Momentum-resolved time evolution with matrix product states

Laurens Vanderstraeten
University of Ghent

Overview

Motivation: spectral functions in quantum matter

Momentum methods: quasiparticle ansatz

Time evolution in real space

Time evolution in momentum space

Results

Outlook

Maarten Van Damme & LV
arXiv::2201.07314

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Motivation: spectral functions

Important probe for relating theory and experiment

$$S(q,\omega) = \int dt e^{i\omega t} \langle e^{iHt} O_{-q} \mathrm{e}^{-iHt} O_q \rangle$$

with $O(q) = \frac{1}{\sqrt{N}} \sum_n e^{iqn} O_n$ → direct probe for low-lying excitations

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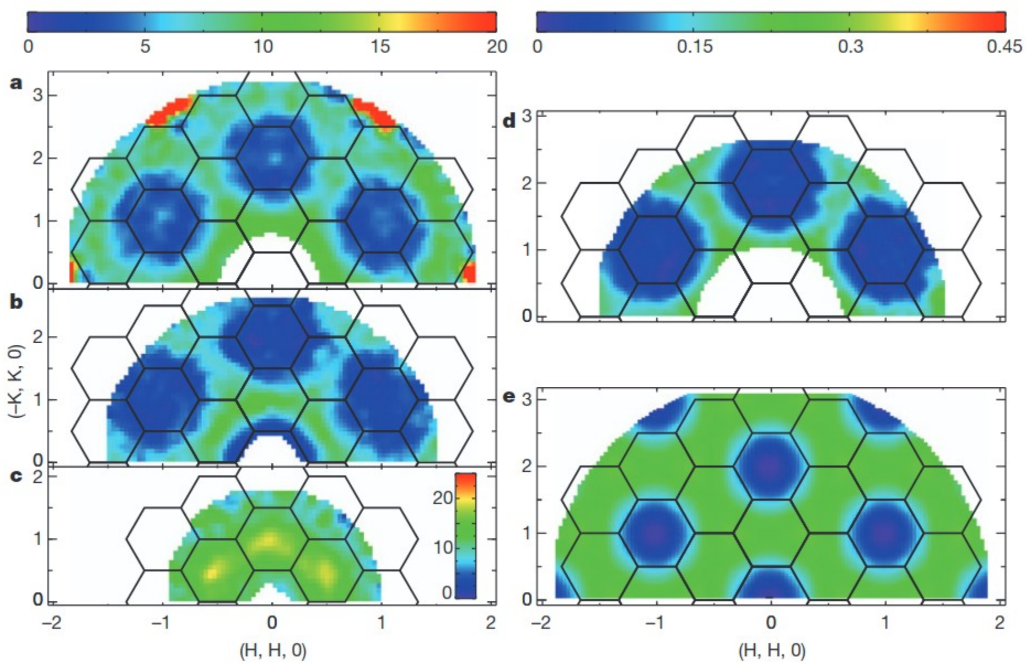
Example: inelastic neutron scattering (INS) for magnetic materials



Han et al., Nature 492, 406 (2012)

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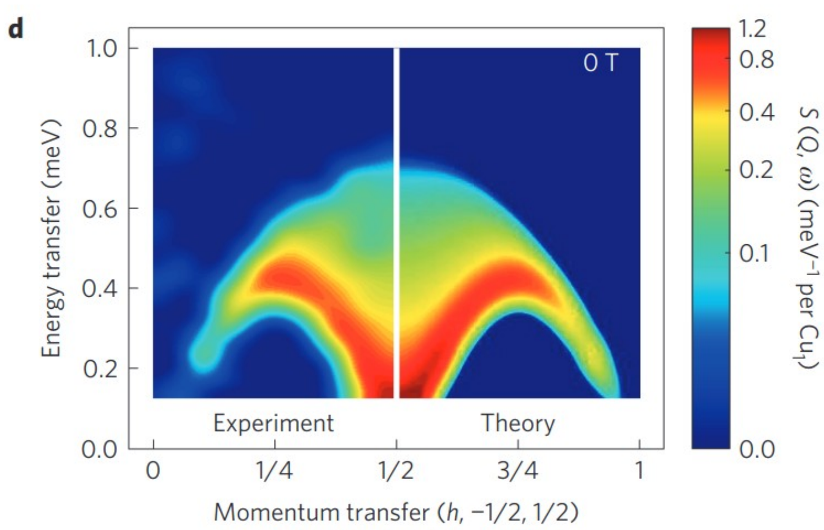

Mourigal et al. Nat. Phys. 9, 435 (2013)

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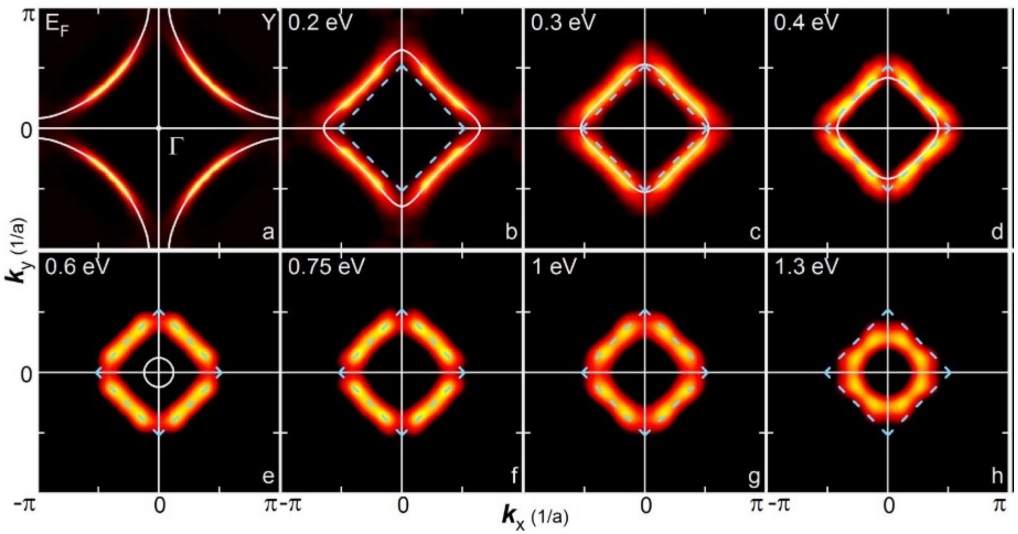
Example: angle-resolved photo emission spectroscopy (ARPES) for electronic systems



Graf, et al, Phys. Rev. Lett. 98, 067004 (2007)

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Numerical approaches

- exact diagonalization
- quantum Monte Carlo: analytic continuation
- matrix product states (MPS)

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Numerical approaches

- exact diagonalization
- quantum Monte Carlo: analytic continuation
- matrix product states (MPS)
    - correction vector approach
    - Chebyshev expansion
    - real-time evolution

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MPS methods all break translation symmetry

→ spectral function is a momentum-resolved quantity

→ use symmetries and associated quantum numbers in MPS simulations!

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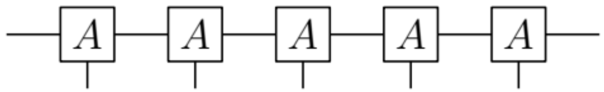
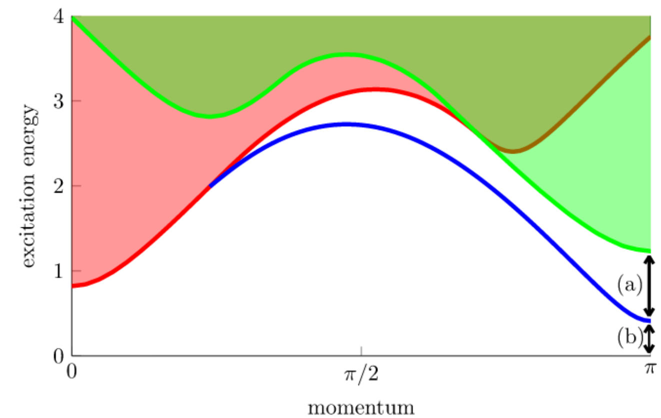
MPS quasiparticle ansatz

The ground state is described by a uniform MPS

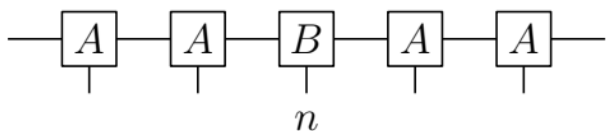
$$|\Psi(A)\rangle =$$





Isolated lines in the excitation spectrum can be captured by the momentum superposition of a local perturbation

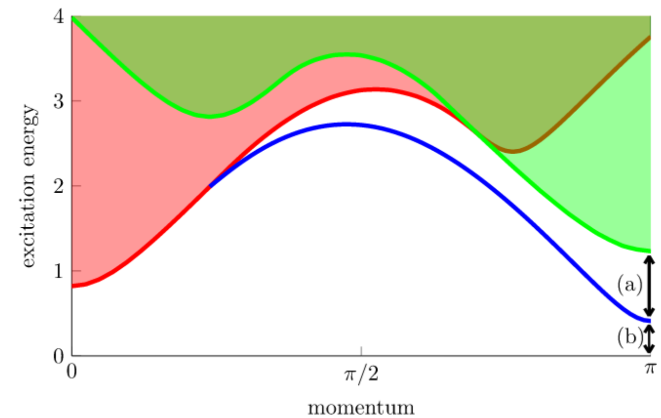
$$|\Phi_q(B)\rangle = \sum_n e^{iqn}$$



Optimization of variational parameters

- → orthogonal to the ground state
- → energy as a function of momentum
- → spectral weights

MPS quasiparticle ansatz



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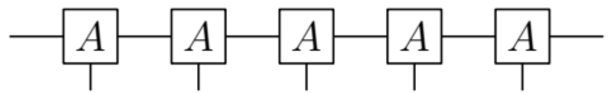
$|\Psi(A)\rangle =$ 

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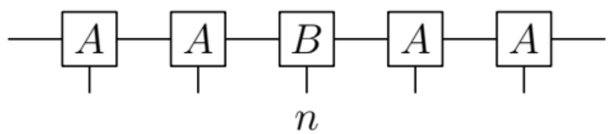
$|\Phi_q(B)\rangle = \sum_n e^{iqn}$ 

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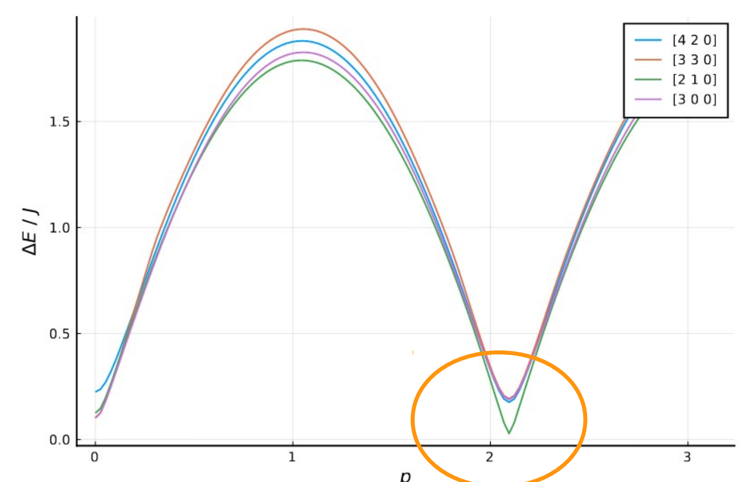


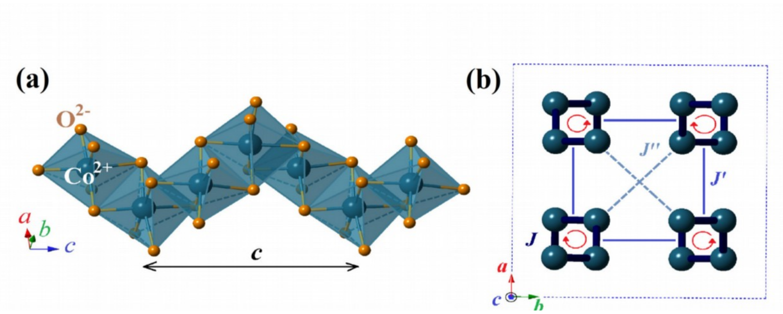
"Haldane gap" in SU(3) chain

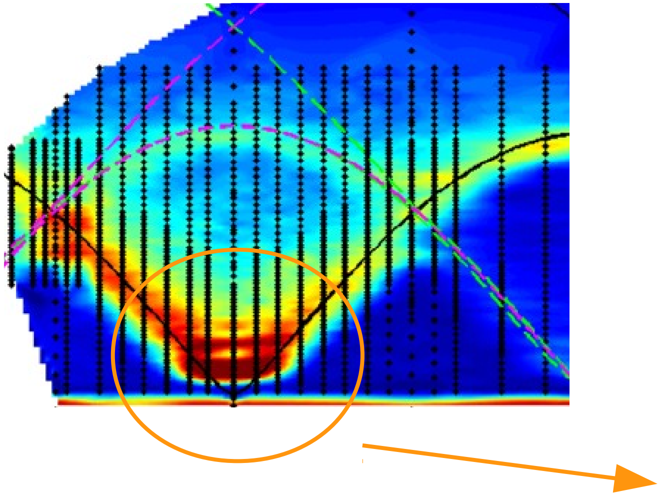
$\Delta = 0.0263$

Devos, LV, Verstraete
arXiv: 2202.09279

MPS quasiparticle ansatz

Confinement of spinons in quasi-1D Heisenberg magnet ($SrCo_2V_2O_8$)





inelastic neutron-scattering measurement of the spectral function

bound states of spinons

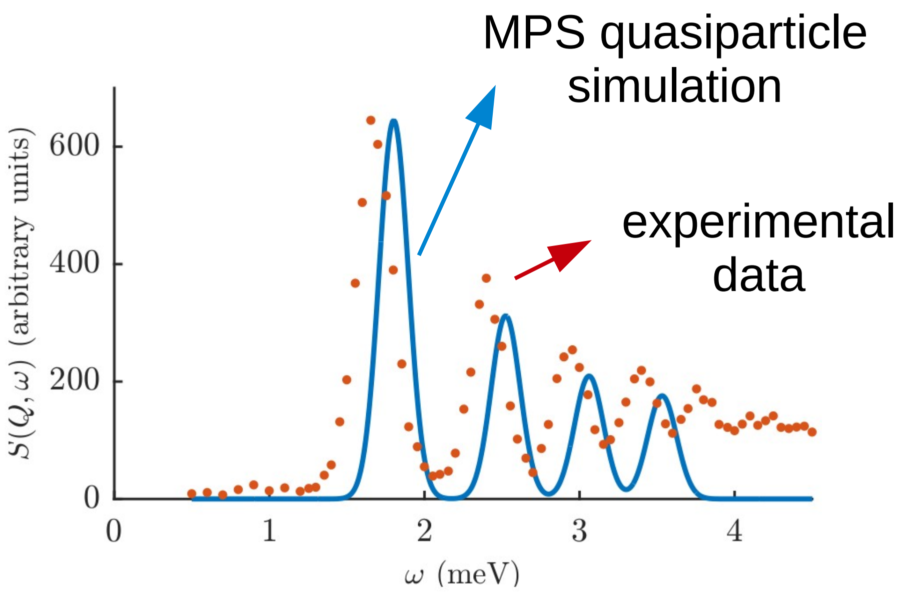
Bera, Lake, Essler, LV, Hubig, Schollwöck, Islam, Schneidewind, Quintero-Castro, PRB 96, 054423 (2017)

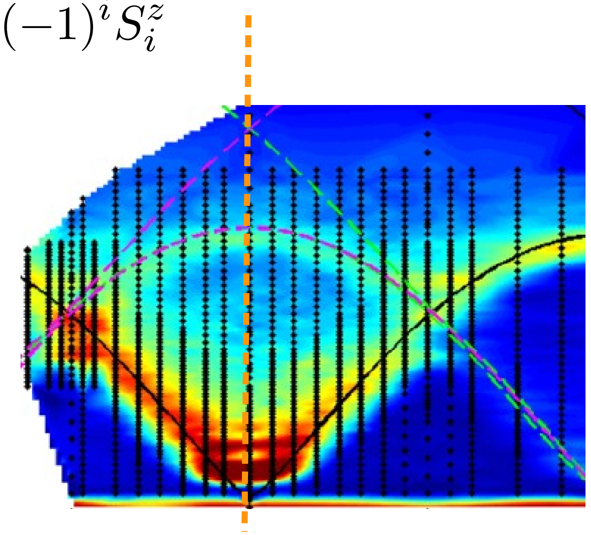
MPS quasiparticle ansatz

Confinement of spinons in quasi-1D Heisenberg magnet ($SrCo_2V_2O_8$)

→ effective 1D model

$$H = \sum_i \epsilon \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + S_i^z S_{i+1}^z + h \sum_i (-1)^i S_i^z$$





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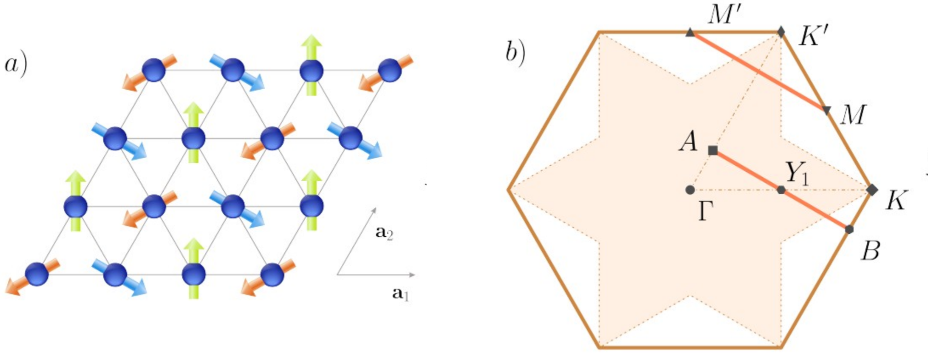
MPS quasiparticle ansatz

Spin spectral function for the
Heisenberg model on the triangular lattice
(six-leg cylinder)



Drescher, LV, Moessner, Pollmann, *in preparation*

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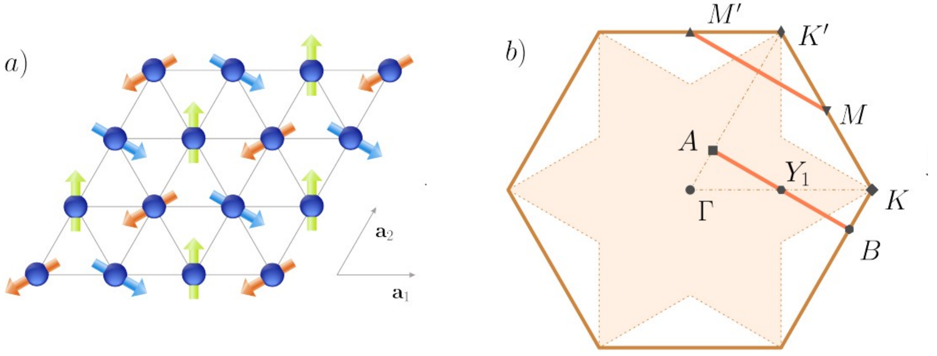
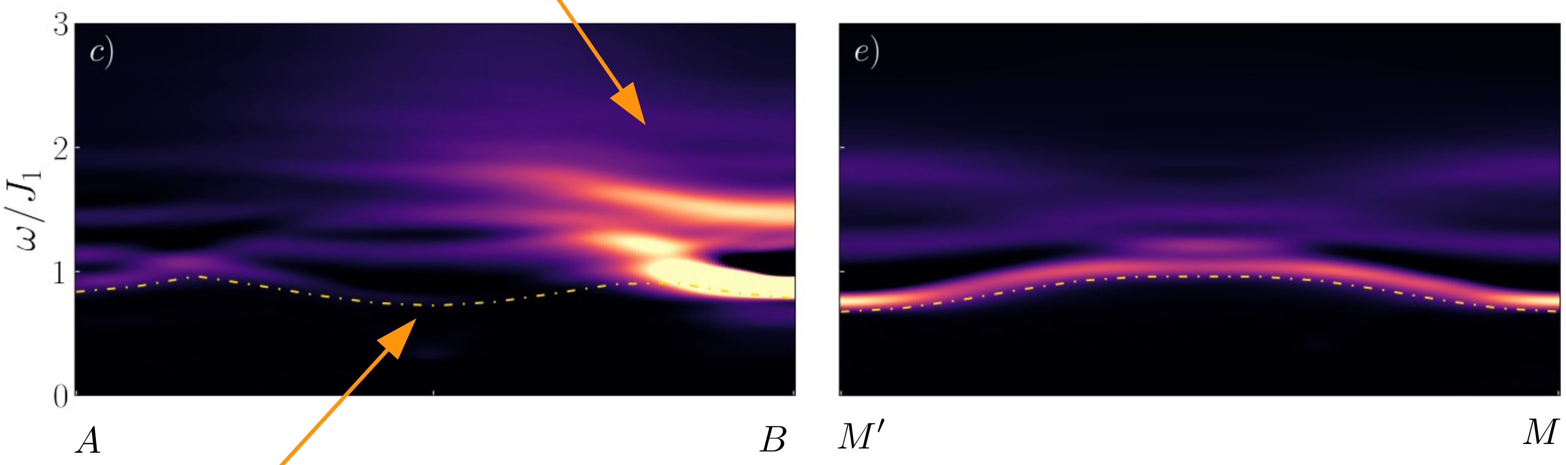


time-dependent MPS methods

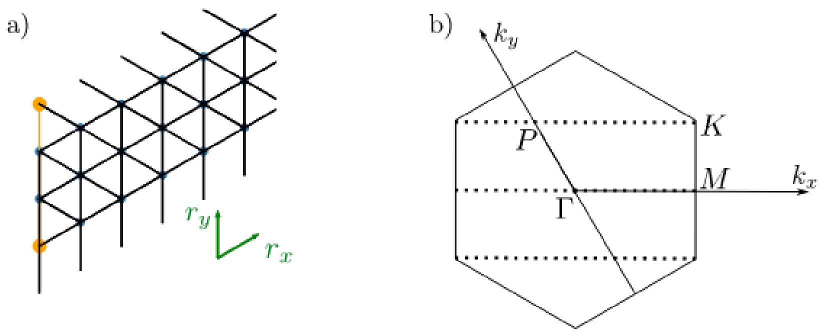


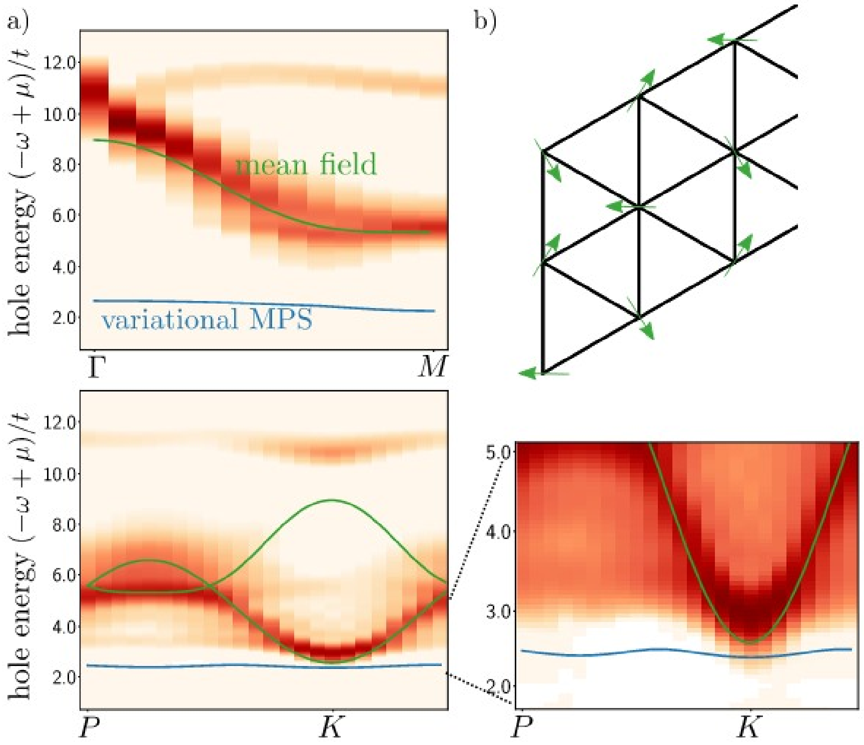
quasiparticle ansatz

Drescher, LV, Moessner, Pollmann, *in preparation*

MPS quasiparticle ansatz

Hole spectral function for the Hubbard model on the triangular lattice (three-leg cylinder)





Kadow, LV, Knap, arXiv:2202.03458

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Time evolution in real space

We compute the real-space and real-time correlator

$$S(n', t) = \langle \Psi_0 | \, O_{n+n'} \mathrm{e}^{-i(H-E_0)t} O_n \, | \Psi_0 \rangle$$

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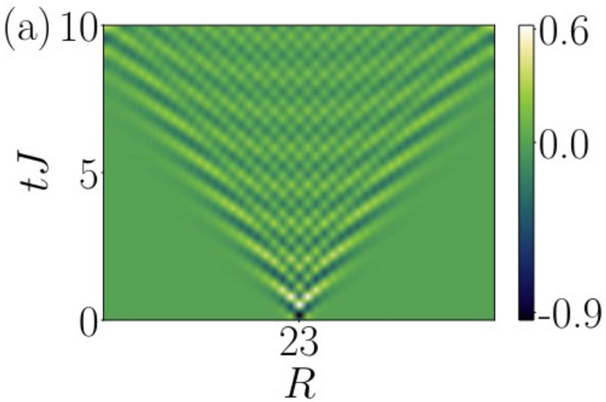

Villa et al, PRA 102, 033337 (2020)

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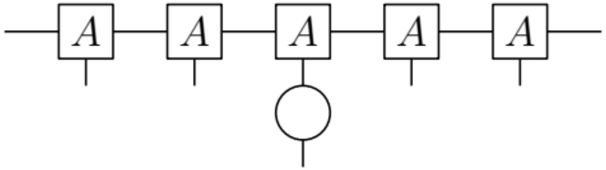
$$O_n|\Psi_0\rangle =$$



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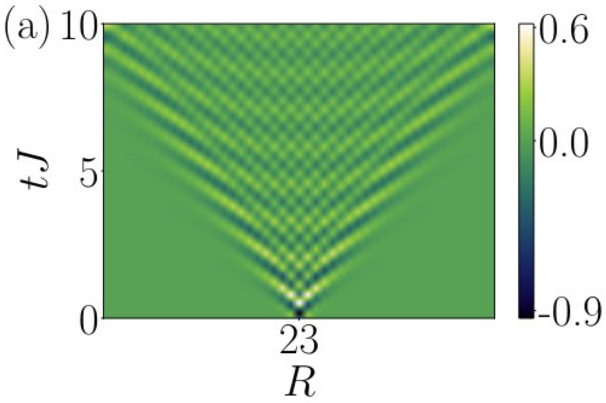

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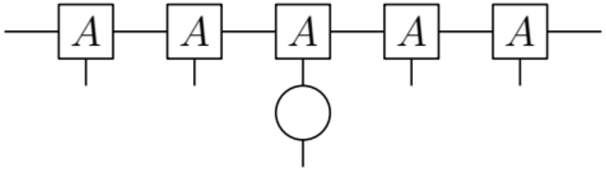

2. Apply time-evolution operator and approximate as window-MPS

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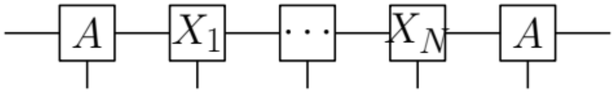

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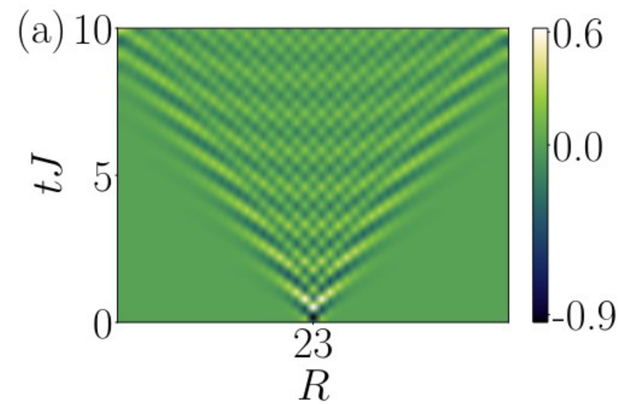

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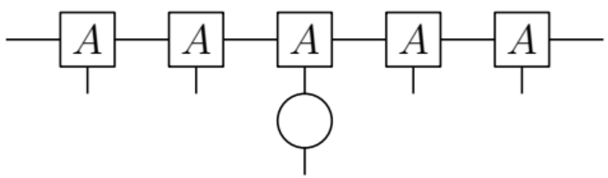

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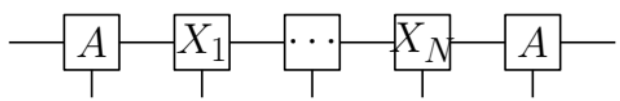
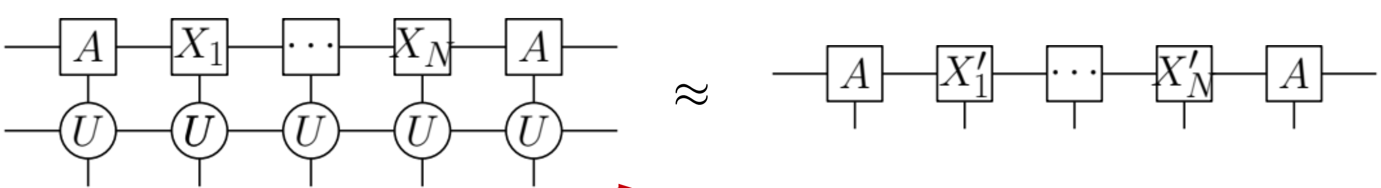


3. In each time step, perform sweep optimization for new window tensors



MPO approximation of time-evolution operator

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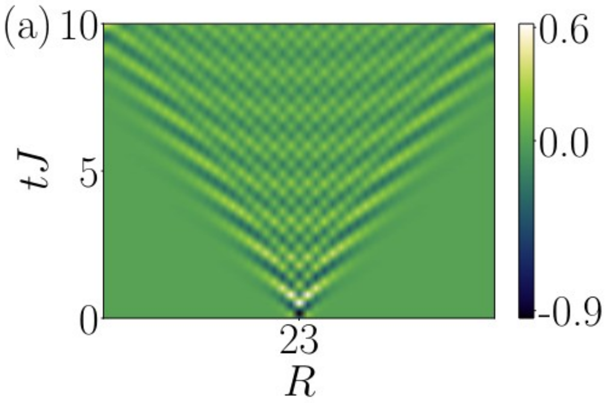

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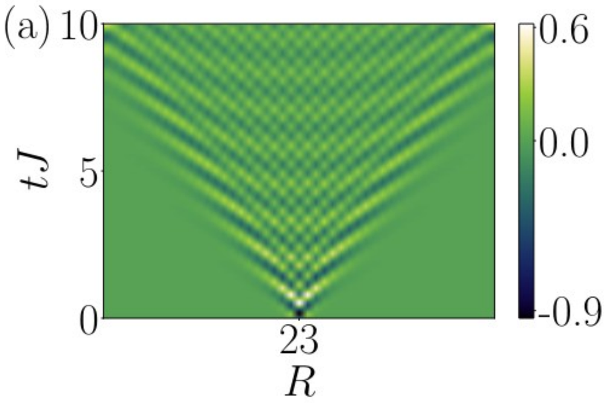

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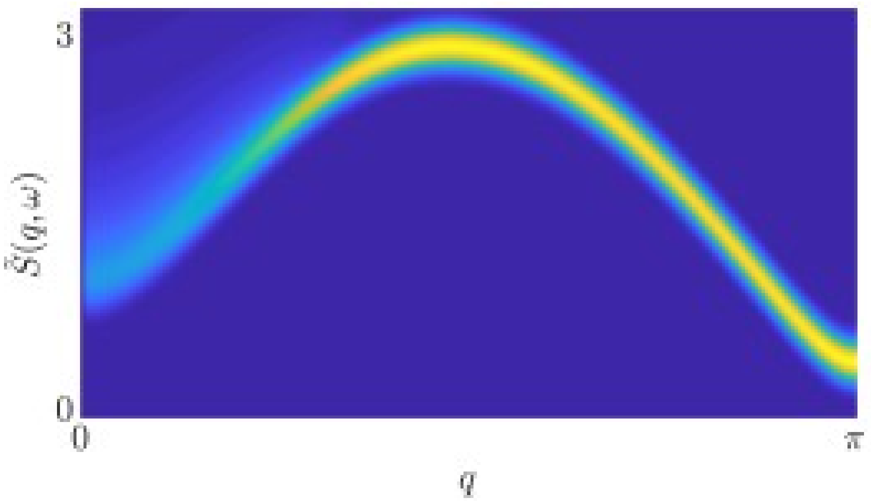
5. Fourier transform to momentum and frequency space

$$S(q, \omega) = \int dt \mathrm{e}^{i\omega t} \sum_{n'} \mathrm{e}^{iqn} S(n', t)$$

Time evolution in real space

Example: spin-1 Heisenberg chain



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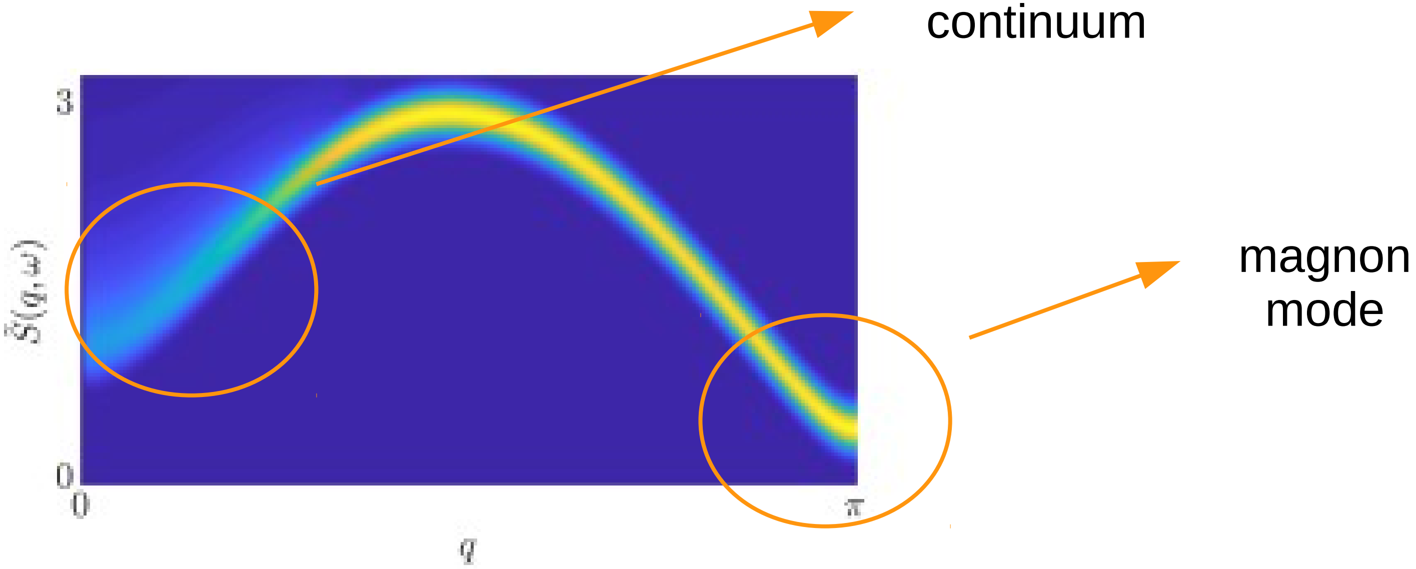

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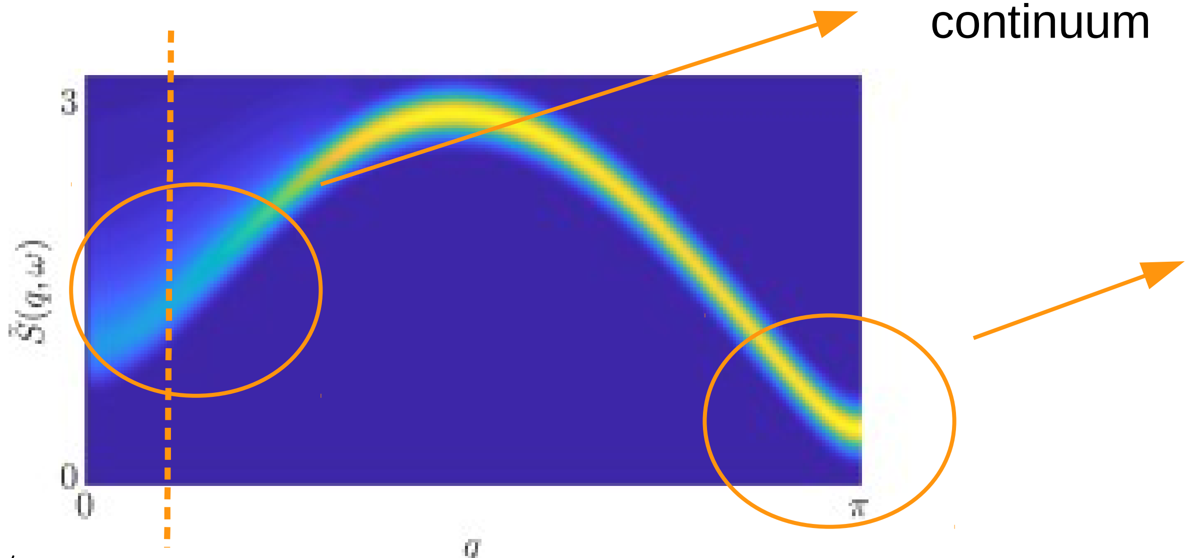
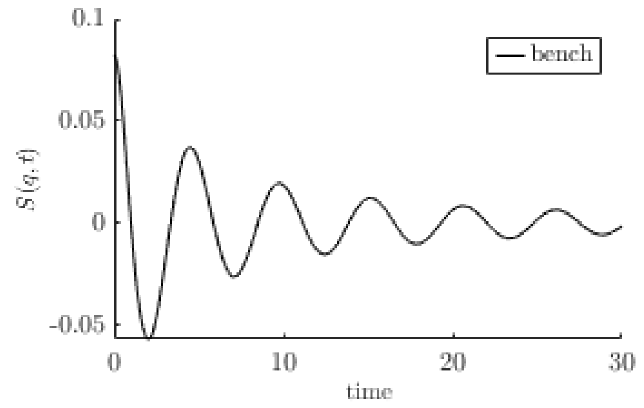
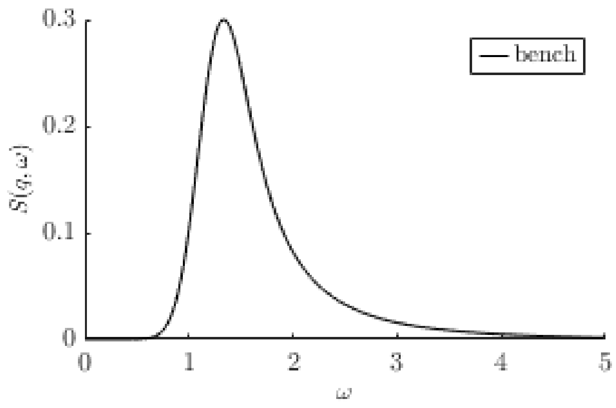
two-magnon continuum



magnon mode

$q = \pi/10$





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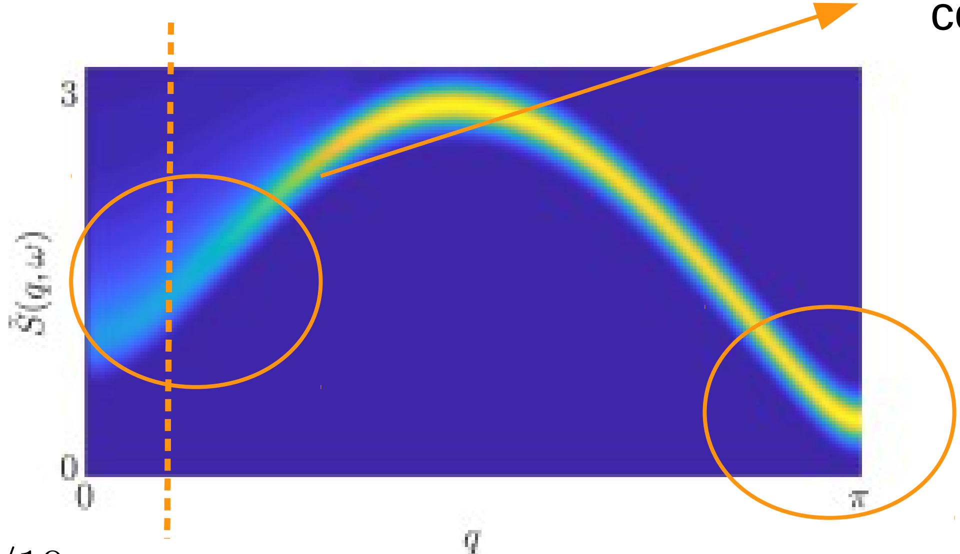

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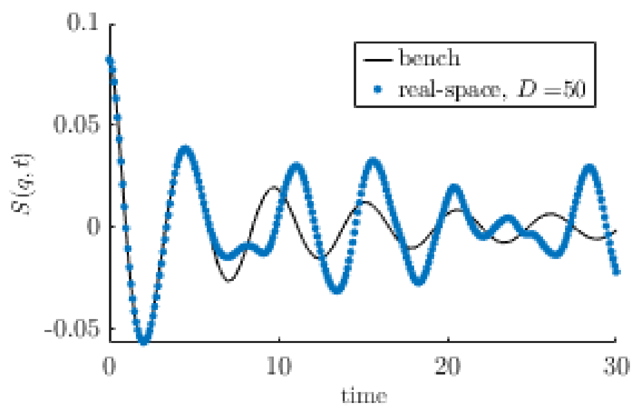

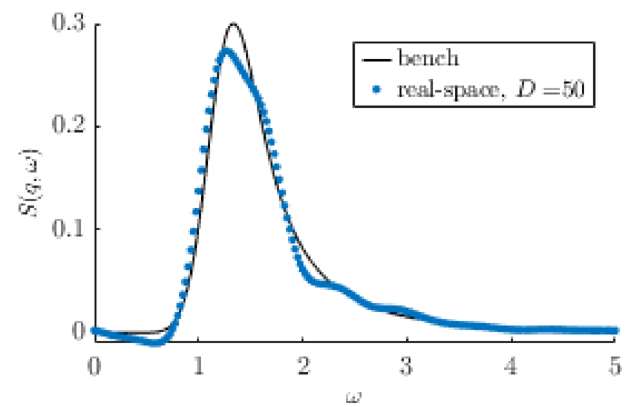

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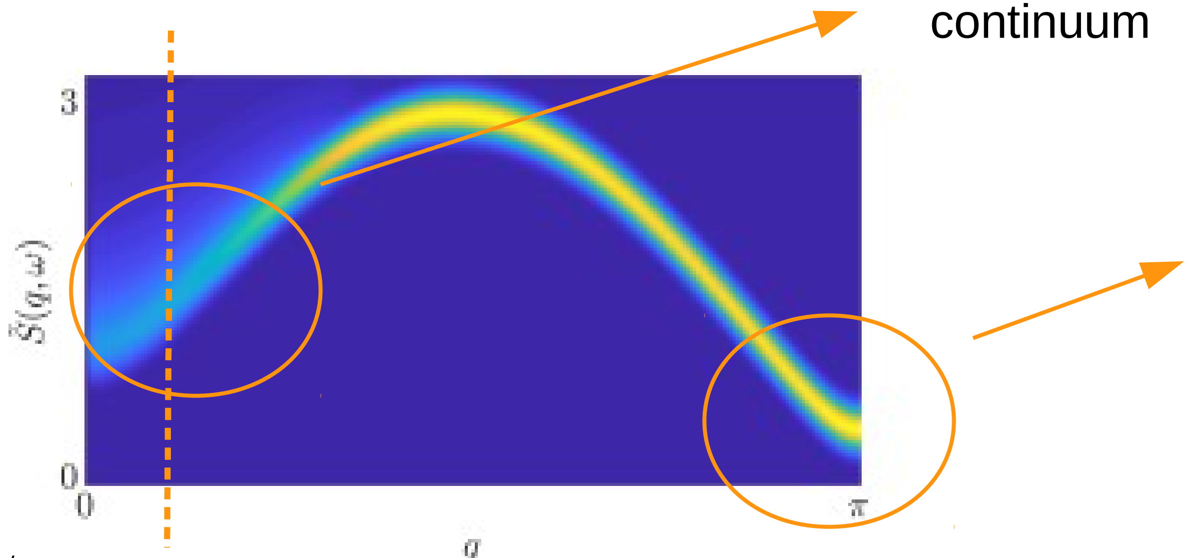

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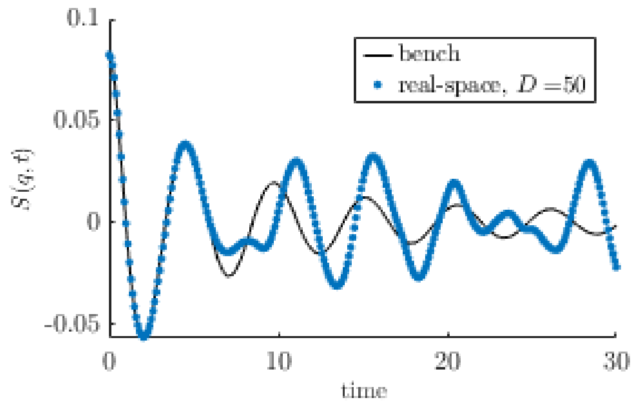

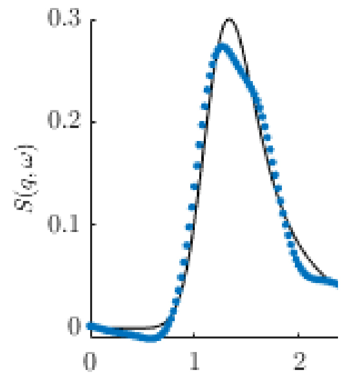

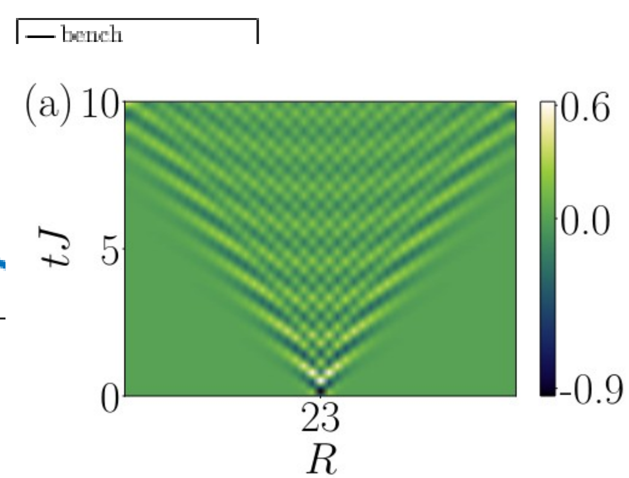

→ Can we do better??

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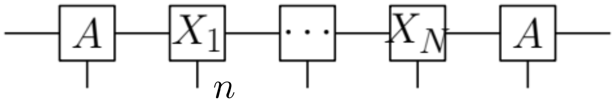
Spectral function is a momentum-resolved quantity!

$$S(q,\omega) = \int dt \mathrm{e}^{i\omega t} \langle e^{iHt} O_{-q} \mathrm{e}^{-iHt} O_q \rangle$$

$$\propto \int dt \mathrm{e}^{i\omega t} \langle \Psi_q(0) | \Psi_q(t) \rangle \qquad \text{with} \quad |\Psi_q(t)\rangle = \mathrm{e}^{-i(H-E_0)t} \sum_n \mathrm{e}^{iqn} O_n |\Psi_0\rangle$$

Represent this time-evolved state as a “momentum-window MPS”

$$|\Psi_q(t)\rangle \approx \sum_n \mathrm{e}^{iqn}$$



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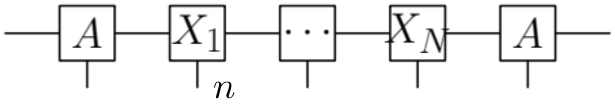


The time-evolution scheme is similar to the real-space version

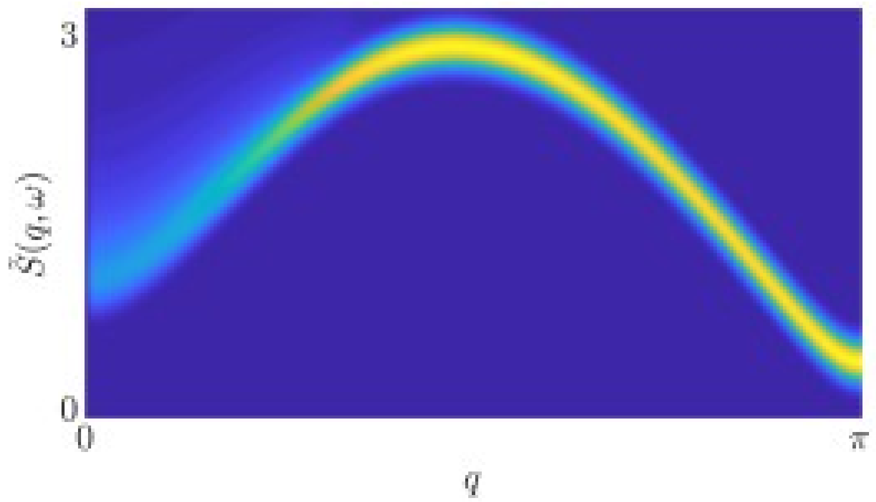
- in each time step, apply time-evolution MPO variationally

- smart gauge fixing of the tensors

- extra linear scaling in window size due to momentum superposition

Time evolution in momentum space

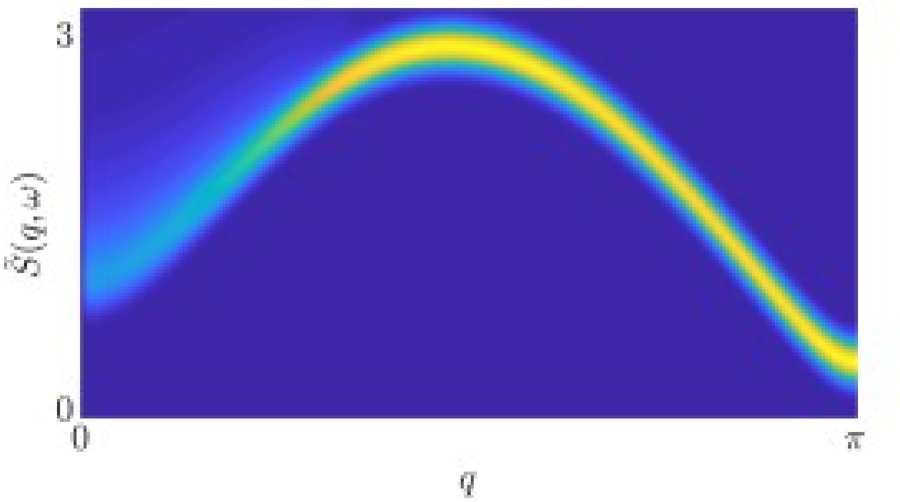
Example: spin-1 Heisenberg chain



For isolated lines in the spectrum, momentum-space window works for infinite times!

Time evolution in momentum space

Example: spin-1 Heisenberg chain



For isolated lines in the spectrum, momentum-space window works for infinite times!

What about continua?

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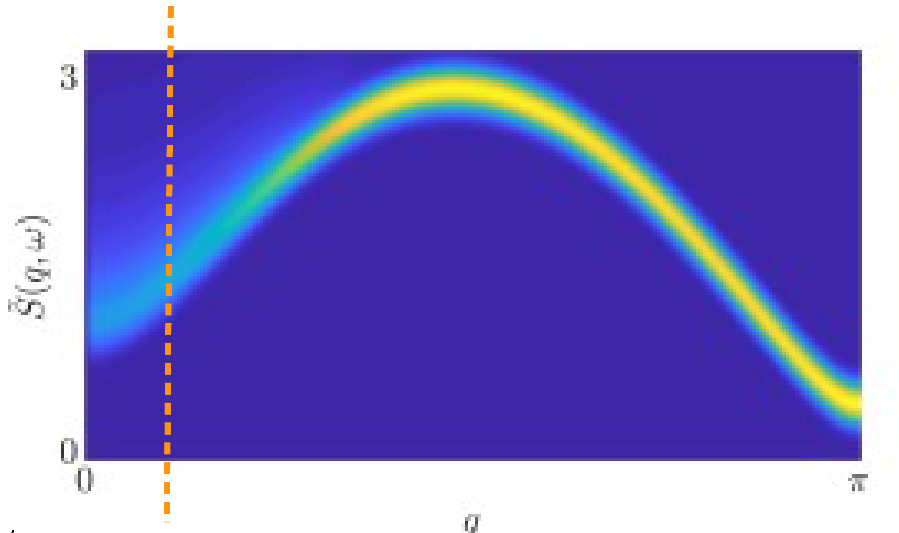

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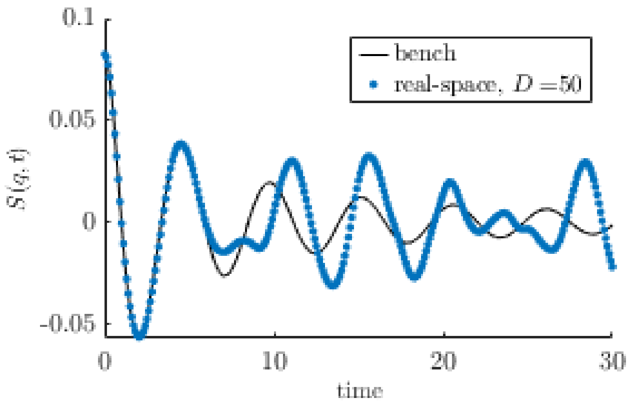
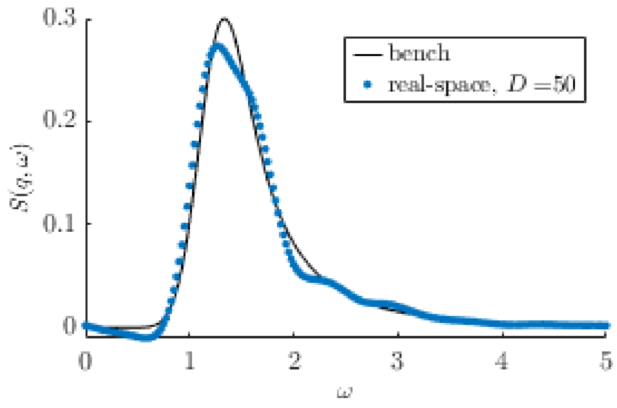
$q = \pi/10$





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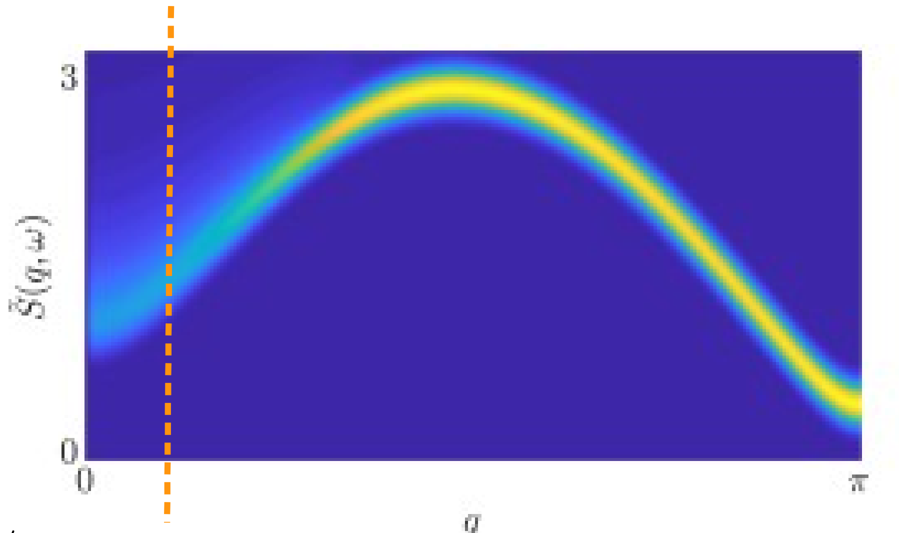

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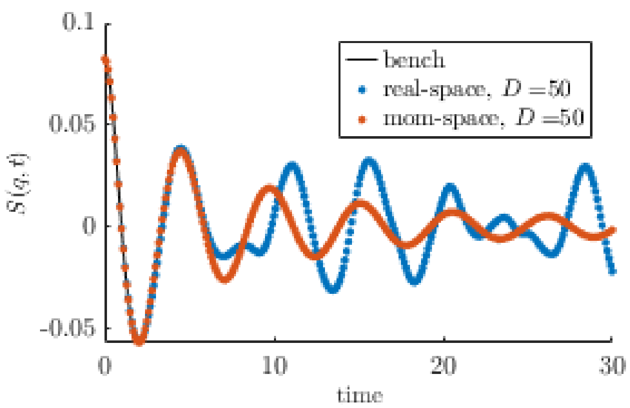
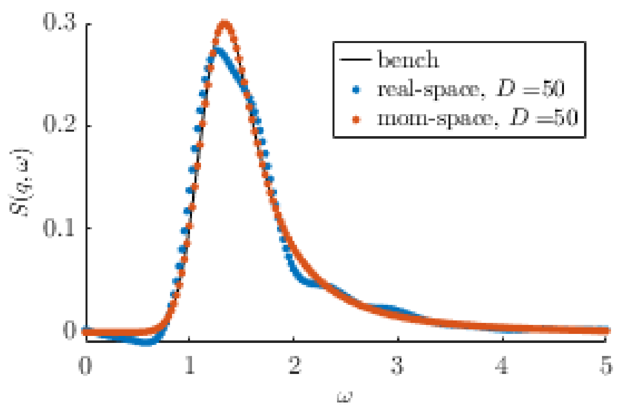




Overview

Motivation: spectral functions in quantum matter

Momentum methods: quasiparticle ansatz

Time evolution in real space

Time evolution in momentum space

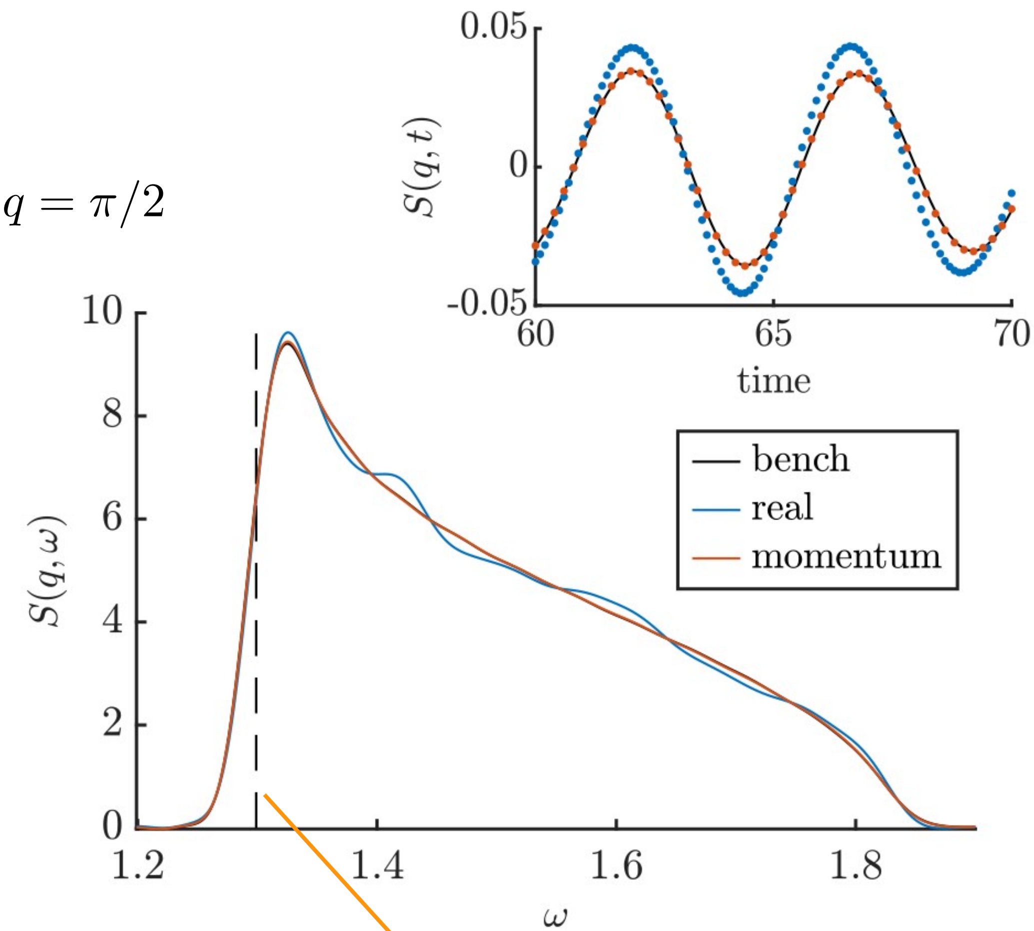
Results

Outlook

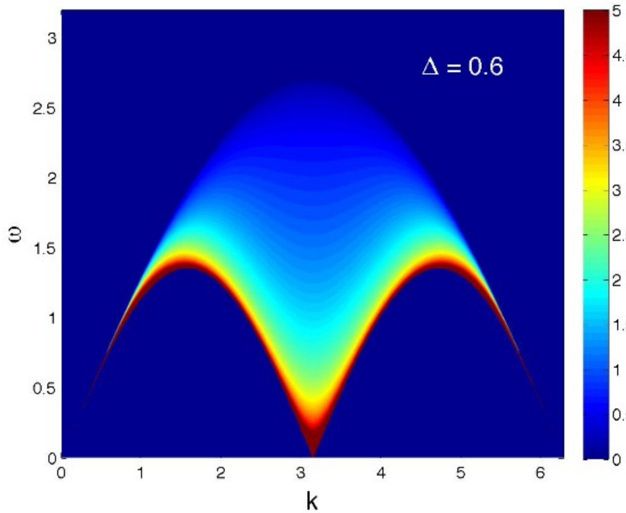
Results

Benchmark: XXZ chain

$q = \pi/2$



edge of the continuum

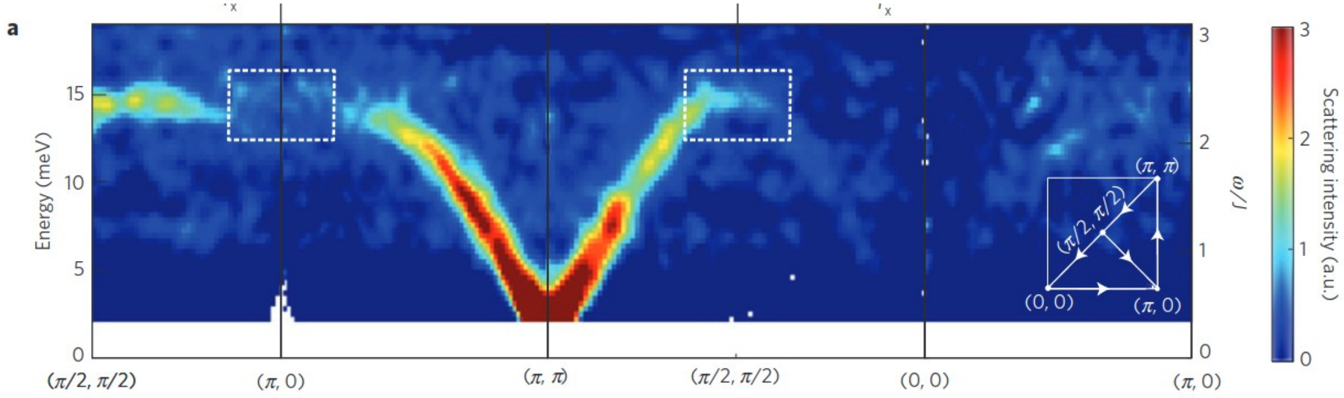


Caux et al, J. Stat. Mech. P01007 (2012)

Results

Application: J1-J2 Heisenberg model on 6-leg cylinder

→ we compute the spectral lineshape for M point: $q = (\pi, 0)$



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

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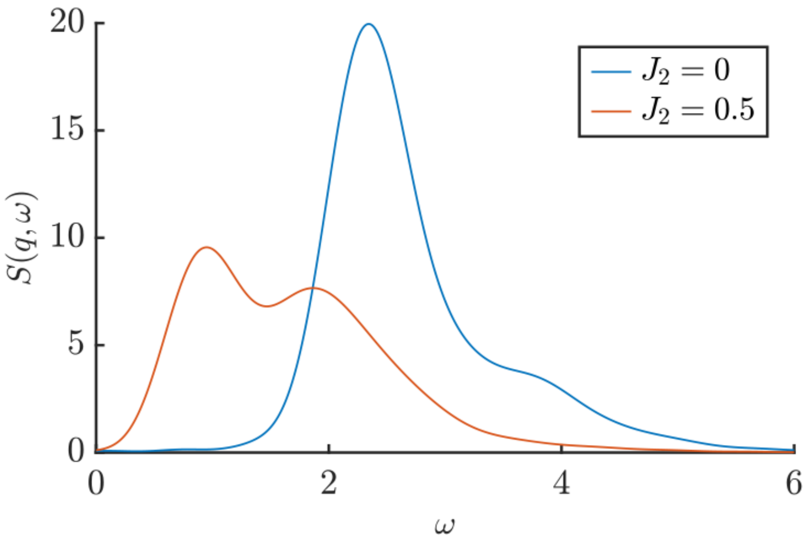

→ huge finite-circumference effect

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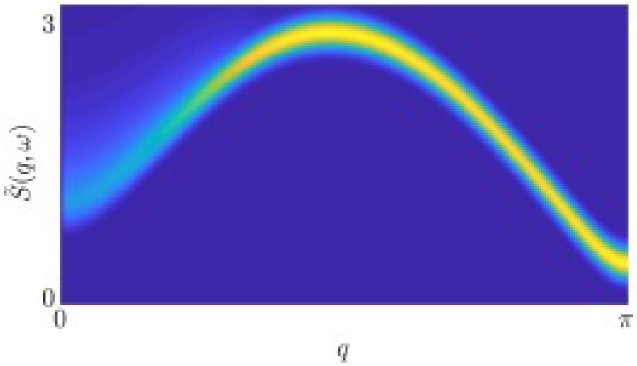
Complementary methods

real-space: get full spectral function in one run

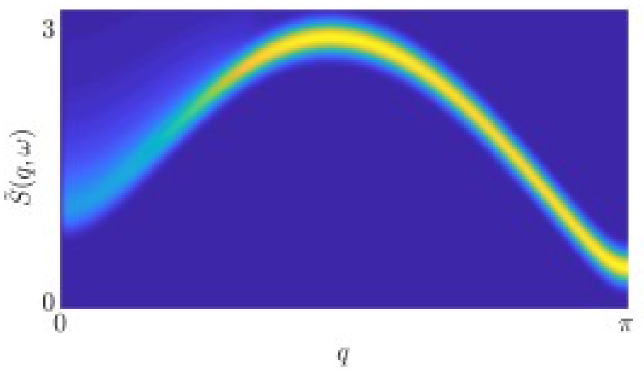


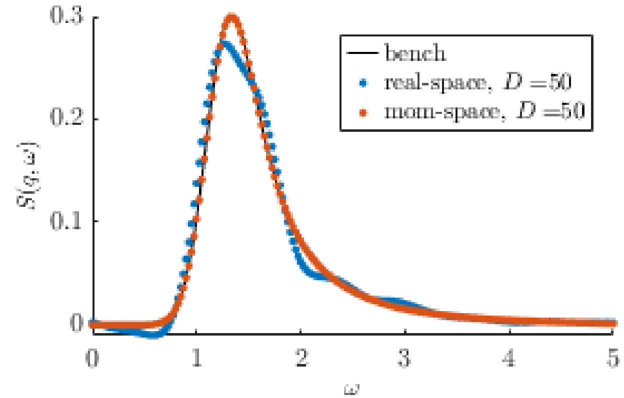
Outlook

Complementary methods

real-space: get full spectral function in one run

momentum space: fine-grained lineshapes





Outlook

Complementary methods

- real-space: get full spectral function in one run
- momentum space: fine-grained lineshapes

Other approaches than time evolution?

- correction vector or Chebyshev expansions
- extrapolation techniques, e.g. linear prediction

Outlook

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PEPS methods for spectral functions

Outlook

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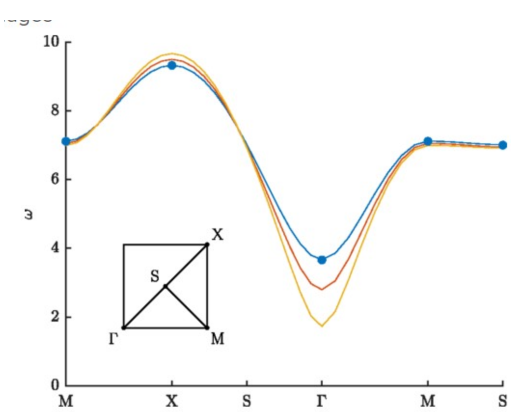
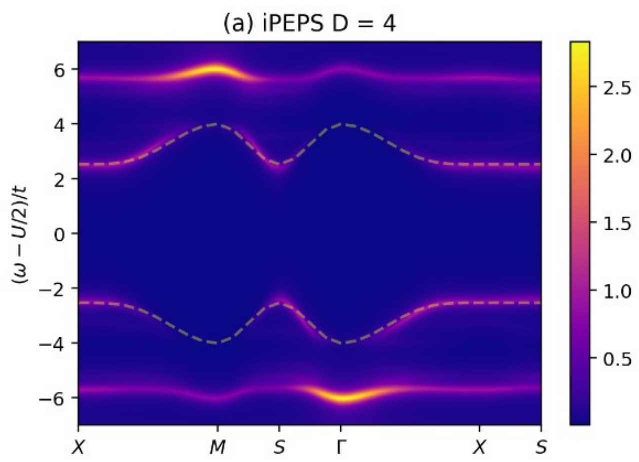
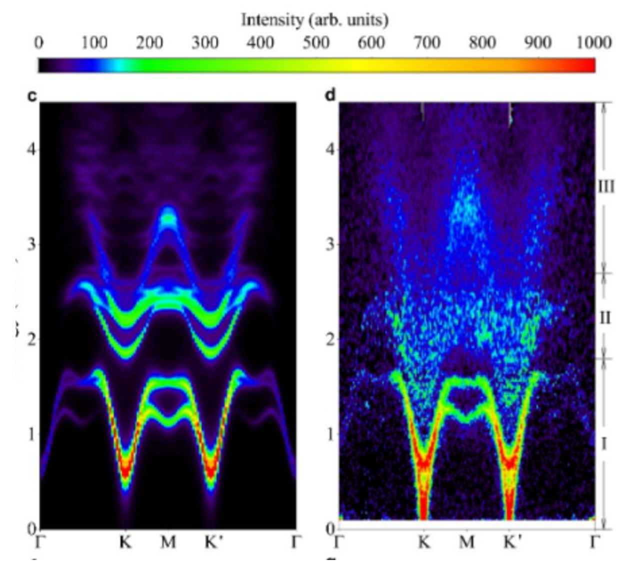
quasiparticle excitation ansatz







LV et al, Phys. Rev. B 99, 165121 (2019)
Ponsioen et al, SciPost 12, 6 (2022)
Chi et al, arXiv:2201.12121

Outlook

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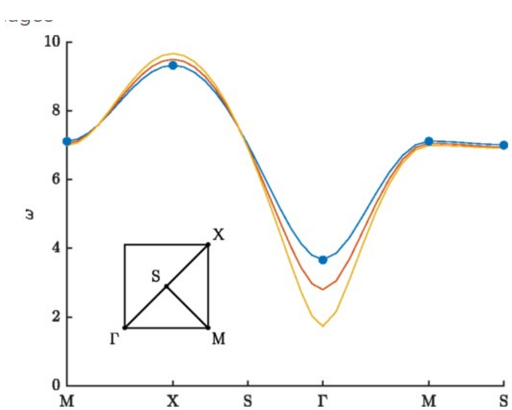

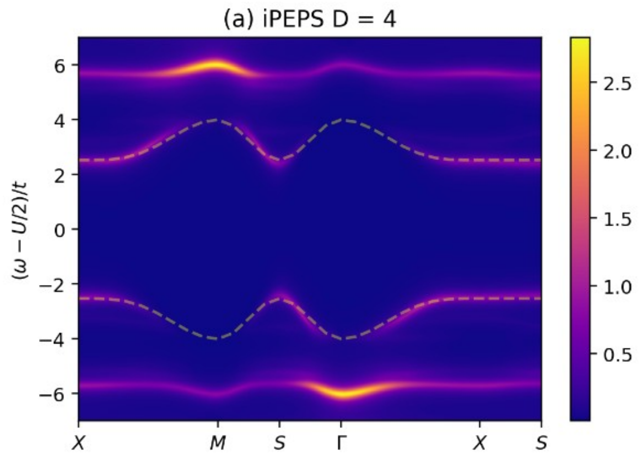

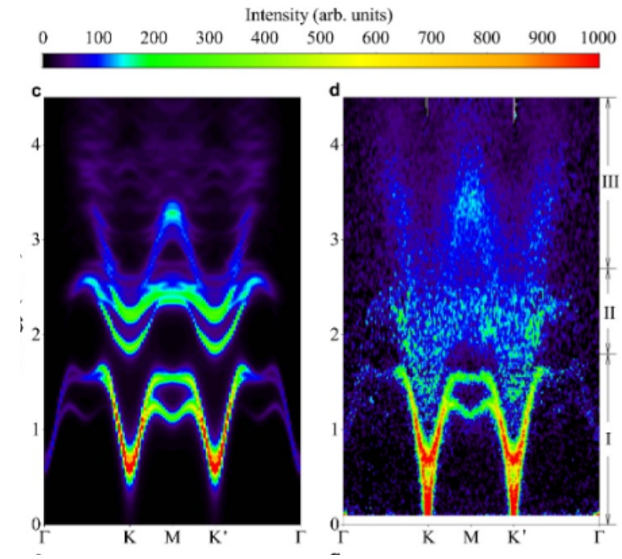

Can we extend to momentum-resolved time evolution?

LV et al, Phys. Rev. B 99, 165121 (2019)
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Thank you!