Spectral signatures of fractionalization in the frustrated Heisenberg model on the square lattice

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

Topological phases of matter: from the quantum Hall effect to spin liquids

Istituto Officina dei Materiali

F. Ferrari, S. Sorella (SISSA, Trieste), and A. Parola (University of Insubria, Como)

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

F. Ferrari and FB, arXiv preprint arXiv:1805.09287

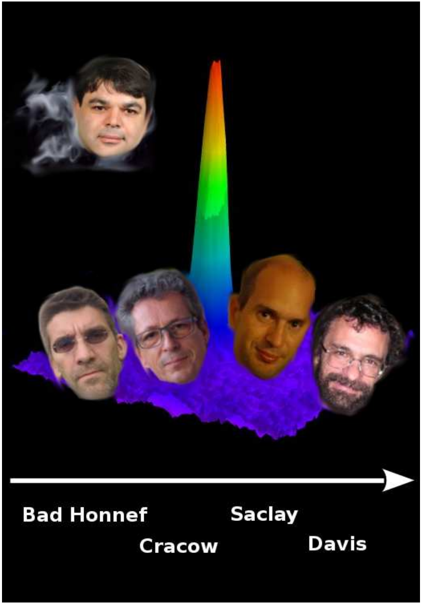
1. Motivations

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
   - Towards two dimensions: the (unfrustrated) anisotropic Heisenberg model
   - Two-dimensional $J_1 - J_2$ Heisenberg model

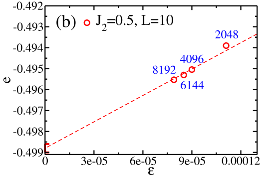
4. Conclusions

Apologise to people who have already seen this talk

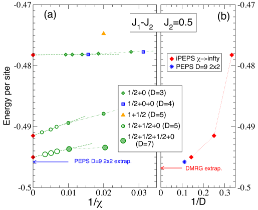


Brute-force approaches, e.g., DMRG or tensor networks

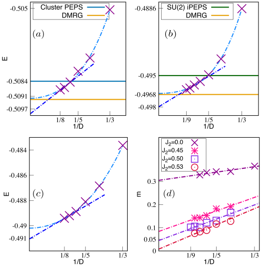
Educated guesses based on "traditional" Jastrow-Slater wave functions



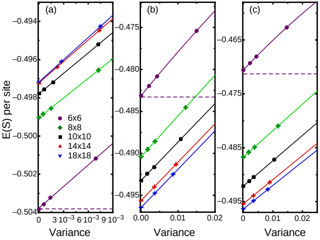
S.-S. Gong *et al.*, Phys. Rev. Lett. **113**, 027201 (2014)



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



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



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

From the ground state to the excitation spectra

- Low-energy excitations could be obtained by **independent** calculations

Is it possible to describe excitations by acting on the ground-state wave function?

- Mean-field approaches (trivial)

$$|\Phi_k\rangle = \prod_i c^\dagger_{k_i} \prod_j c_{k_j} |\Upsilon_0\rangle \qquad k = \sum_i k_i - \sum_j k_j$$

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

R.P. Feynman, *Statistical Mechanics*

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

- Composite-fermion approach for the fractional quantum Hall effect

J. Jain, *Composite Fermions*

$$\Psi^\alpha_\nu = \mathcal{P}_{\rm LLL} \prod_{i<j} (z_i - z_j)^{2p} \Phi^\alpha_{\nu^*}$$

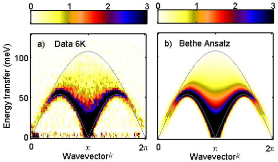
The dynamical spin structure factor

$$S^a(q,\omega) = \sum_\alpha |\langle \Upsilon_\alpha^q | S_q^a | \Upsilon_0 \rangle|^2 \delta(\omega - E_\alpha^q + E_0),$$

$$S_q^a = \frac{1}{\sqrt{L}} \sum_R e^{iqR} S_R^a$$

- 1D Heisenberg model and $KCuF_3$

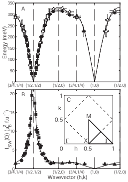
  B. Lake *et al.*, PRL **111**, 137205 (2013)

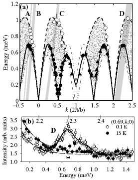


- 2D Heisenberg model
  for La_2CuO_4 and Cs_2CuCl_4

  R. Coldea *et al.*, Phys. Rev. Lett. **86**, 1335 (2001)

  R. Coldea *et al.*, Phys. Rev. Lett. **86**, 5377 (2001)





Theoretical attempts to evaluate the dynamical structure factor

- Magnons and multi-magnon decay in ordered antiferromagnets

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

M.E. Zhitomirsky and A.L. Chernyshev, Rev. Mod. Phys. **85**, 219 (2013)

- Fractionalization in the Kitaev and Kitaev-Heisenberg models

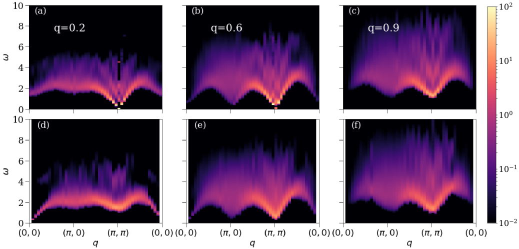
J. Knolle, D.L. Kovrizhin, J.T. Chalker, and R. Moessner, Phys. Rev. Lett. **112**, 207203 (2014)

M. Gohlke, R. Verresen, R. Moessner, and F. Pollmann, Phys. Rev. Lett. **119**, 157203 (2017)

J. Knolle, S. Bhattacharjee, and R. Moessner, Phys. Rev. B **97**, 134432 (2018)

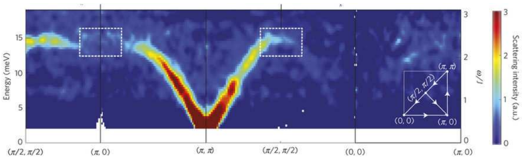
- Fractionalization at a deconfined quantum critical point (AF $\rightarrow$ VBC)

N. Ma, G.-Y. Sun, Y.-Z. You, C. Xu, A. Vishwanath, A.W. Sandvik, and Z.Y. Meng, arXiv:1803.01180

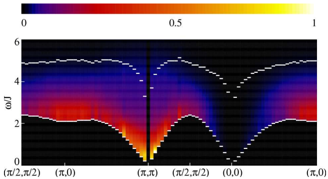


Fractionalization in ordered antiferromagnets?

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



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



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

- They claim for a coexistence of magnons (low energy) and spinons (high energy)

- 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

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

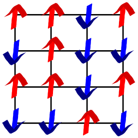
$\{t_{R,R'}\}$ and $\{\Delta_{R,R'}\}$ define the mean-field Ansatz $\longrightarrow$ BCS spectrum $\{\epsilon_\alpha\}$

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

- The constraint can be inserted by the Gutzwiller projector → **RVB**

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

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



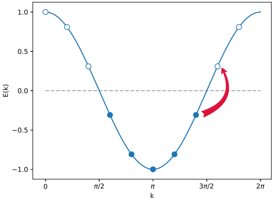
- The exact projection can be treated within the variational Monte Carlo approach

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

Gutzwiller-projected fermionic states

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

- Excitations in the electronic occupation (before Gutzwiller projection)



Spinons

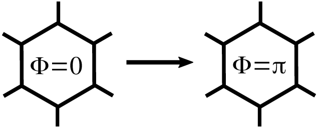
1D Haldane-Shastry model

F.D.M. Haldane, Phys. Rev. Lett. **60**, 635 (1988)

B.S. Shastry, Phys. Rev. Lett. **60**, 639 (1988)

F.D.M. Haldane, Phys. Rev. Lett. **66**, 1529 (1991)

- Modifications of the $\{t_{R,R'}\}$ and $\{\Delta_{R,R'}\}$ pattern (gauge fluctuations)



Magnetic flux/visons

2D Kitaev model

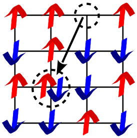
A. Kitaev, Annals of Physics **321**, 2 (2006)

visons and spinons are decoupled

mean-field is exact

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

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



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

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

- 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 $S^z = 0$)

Dynamical variational Monte Carlo

- The generic "eigenstate" of the Hamiltonian is

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

If $A_R^{n,q} = \delta_{R,0}$, on-site particle-hole excitations in $|q, R\rangle$
We obtain the the single-mode approximation (magnon)

$$|\Psi_n^q\rangle = S_q^z |\Psi_0\rangle$$

In general, $A_R^{n,q} \neq \delta_{R,0}$, non-local particle-hole excitations in $|q, R\rangle$

- The dynamical structure factor is approximated by

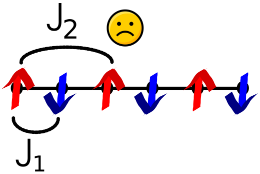
$$S^z(q,\omega) = \sum_n \left| \sum_R (A_R^{n,q})^* O_{R,0}^q \right|^2 \delta(\omega - E_n^q + E_0)$$

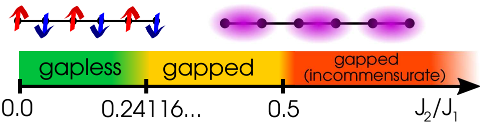
At most L states for each momentum q

The frustrated Heisenberg model in one dimension

- 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 $J_2/J_1 \gtrsim 0.5$

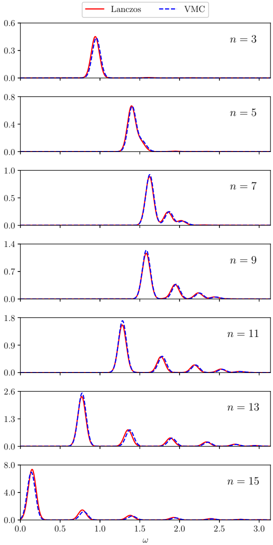
H. Bethe, Z. Phys. **71**, 205 (1931)

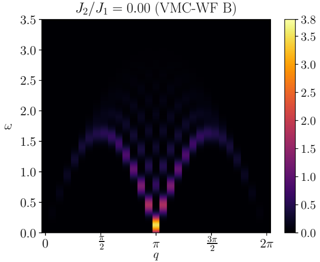
C.K. Majumdar and D.K. Ghosh, J. Math. Phys. **10**, 1388 (1969)

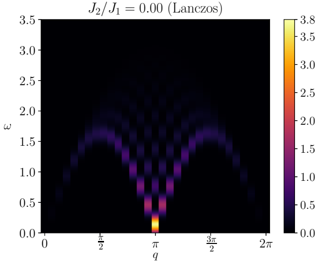
S.R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996)

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

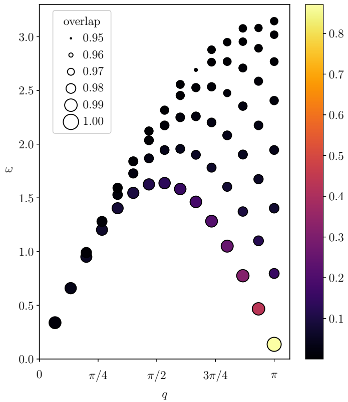
- NN hopping t_1 and both onsite Δ_0 and NNN (Δ_2) pairing
  $q = \frac{2\pi}{L} n$



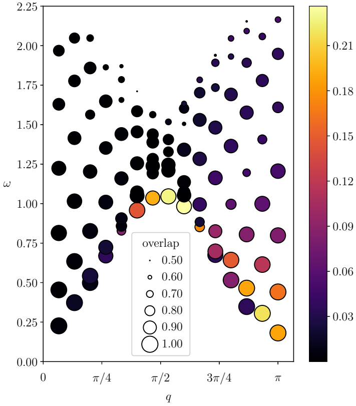




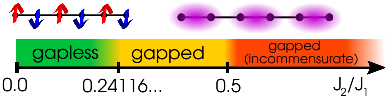
$J_2/J_1 = 0$

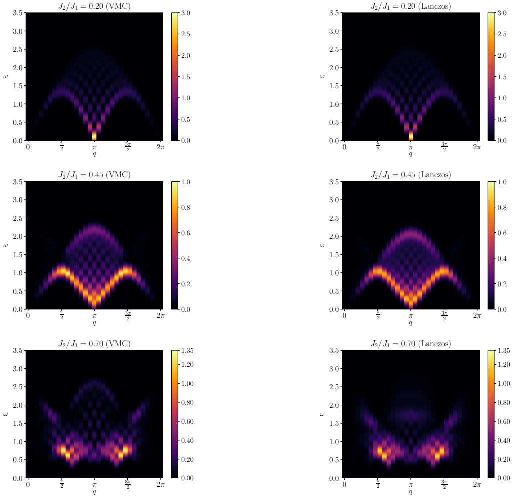


$J_2/J_1 = 0.45$

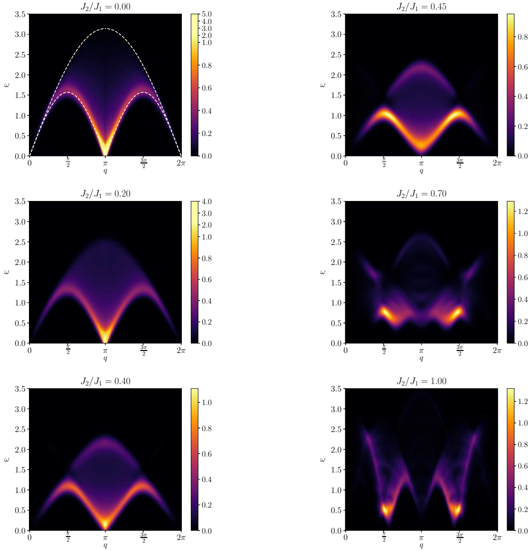


Our variational states describe spinons in 1D

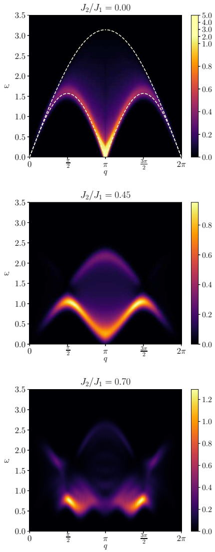

gapless
gapped
gapped (incommensurate)
0.0
0.24116...
0.5
J2/J1


$J_2/J_1 = 0.20$ (VMC)
$J_2/J_1 = 0.20$ (Lanczos)
$J_2/J_1 = 0.45$ (VMC)
$J_2/J_1 = 0.45$ (Lanczos)
$J_2/J_1 = 0.70$ (VMC)
$J_2/J_1 = 0.70$ (Lanczos)
ω
q

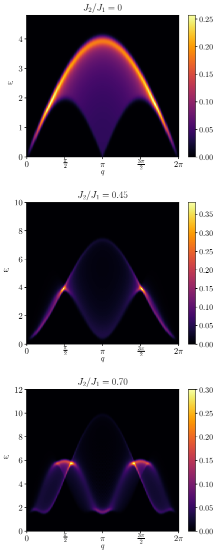
One-dimensional $J_1 - J_2$ model: Results on $L = 198$ sites



With Gutzwiller Projector



Without Gutzwiller Projector



Variational wave functions for the ground-state wave function

- 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

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

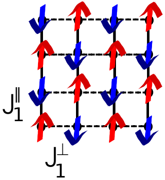
$$\mathcal{H}_0 = \sum_{R,R',\sigma} t_{R,R'} c^\dagger_{R,\sigma} c_{R',\sigma} + \Delta_{\mathrm{AF}} \sum_{R} e^{iQR} \left(c^\dagger_{R,\uparrow} c_{R,\downarrow} + c^\dagger_{R,\downarrow} c_{R,\uparrow} \right)$$

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)

- The transverse dynamical structure factor is considered

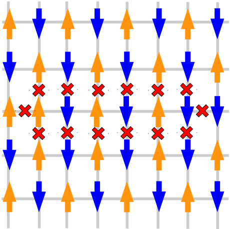


$J_{\parallel} = 1 \qquad J_{\perp} = 0, \ldots, 1$

- AF order as soon as $J_{\perp} > 0$

I. Affleck, M.P. Gelfand, and R.R.P. Singh, J. Phys. A: Math. Gen. **27**, 7313 (1994)

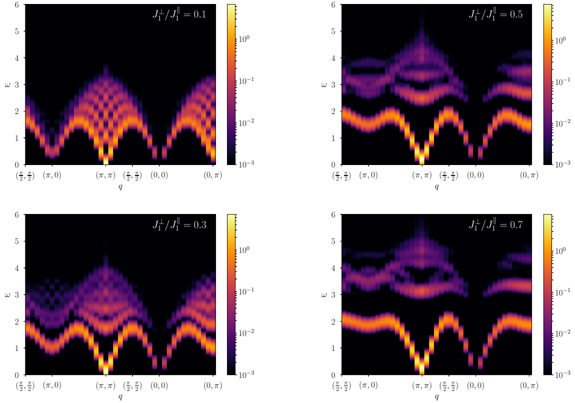
- Spinons become confined as soon as $J_{\perp} > 0$



Spinons look deconfined for $\xi > L$
Weak confinement $\approx$ deconfinement

- NN hopping t (staggered flux phase) and $\Delta_{\rm AF}$

The anisotropic Heisenberg model on the square lattice



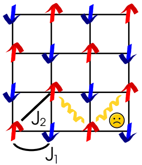
- The magnon signal acquires more weight around $q = (\pi, \pi)$
- The continuum is pushed at high energies

  Multimagnon processes are probably beyond our approach

  Our Ansatz for excitations is not good for the "low energy" continuum

- 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)

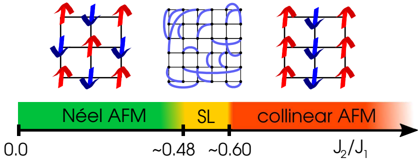
L. Wang *et al.*, Phys. Rev. B **94**, 075143 (2016)

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, arXiv:1702.08197

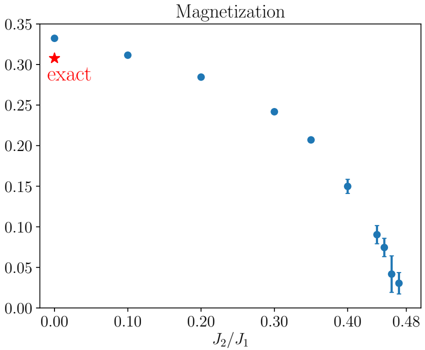
- Possibly, a gapless spin liquid (SL) emerges between two AF phases



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

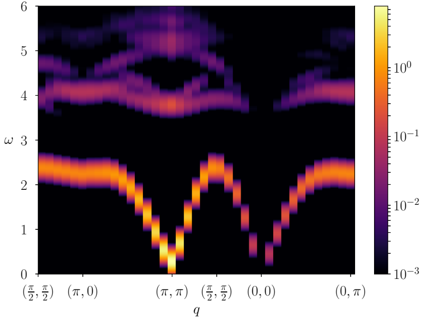
$$m^2 = \lim_{r \to \infty} \langle \mathbf{S}_r \cdot \mathbf{S}_0 \rangle$$

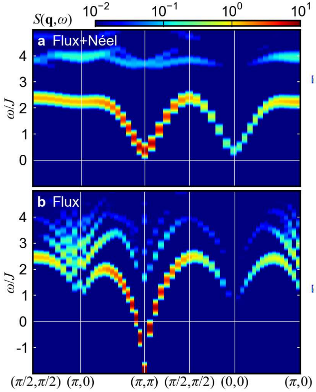
- Magnetization computed for finite clusters from 10×10 to 22×22



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

The unfrustrated Heisenberg model

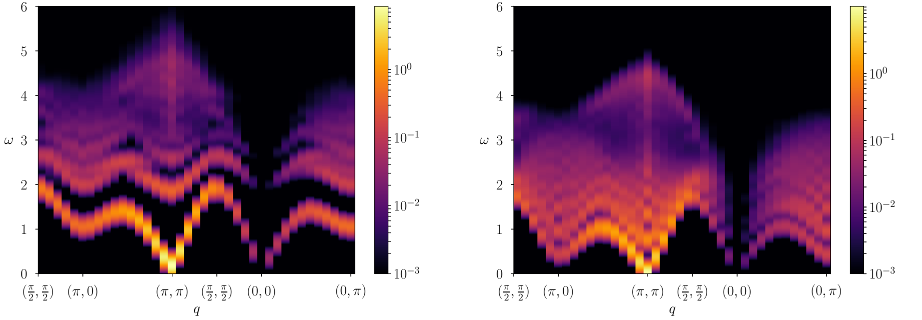




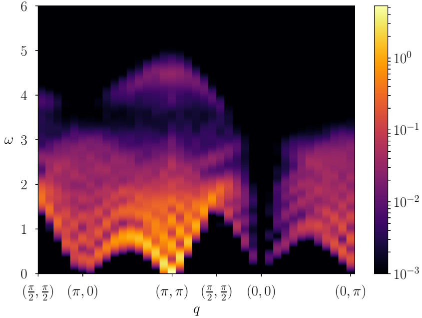
B. Dalla Piazza *et al.*, Nat. Phys. **11**, 62, (2015)

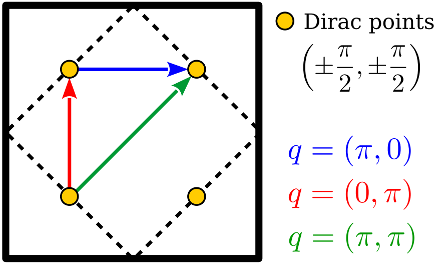
- Strong magnon branch
- Very weak (almost no) three-magnon continuum

The frustrated cases with $J_2/J_1 = 0.3$ and 0.45 (still magnetically ordered)



- The magnon signal looses its intensity around $q = (\pi, 0)$ and $(0, \pi)$
- Softening of the lowest-energy excitation at $q = (\pi, 0)$ and $(0, \pi)$
- Significant continuum above the single magnon branch



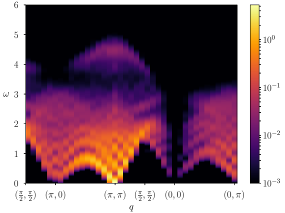


A $\mathbb{Z}_2$ gapless spin liquid

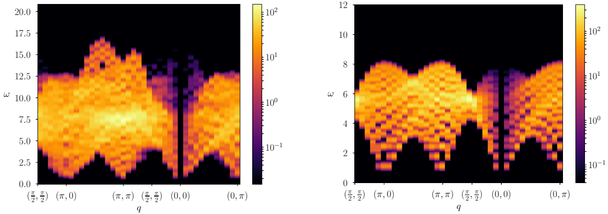
- NN hopping t (staggered flux phase) and $\Delta(k) = \Delta_{xy} \sin(2k_x) \sin(2k_y)$
- Gapless excitations at $q = (0,0)$, (π,π), $(\pi,0)$, and $(0,\pi)$.

Role of the Gutzwiller projector

With Gutzwiller Projector



Without Gutzwiller Projector



Pros and cons

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
- Other kind of excitations (visons)?
  Finite overlap thanks to the Gutzwiller projector? (Kitaev model)

A stable variational approach is possible to describe low-energy excitations

- Excellent accuracy in the 1D models with spinon excitations

  Gapless and gapped phases in the 1D $J_1 - J_2$ model

- Gradual confinement of spinons in (unfrustrated) coupled chains

  Single magnon excitation in presence of AF order

- Tendency toward spinon deconfinement in the 2D $J_1 - J_2$ model

  Gradual softening at $q = (\pi, 0)$ for AF $\longrightarrow$ SL

  Stability of a gapless $\mathbb{Z}_2$ spin liquid for $0.48 \lesssim J_2/J_1 \lesssim 0.6$

Gutzwiller-projected fermionic wave functions:
the correct framework for low-energy excitations