Dynamical structure factor of frustrated spin models: a variational Monte Carlo approach

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CNR IOM-DEMOCRITOS

International Conference on Highly Frusturated Magnetism

Istituto Officina dei Materiali

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

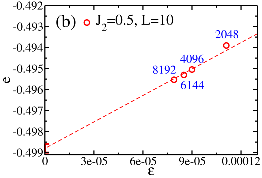
F. Ferrari, A. Parola, S. Sorella, and FB, Phys. Rev. B **97**, 235103 (2018)

F. Ferrari and FB, arXiv preprint arXiv:1805.09287

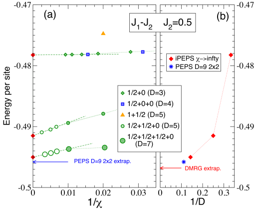
Numerical approaches for ground state properties

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

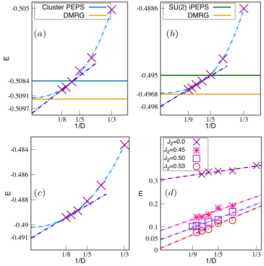
Educated guesses based on "traditional" Jastrow-Slater wave functions



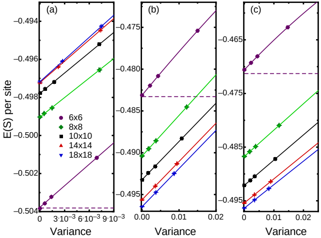
S.-S. Gong *et al.*, Phys. Rev. Lett. **113**, 027201 (2014)



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?

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

R.P. Feynman, *Statistical Mechanics*

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

- Composite-fermion approach for the fractional quantum Hall effect

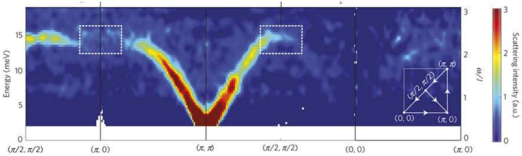
J. Jain, *Composite Fermions*

$$\Psi_\nu^\alpha = \mathcal{P}_{\mathrm{LLL}} \prod_{i<j} (z_i - z_j)^{2p} \Phi_{\nu^*}^\alpha$$

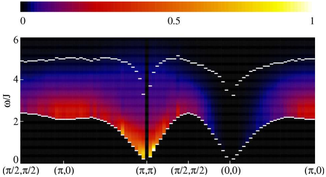
The dynamical spin structure factor

$$\boxed{S^a(q,\omega) = \sum_\alpha |\langle \Upsilon_\alpha^q | S_q^a | \Upsilon_0 \rangle|^2 \delta(\omega - E_\alpha^q + E_0),} \qquad S_q^a = \frac{1}{\sqrt{L}} \sum_R e^{iqR} S_R^a$$

- 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)

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

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

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 $\rightarrow$ we must impose the constraint

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

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

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

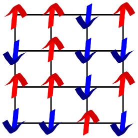
$\{t_{R,R'}\}$ and $\{\Delta_{R,R'}\}$ define the mean-field Ansatz $\longrightarrow$ BCS spectrum $\{\epsilon_\alpha\}$

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

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

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

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

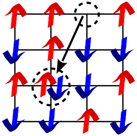


- The exact projection can be treated within the variational Monte Carlo approach

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

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

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



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

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

- The dynamical structure factor is approximated by

$$\boxed{S^z(q,\omega) = \sum_n \left| \sum_R (A^{n,q}_R)^* O^q_{R,0} \right|^2 \delta(\omega - E^q_n + E_0)}$$

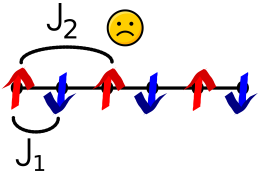
At most L states for each momentum q

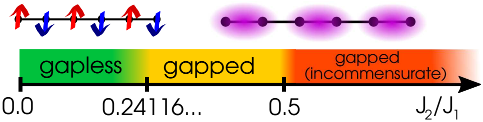
T. Li and F. Yang, Phys. Rev. B **81**, 214509 (2010)

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)

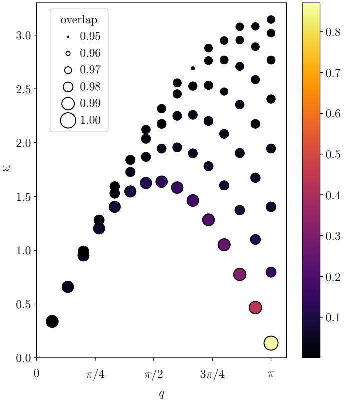
S.R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996)

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

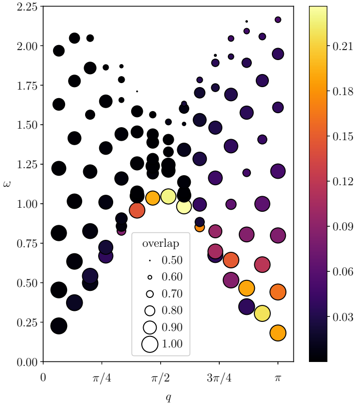
One-dimensional $J_1 - J_2$ model: A benchmark on 30-site cluster (I)

- NN hopping t_1 and both onsite Δ_0 and NNN (Δ_2) pairing

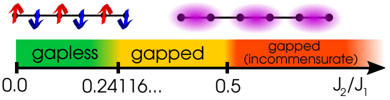
$J_2/J_1 = 0$

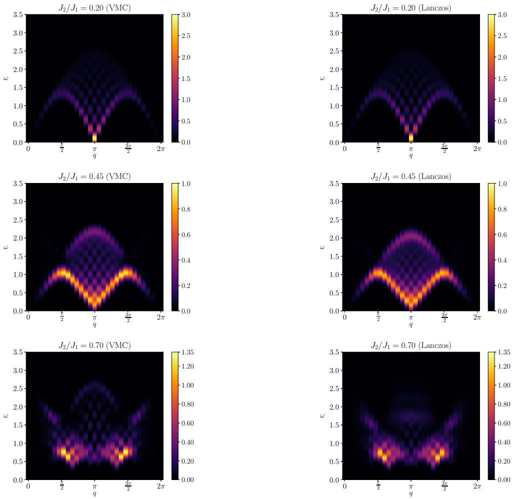


$J_2/J_1 = 0.45$

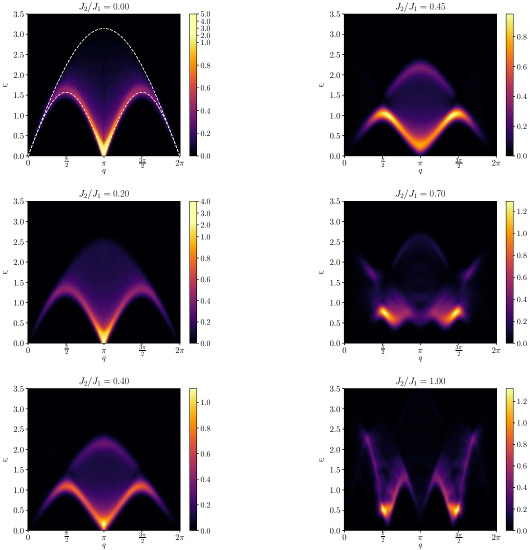


One-dimensional $J_1 - J_2$ model: A benchmark on 30-site cluster (II)





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



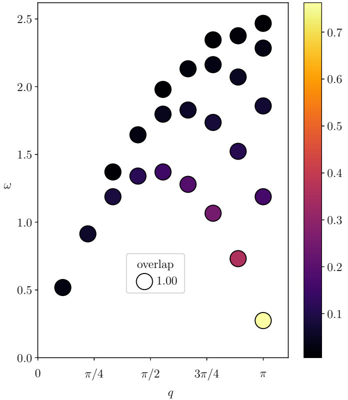
$$\mathcal{H} = \sum_{R,R'} J(|R-R'|)\, \mathbf{S}_R \cdot \mathbf{S}_{R'}$$

$$J(|R-R'|) = \frac{J}{\left| \frac{L}{\pi} \sin\left[\frac{\pi(R-R')}{L} \right] \right|^2}$$

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

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

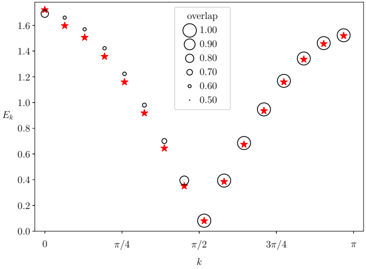
F.D.M. Haldane and M.R. Zirnbauer, Phys. Rev. Lett. **71**, 4055 (1993)



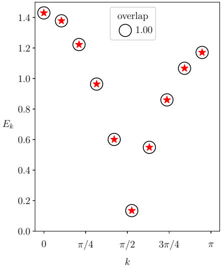
Odd number of sites L

- $|\Phi_{\mathrm{FS}}\rangle = \prod_{p<\pi/2,\sigma} c^\dagger_{p,\sigma}|0\rangle$ — Fermi sea with $L-1$ electrons
- $|\Psi_k\rangle = \mathcal{P}_G c^\dagger_{k,\uparrow}|\Phi_{\mathrm{FS}}\rangle$ — $|k| > \pi/2$
- $|\Psi_k\rangle = \mathcal{P}_G c_{k,\uparrow} c^\dagger_{k_F,\uparrow} c^\dagger_{-k_F,\uparrow}|\Phi_{\mathrm{FS}}\rangle$ — $|k| < \pi/2$ with $k_F = \pi(L+1)/L$

Spinon energy $E_k = [E(L)/L - E(L-1)/(L-1)] \times L$



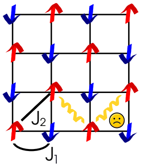
Heisenberg on $L = 31$ sites



Haldane-Shastry on $L = 19$ sites

- 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)

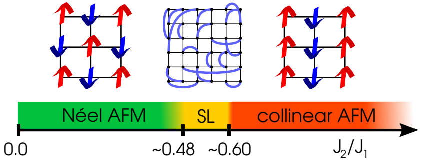
L. Wang *et al.*, Phys. Rev. B **94**, 075143 (2016)

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)

- 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

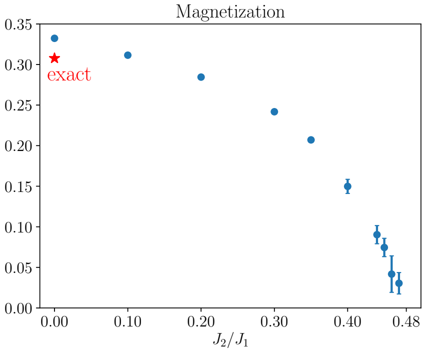
E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991)

- The transverse dynamical structure factor is considered

Two-dimensional $J_1 - J_2$ model: From Néel to spin liquid

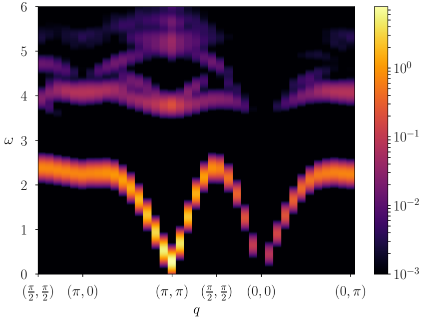
$$m^2 = \lim_{r \to \infty} \langle \mathbf{S}_r \cdot \mathbf{S}_0 \rangle$$

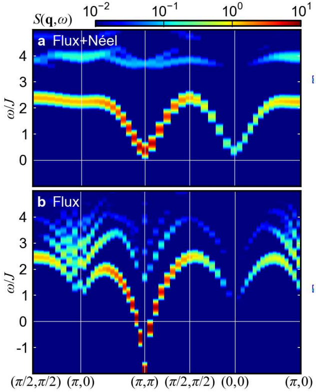
- Magnetization computed for finite clusters from 10×10 to 22×22



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

The unfrustrated Heisenberg model

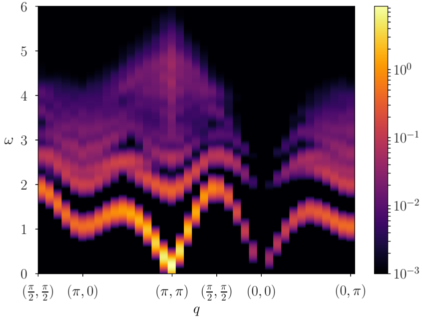


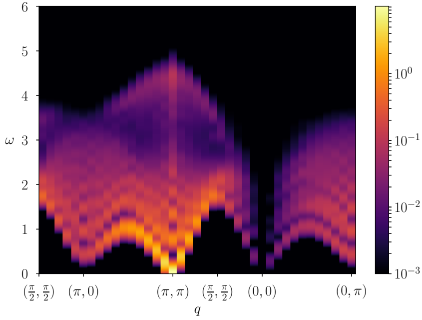


B. Dalla Piazza *et al.*, Nat. Phys. **11**, 62, (2015)

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

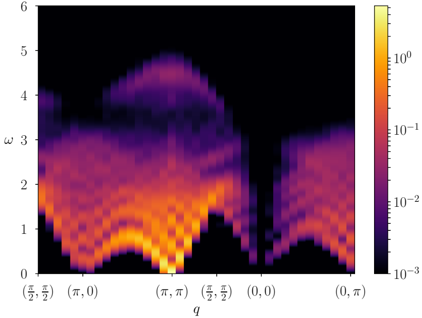
The frustrated cases with $J_2/J_1 = 0.3$ and 0.45 (still magnetically ordered)

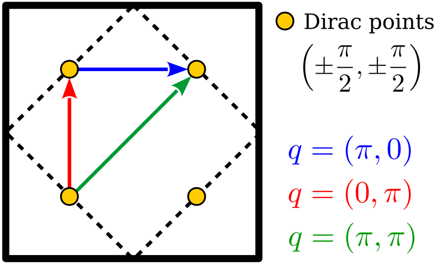




- The magnon signal looses its intensity around $q = (\pi, 0)$ and $(0, \pi)$
- Softening of the lowest-energy excitation at $q = (\pi, 0)$ and $(0, \pi)$
- Significant continuum above the single magnon branch

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 $(0, \pi)$.

Conclusions

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

- 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