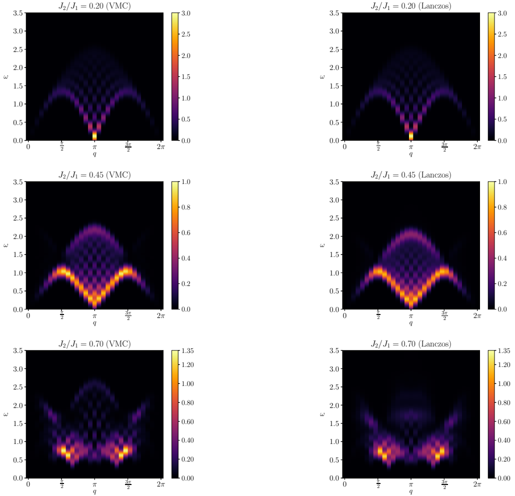
$$|\Psi_n^q\rangle = \sum_R A_R^{n,q} |q, R\rangle$$

- By using triplet states, the dynamical structure factor is approximated by

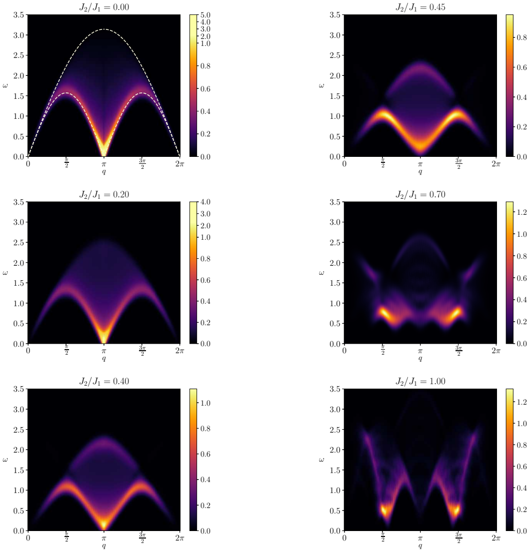
$$S^z(q,\omega) = \sum_n \left| \sum_R (A_R^{n,q})^* O_{R,0}^q \right|^2 \delta(\omega - E_n^q + E_0)$$

At most L states for each momentum q

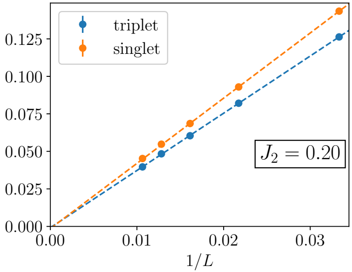
The dynamical structure factor

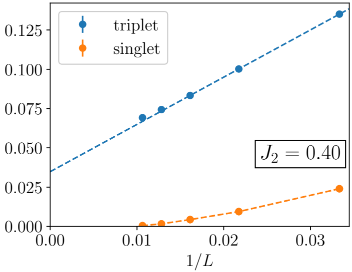


One-dimensional $J_1 - J_2$ model: Results on 198 sites



One-dimensional $J_1 - J_2$ model: level crossing





- **For small J_2/J_1**

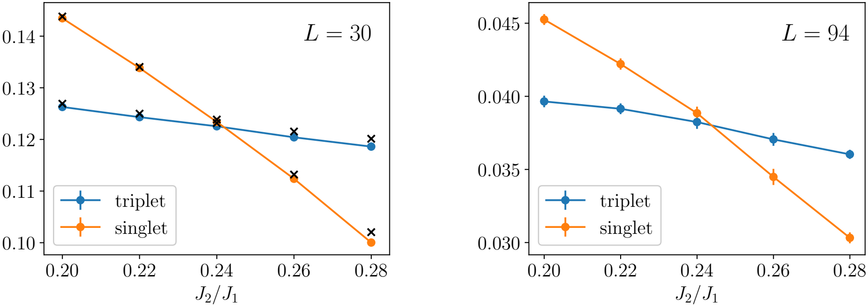
  The triplet is lower than the singlet

  Both excitations are gapless in the thermodynamic limit

- **For large J_2/J_1**

  The singlet is lower than the triplet

  The triplet is gapped, the singlet is degenerate with the ground state



The level crossing comes out to be quite accurate

- For a non-magnetic (spin liquid or valence-bond solid) state

$$\boxed{|\Psi_0\rangle = \mathcal{P}_G|\Phi_0\rangle}$$

$$\mathcal{H}_0 = \sum_{R,R',\sigma} t_{R,R'} c^\dagger_{R,\sigma} c_{R',\sigma} + \sum_{R,R'} \Delta_{R,R'} c^\dagger_{R,\uparrow} c^\dagger_{R',\downarrow} + h.c.$$

- For an antiferromagnetic state

$$\boxed{|\Psi_0\rangle = \mathcal{P}_{S_z}\mathcal{J}\mathcal{P}_G|\Phi_0\rangle}$$

$$\mathcal{H}_0 = \sum_{R,R',\sigma} t_{R,R'} c^\dagger_{R,\sigma} c_{R',\sigma} + \Delta_{\mathrm{AF}} \sum_{R} e^{iQR} \left(c^\dagger_{R,\uparrow} c_{R,\downarrow} + c^\dagger_{R,\downarrow} c_{R,\uparrow}\right)$$

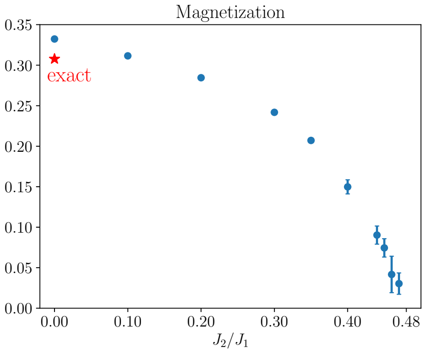
The magnetic moment in the $x - y$ plane (because of $\mathcal{P}_{S_z}$)

$\mathcal{J} = \exp\left(\frac{1}{2}\sum_{R,R'} v_{R,R'} S^z_R S^z_{R'}\right)$ is the spin-spin Jastrow factor

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

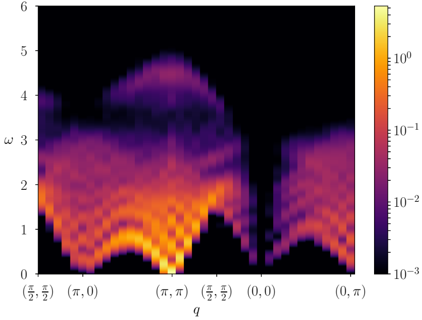
$$m^2 = \lim_{r \to \infty} \langle \mathbf{S}_r \cdot \mathbf{S}_0 \rangle$$

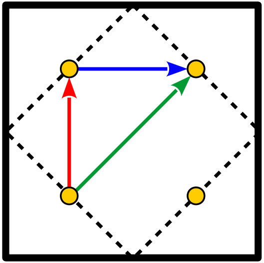
- Magnetization computed for finite clusters from 10×10 to 22×22



- NN hopping t (staggered flux phase), no pairing
- A finite staggered magnetization is related to a finite Δ_{AF} in the wave function

The spin-liquid phase with $J_2/J_1 = 0.55$





A $\mathbb{Z}_2$ gapless spin liquid

- NN hopping t (staggered flux phase) and $\Delta(k) = \Delta_{xy} \sin(2k_x) \sin(2k_y)$
- Gapless excitations at $q = (0, 0)$, (π, π), $(\pi, 0)$, and $(0, \pi)$.

- On finite sizes the gapless points can be avoided by suitable boundary conditions
- Let us fix $L_y = 6$ and perform $L_x \to \infty$

With PBC along y, Dirac points are always avoided (**gapped spectrum**)

$$E_0/J_1 = -0.48655(1)$$

With APBC along y, Dirac points are avoided for

1) $L_x = 4n$ and APBC along x

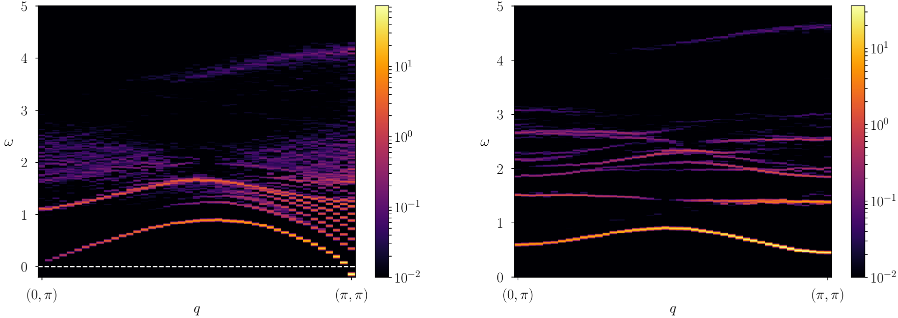
2) $L_x = 4n + 2$ and PBC along x

Dirac points are reached for $L_x \to \infty$ (**gapless spectrum**)

$$E_0/J_1 = -0.47543(1)$$

The gapped wave function has a lower energy than the gapless one!

Dynamical structure factor for gapless/gapped states



- The gapped state gives a gapped spectrum (stable)
- The gapless state gives "antivariational" excited states (unstable)
  (still much higher in energy than the gapped wave function)

Two-dimensional $J_1 - J_2$ model: level crossing

- On 6×6 for $J_2/J_1 = 0.5$:

  Ground-state accuracy 0.005% ($E_{ex}/J_1 = -0.50381$ vs $E_{var}/J_1 = -0.50116$)

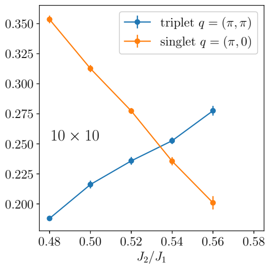
  Triplet-state accuracy 0.007% ($E_{ex}/J_1 = -0.49072$ vs $E_{var}/J_1 = -0.48706$)

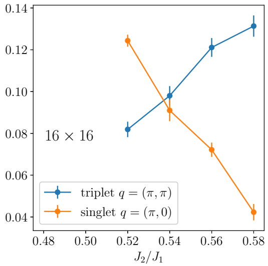
  Singlet-state accuracy 0.014% ($E_{ex}/J_1 = -0.49054$ vs $E_{var}/J_1 = -0.48375$)

  Triplet gap $\Delta_{\rm ex}/J_1 = 0.471$ vs $\Delta_{\rm var}/J_1 = 0.508$

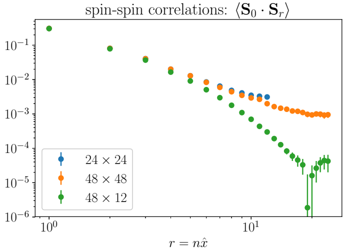
  Singlet gap $\Delta_{\rm ex}/J_1 = 0.477$ vs $\Delta_{\rm var}/J_1 = 0.627$

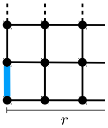
- On larger clusters:

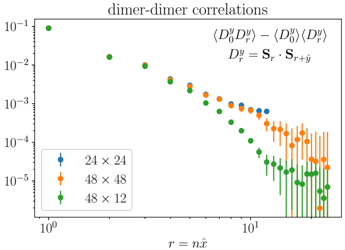


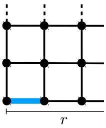


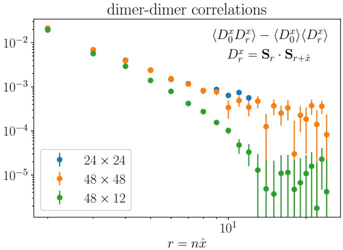
Two-dimensional $J_1 - J_2$ model: correlation functions







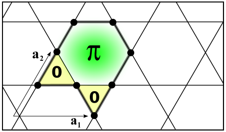


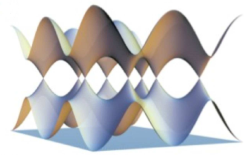


$$\mathcal{H} = J \sum_{\langle R,R' \rangle} \mathbf{S}_R \cdot \mathbf{S}_{R'}$$

- A variational ansatz with only hopping but non-trivial fluxes has been proposed

$$\mathcal{H}_0 = \sum_{R,R',\sigma} t_{R,R'} c^\dagger_{R,\sigma} c_{R',\sigma}$$





Y. Ran, M. Hermele, P.A. Lee, and X.-G. Wen, Phys. Rev. Lett. **98**, 117205 (2007)

- Recently, DMRG calculations suggested the existence of Dirac points

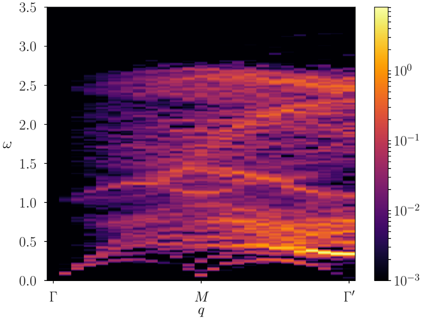
  On cylinders, a finite spin gap may exist

  By using an adiabatic flux insertion a gapless spectrum may be recovered

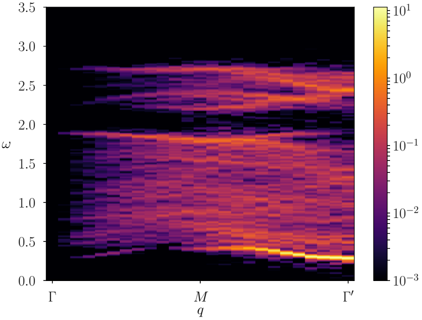
Y.-C. He, M.P. Zaletel, M. Oshikawa, and F. Pollmann, Phys. Rev. X **7**, 031020 (2017)

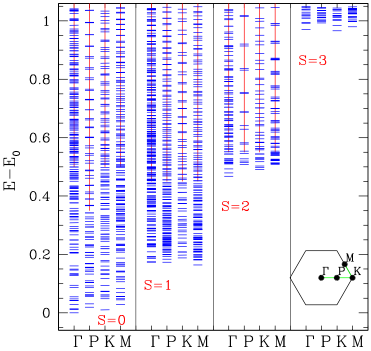
- According to boundary conditions both "gapless" and gapped states are possible ($24 \times 4 \times 3$ cluster)
- **The gapped wave function has the lowest variational energy**

Gapless: $E/J = -0.42674(1)$



Gapped: $E/J = -0.43023(1)$



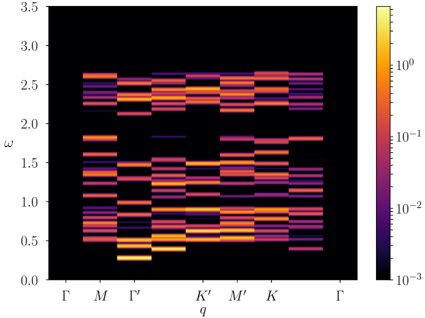


P. Lecheminant, B. Bernu, C. Lhuillier, L. Pierre, and P. Sindzingre, Phys. Rev. B **56**, 2521 (1997)

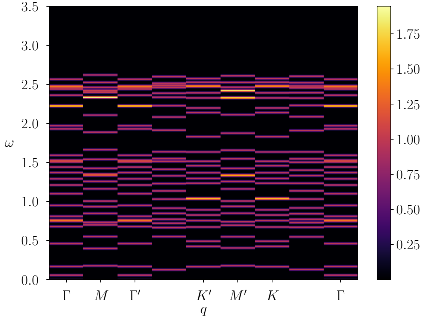
- Several (exponentially large) number of singlets below the first triplet excitation
- What is the origin? Nearest-neighbor dimer covering (short-range RVB physics)?

F. Mila, Phys. Rev. Lett. **81**, 2356 (1998)

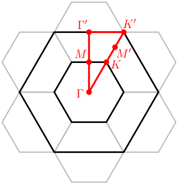
Dynamical structure factor (triplets)



Density of states (singlets)

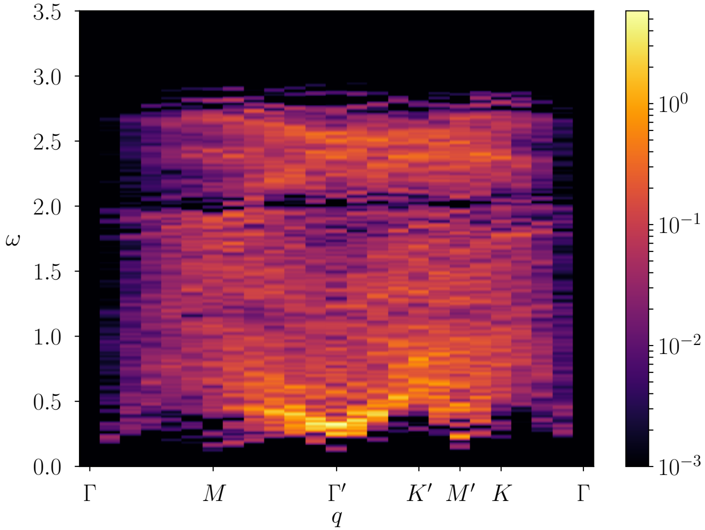


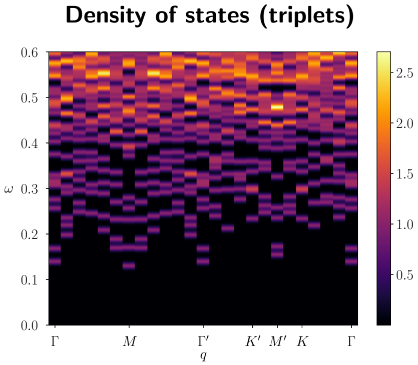
- **Quite flat triplet dispersion**
- **Several singlets below the triplets**
- **Singlet and triplet gaps overestimated**
- **Are we capturing the actual low-energy states?**

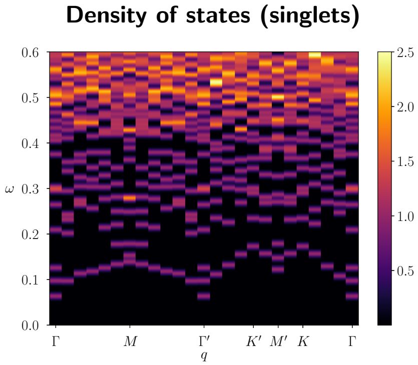


A. Lauchli and C. Lhuillier, arXiv:0901.1065

THE 12×12 CLUSTER: DYNAMICAL STRUCTURE FACTOR




Density of states (triplets)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
ω
Γ
M
Γ′
K′
M′
K
Γ
q
2.5
2.0
1.5
1.0
0.5


Density of states (singlets)
0.6
0.5
0.4
0.3
0.2
0.1
0.0
ω
Γ
M
Γ′
K′
M′
K
Γ
q
2.5
2.0
1.5
1.0
0.5

PROS

- Monte Carlo sampling with no sign problem
- No analytic continuation is required (see below)
- Transparent interpretation in terms of spinon excitations
- Particularly suited to study the spreading (delocalization) of magnons
  Excellent for systems with free (or nearly-free) spinons

CONS

- No analytic continuation is required (see above)
  For each momentum, a set of delta functions are obtained
  Difficult to distinguish between real poles (magnons) and continuum
- For the kagome lattice: is it a quantitative or qualitative problem?
  Are low-energy singlet (and triplet) states only due to nearly-free spinons?