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

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Topological Quantum Matter: Concepts and Realizations
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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, Phys. Rev. X **9**, 031026 (2019)

Special thanks to S. Chernyshev

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

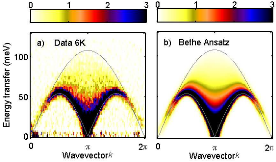
$$\boxed{S^a(q,\omega) = \sum_\alpha |\langle \Upsilon_\alpha^q | S_q^a | \Upsilon_0\rangle|^2 \delta(\omega - E_\alpha^q + E_0),}$$

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

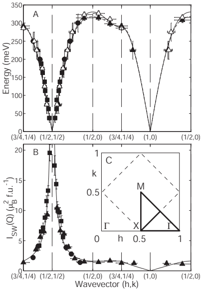
The dynamical spin structure factor

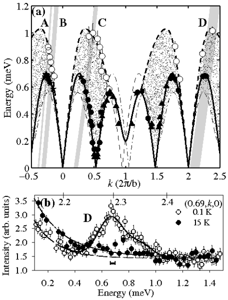
- 1D Heisenberg model and $KCuF_3$

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



- 2D Heisenberg model
  for La_2CuO_4 and Cs_2CuCl_4



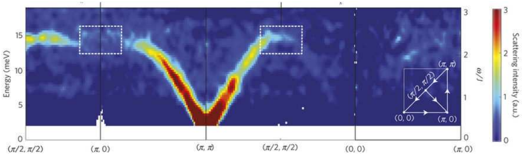


R. Coldea, D.A. Tennant, A.M. Tsvelik, and Z. Tylczynski, Phys. Rev. Lett. **86**, 1335 (2001)

R. Coldea, S.M. Hayden, G. Aeppli, T.G. Perring, C.D. Frost, T.E. Mason, S.-W. Cheong, and Z. Fisk, Phys. Rev. Lett. **86**, 5377 (2001)

- 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

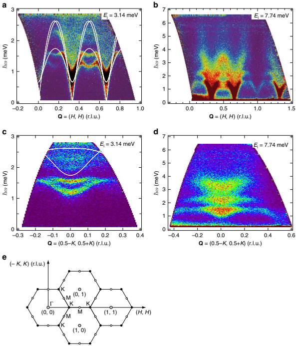
M. Powalski, K.P. Schmidt, and G.S. Uhrig, SciPost **4**, 001 (2018)

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

L. Vanderstraeten, J. Haegeman, and F. Verstraete, Phys. Rev. B, **99**, 165121 (2019)

- $Ba_3CoSb_2O_9$: a realization of an almost isotropic triangular lattice

S. Ito, N. Kurita, H. Tanaka, S. Ohira-Kawamura, K. Nakajima, S. Itoh, K. Kuwahara, and K. Kakurai, Nat. Comm. **8**, 235 (2017)



- Schwinger boson approach: relevance of strong quantum fluctuations

E.A. Ghioldi, M.G. Gonzalez, S.-S. Zhang, Y. Kamiya, L.O. Manuel, A.E. Trumper, and C.D. Batista, Phys. Rev. B **98**, 184403 (2018)

- DMRG method: strong magnon-continuum repulsion, avoided magnon decay

R. Verresen, F. Pollmann, and R. Moessner, Nat. Phys. **15**, 750 (2019)

- 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

$$S_R^a = \frac{1}{2} c^\dagger_{R,\alpha} \sigma^a_{\alpha,\beta} c_{R,\beta}$$

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

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

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

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

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

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

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

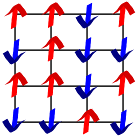
$\{t_{R,R'}\}$ and $\{\Delta_{R,R'}\}$ define the mean-field Ansatz $\longrightarrow$ BCS spectrum $\{\epsilon_\alpha\}$

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

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

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

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



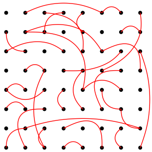
- The exact projection can be treated within the variational Monte Carlo approach

F. Becca and S. Sorella, *Quantum Monte Carlo Approaches for Correlated Systems* (Cambridge University Press, 2017)

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

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

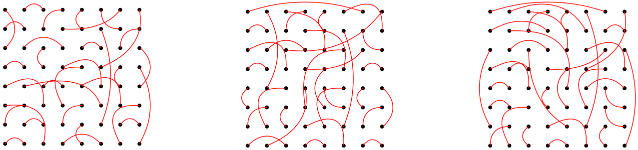
It is a linear superposition of all singlet configurations (that may overlap)



$+ \dots$

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

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



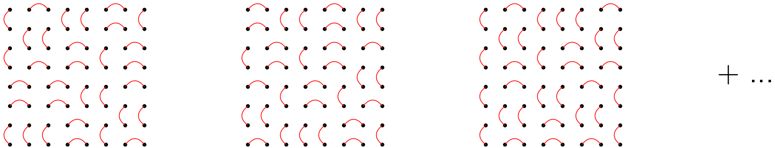
$+ \dots$

The projected wave function

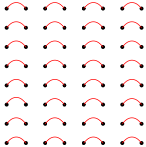
- The mean-field wave function has a BCS-like form

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

- Depending on the pairing function $f_{i,j}$, different RVB states may be obtained...

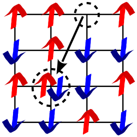


- ...even with valence-bond order (valence-bond crystals)



- 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 $S^z = 0$)

- 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 $|q, R\rangle$

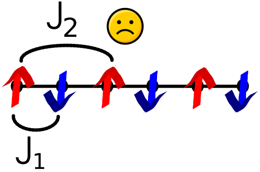
- The dynamical structure factor is approximated by

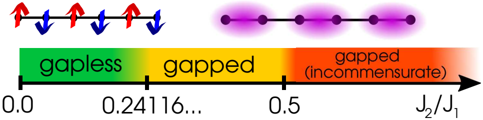
$$S^z(q, \omega) = \sum_n \left| \sum_R (A_R^{n,q})^* O_{R,0}^q \right|^2 \delta(\omega - E_n^q + E_0)$$

At most L states for each momentum q

- The 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)

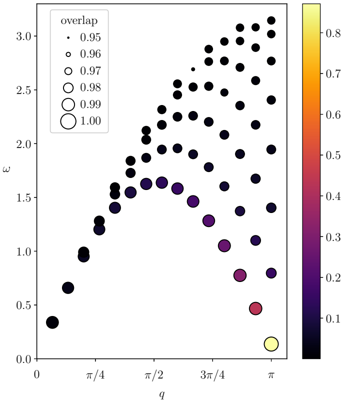
S.R. White and I. Affleck, Phys. Rev. B **54**, 9862 (1996)

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

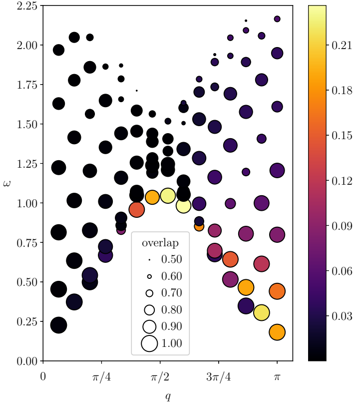
One-dimensional $J_1 - J_2$ model: A benchmark on 30 sites

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

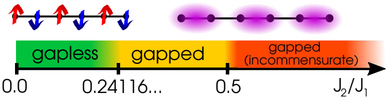
$J_2/J_1 = 0$

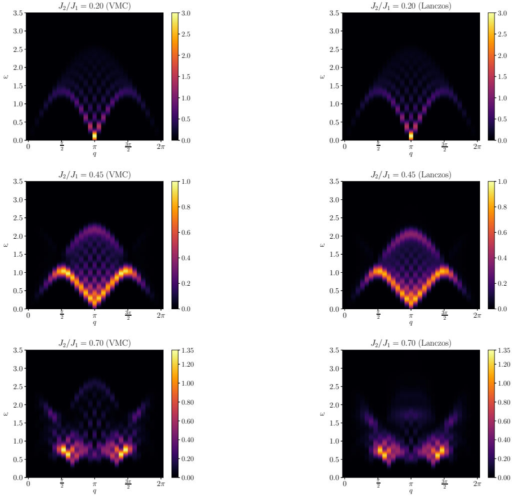


$J_2/J_1 = 0.45$

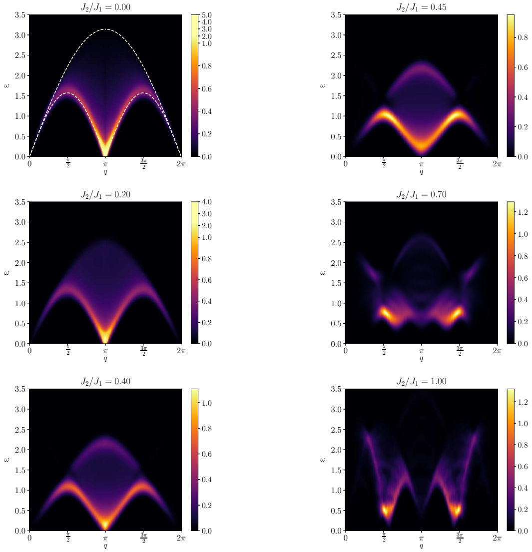


One-dimensional $J_1 - J_2$ model: A benchmark on 30 sites





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



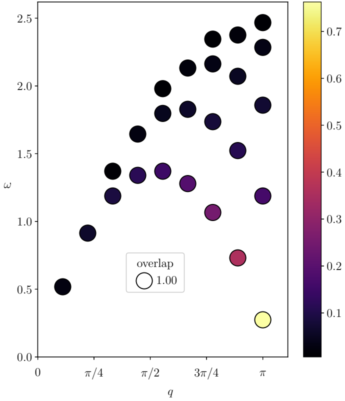
$$\mathcal{H} = \sum_{R,R'} J(|R - R'|)\, \mathbf{S}_R \cdot \mathbf{S}_{R'}$$

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

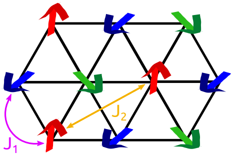
F.D.M. Haldane, Phys. Rev. Lett. **60**, 635 (1988)

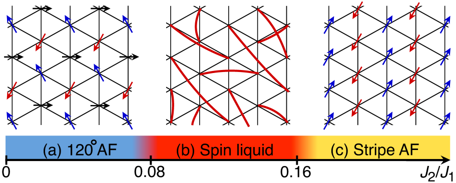
F.D.M. Haldane, Phys. Rev. Lett. **66**, 1529 (1991)

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



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





- Coplanar antiferromagnetic (120°) order for $J_2/J_1 \lesssim 0.07$
- Spin liquid (gapped or gapless?) for $0.07 \lesssim J_2/J_1 \lesssim 0.16$
- Collinear antiferromagnet $0.16 \lesssim J_2/J_1 <$???

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

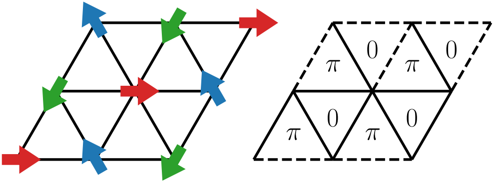
W.-J. Hu, S.-S. Gong, W. Zhu, and D.N. Sheng, Phys. Rev. B **92**, 140403 (2015)

Y. Iqbal, W.-J. Hu, R. Thomale, D. Poilblanc, and F. Becca, Phys. Rev. B **93**, 144411 (2016)

- A fictitious magnetic field h is considered to have AFM order

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

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

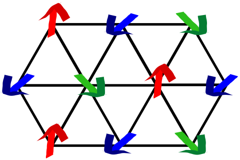


The magnetic moment in the $x - y$ plane

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

Y. Iqbal, W.-J. Hu, R. Thomale, D. Poilblanc, and F. Becca, Phys. Rev. B **93**, 144411 (2016)

- The transverse dynamical structure factor is considered

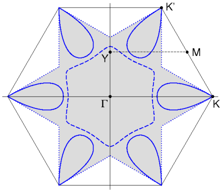


- Spin-wave approach (including $1/S$ corrections): magnon decay

  The sound velocities at Γ and K (K') are different

$$E_{k,q} = \epsilon_q + \epsilon_{k-q} < \epsilon_k$$

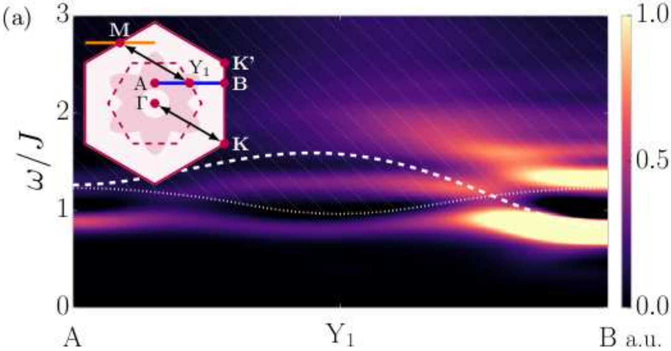
- Decay with one magnon at Γ
- Decay with one magnon at K or K'
- Decay with two generic magnons: $\partial E_{k,q}/\partial q = 0$



A. L. Chernyshev and M.E. Zhitomirsky, Phys. Rev. Lett. **97**, 207202 (2006)

A. L. Chernyshev and M.E. Zhitomirsky, Phys. Rev. B **79**, 144416 (2009)

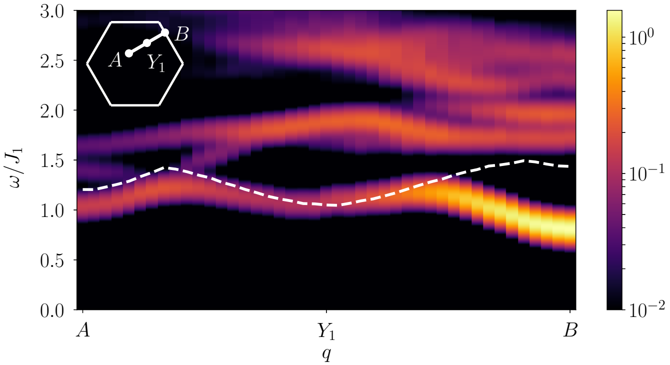
- DMRG on an infinite cylinder of width $L = 6$: no magnon decay
  Strong interactions push the magnon out of the continuum



- From the lowest-energy excitation E_0^q for each momentum q
  see if the magnon decay is possible: $E_q = E_0^{q-K} + E_0^K$ vs E_0^q

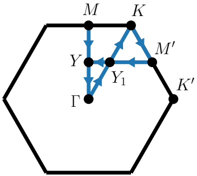
R. Verresen, F. Pollmann, and R. Moessner, Nat. Phys. **15**, 750 (2019)

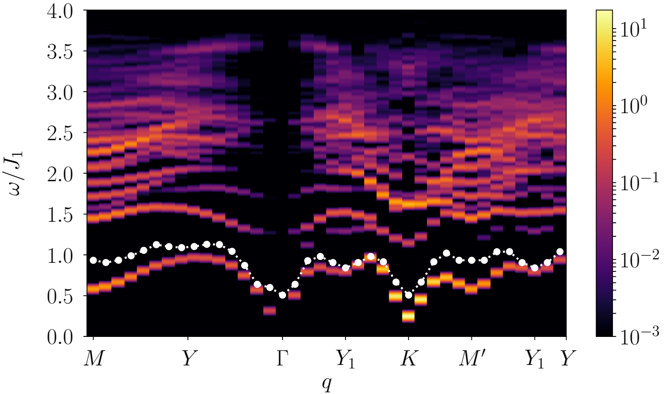
- Calculations on a 84×6 cylinder: no magnon decay



- From the lowest-energy excitation E_0^q for each momentum q see if the magnon decay is possible: $E_q = E_0^{q \mp K} + E_0^{\pm K}$ vs E_0^q

The variational wave function π-flux and the fictitious magnetic field h

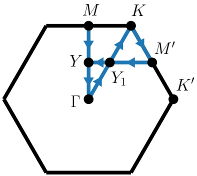


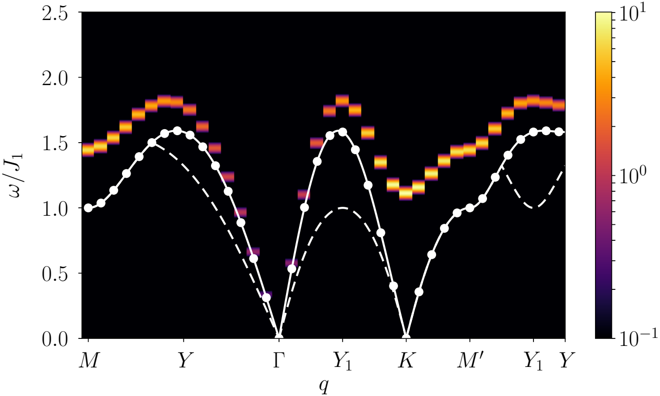


- Calculations on a 30×30 cluster
- No decay with $E_q = E_0^{q-p} + E_0^p$ vs E_0^q

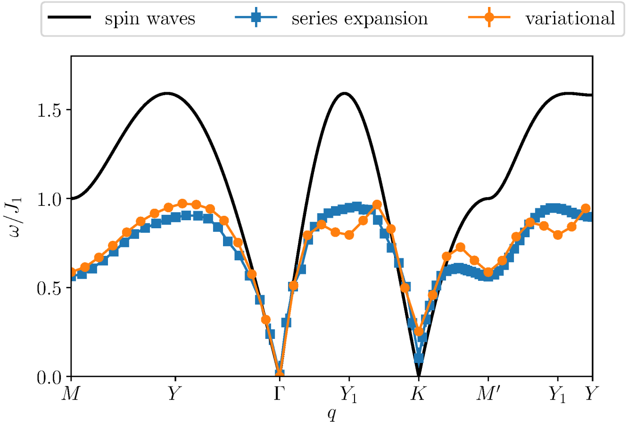
Our variational Monte Carlo approach

The variational wave function with only the fictitious magnetic field h



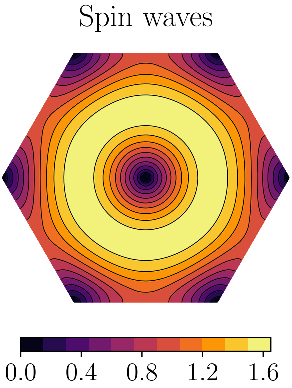


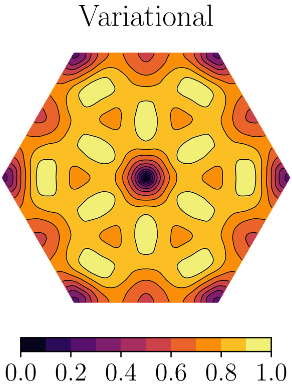
- A single excitation, no continuum is present
- It reproduces the spin-wave calculations (with a gap at K)



- Good agreement with series expansion approach

W. Zheng, J.O. Fjaerestad, R.R.P. Singh, R.H. McKenzie, and R. Coldea, Phys. Rev. Lett. **96**, 057201 (2006); Phys. Rev. B **74**, 224420 (2006)

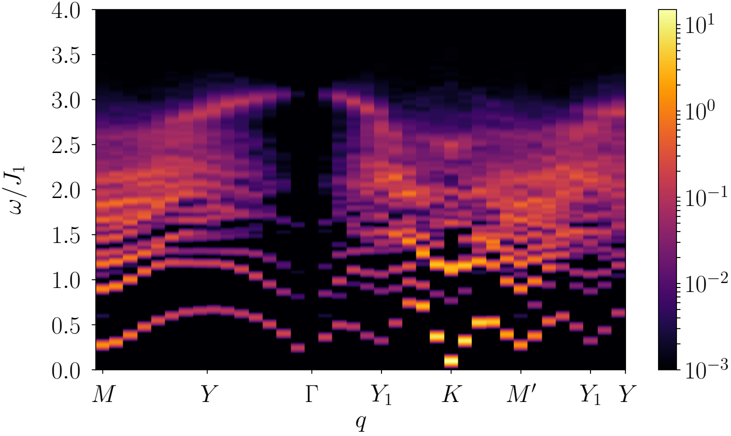




- Local minima at the midpoint of the magnetic Brillouin zone

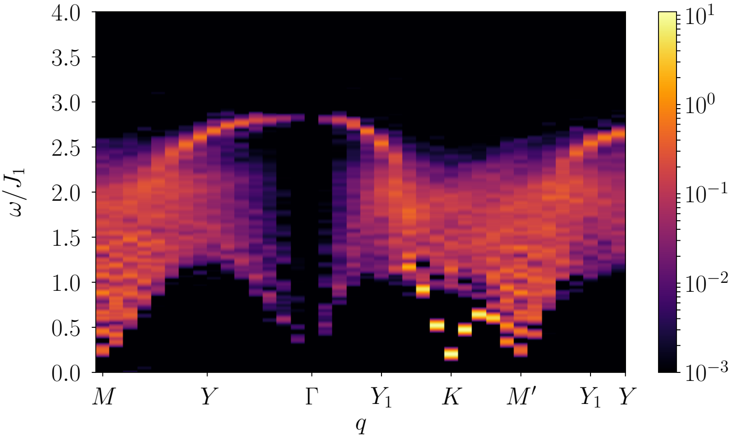
see also R. Verresen, F. Pollmann, and R. Moessner, Nat. Phys. **15**, 750 (2019)

- $J_1 - J_2$ model with $J_2/J_1 = 0.07$
  The variational wave function π-flux and the fictitious magnetic field h



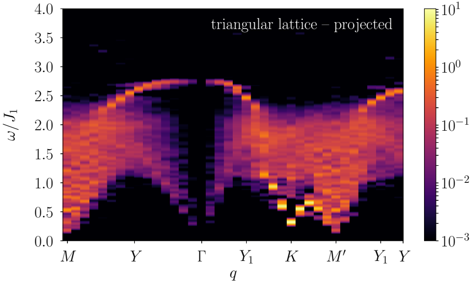
- Low-energy excitations at K and M points

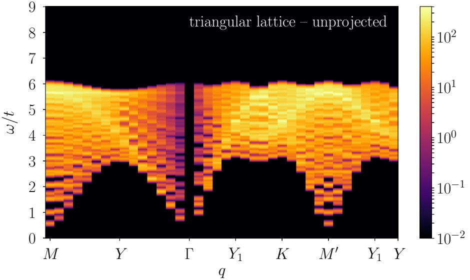
- $J_1 - J_2$ model with $J_2/J_1 = 0.09$
  The variational wave function π-flux and the fictitious magnetic field h



- Low-energy excitations at K and M points

- $J_1 - J_2$ model with $J_2/J_1 = 0.125$
  The variational wave function has only π-flux



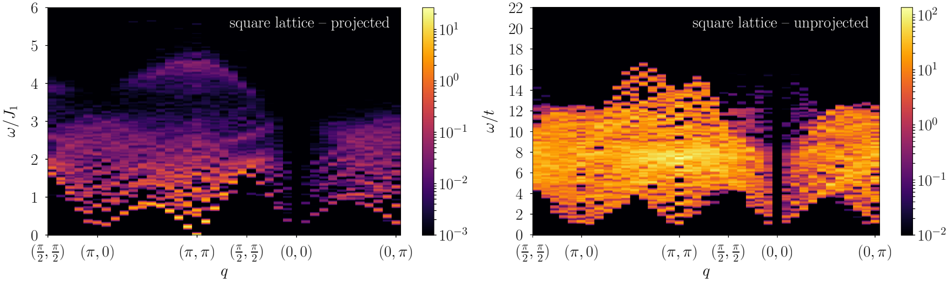


- Qualitative features are not all captured by mean field (no Gutzwiller projection)
- Huge signal at low energies around K points

X.-Y. Song, C. Wang, A. Vishwanath, Y.-C. He, arXiv:1811.11186

Comparison with the square lattice: inside the (gapless) spin-liquid phase

- $J_1 - J_2$ model with $J_2/J_1 = 0.55$
  The variational wave function has BCS pairing at NN and NNN ($\mathcal{Z}_2$)



- Calculations on a 22×22 cluster
- Qualitative features are captured by mean field (no Gutzwiller projection)

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

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)