Simulating excitation spectra with PEPS

Laurens Vanderstraeten
University of Ghent

Overview

Quasiparticles in strongly-correlated quantum systems

The MPS quasiparticle ansatz

Two-particle scattering

The PEPS quasiparticle ansatz

Outlook

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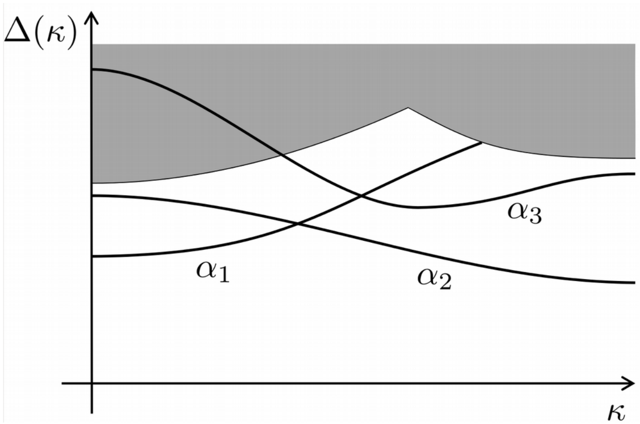
In strongly-correlated systems, the quasiparticles are typically not connected to a free limit

Quasiparticles in strongly-correlated systems

Variational approach

→ can we target low-energy eigenstates directly?



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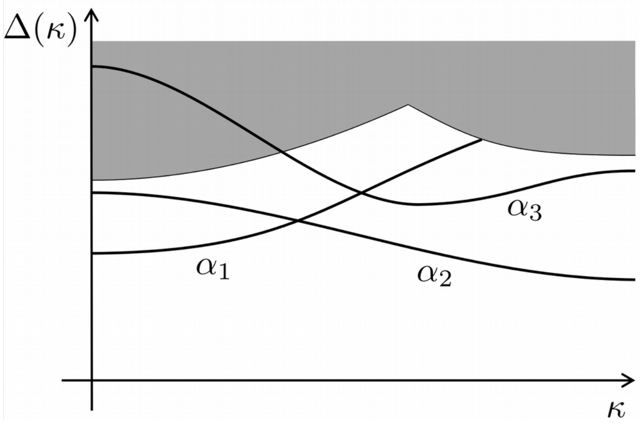

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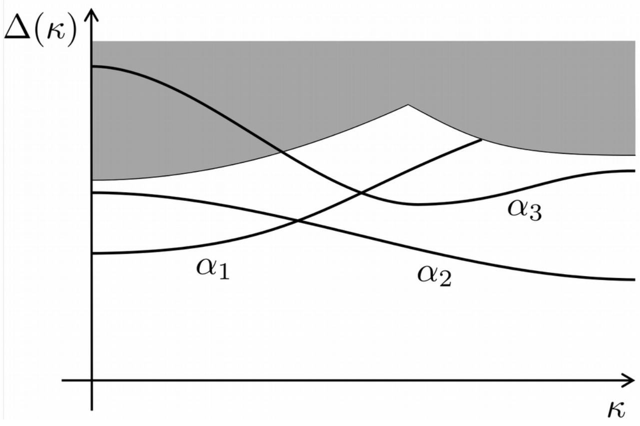

Feynman, Physical Review 94, 262 (1954)

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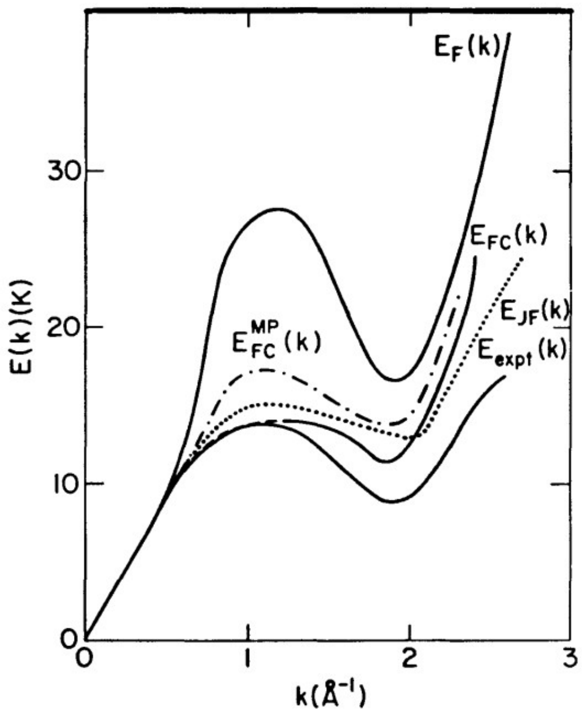

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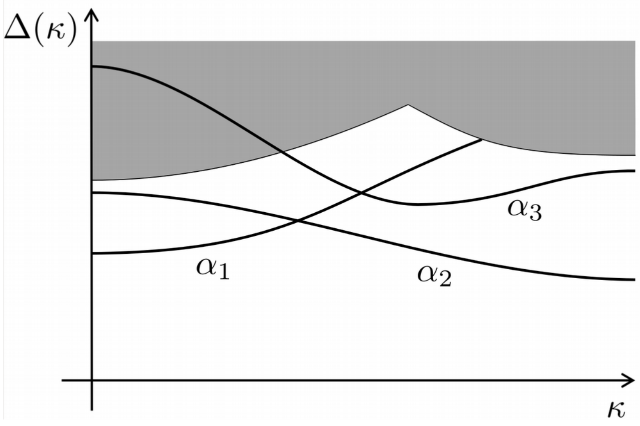

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Arovas, Auerbach & Haldane, PRL 60, 531 (1988)

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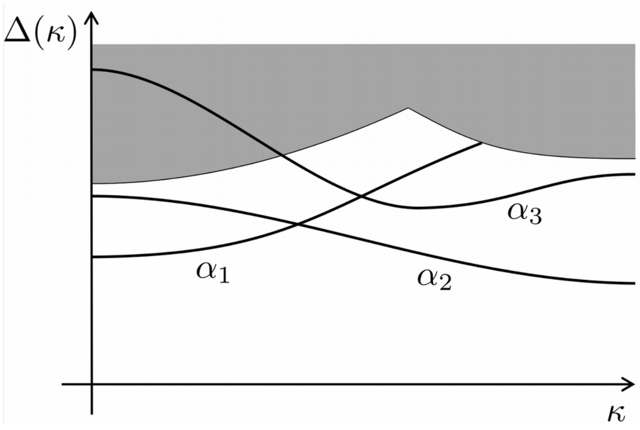

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In general, an excited state is a dressed object on a strongly-correlated background

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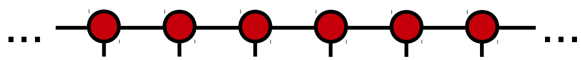
The MPS quasiparticle ansatz

Östlund & Rommer, PRL 75, 3537 (1995)
Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, Verstraete, PRB 85, 100408 (2012).

The MPS quasiparticle ansatz

Start from the MPS ground state in the thermodynamic limit

$$|\Psi\rangle_{\mathrm{MPS}} =$$



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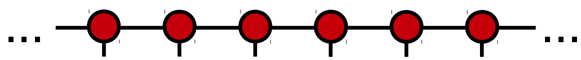
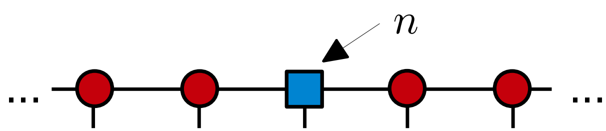


MPS version of the single-mode approximation

$$|\Phi_p\rangle = \sum_n \mathrm{e}^{ipn}$$



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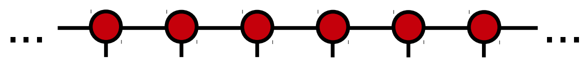

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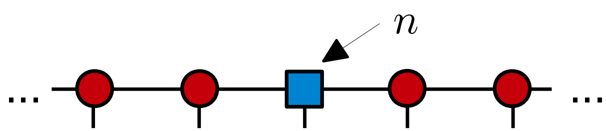

Optimize over blue tensor variationally

- → correlations in the ground state are exploited to make a dressed quasiparticle
- → systematic refining of variational ansatz

Östlund & Rommer, PRL 75, 3537 (1995)
Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, Verstraete, PRB 85, 100408 (2012).

The MPS quasiparticle ansatz

Variational approach is extremely accurate!

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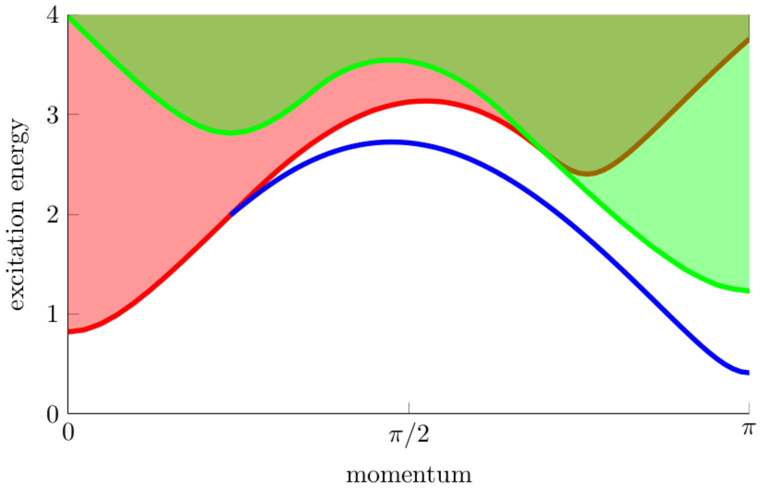
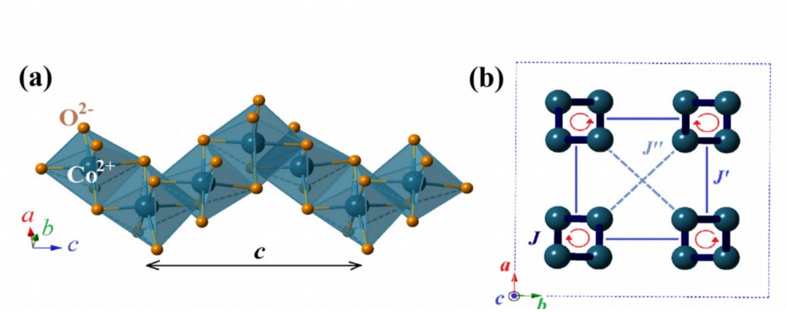
→ example: spin-1 Heisenberg chain



Haldane gap
$\Delta \approx 0.41047924871$

Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, Verstraete, PRB 85, 100408 (2012)

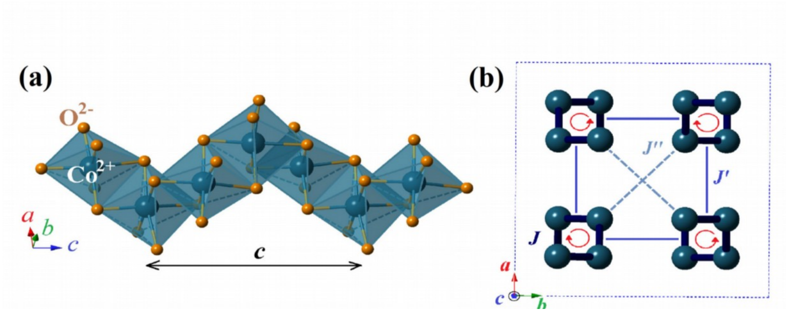
The MPS quasiparticle ansatz



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

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

The MPS quasiparticle ansatz



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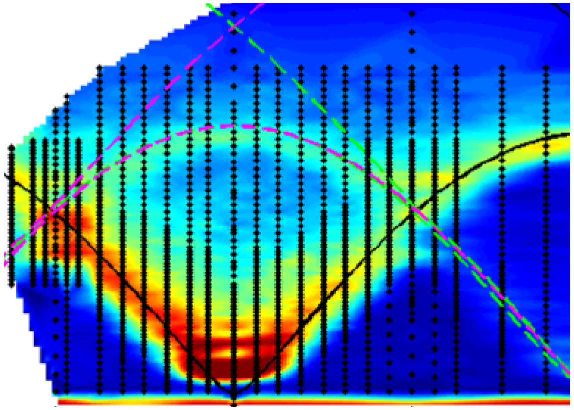

inelastic neutron-scattering measurement of the spin structure factor

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

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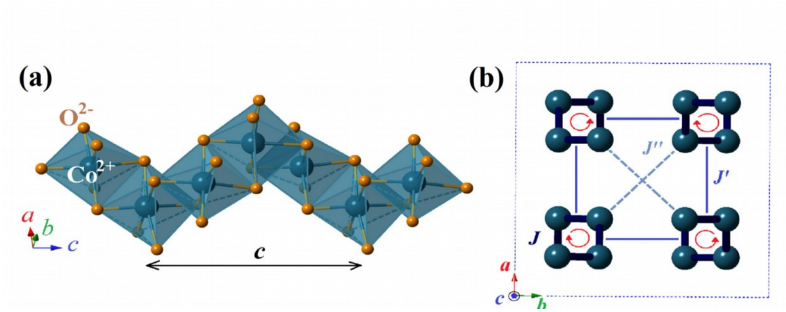

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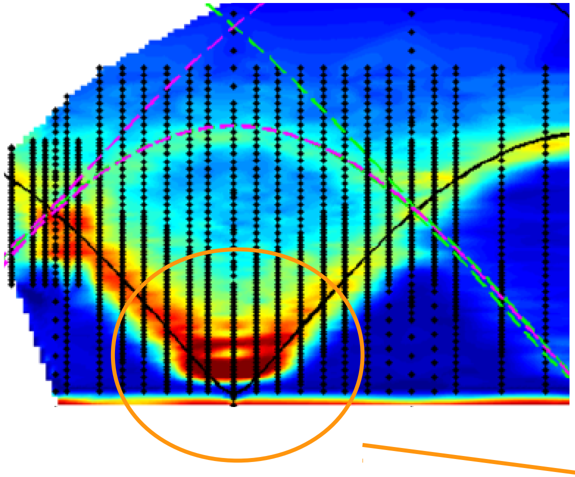

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bound states of spinons

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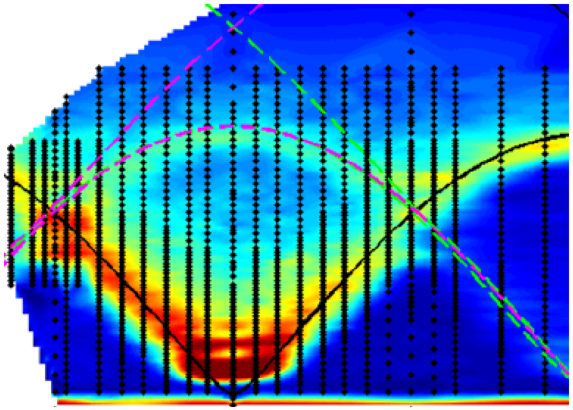

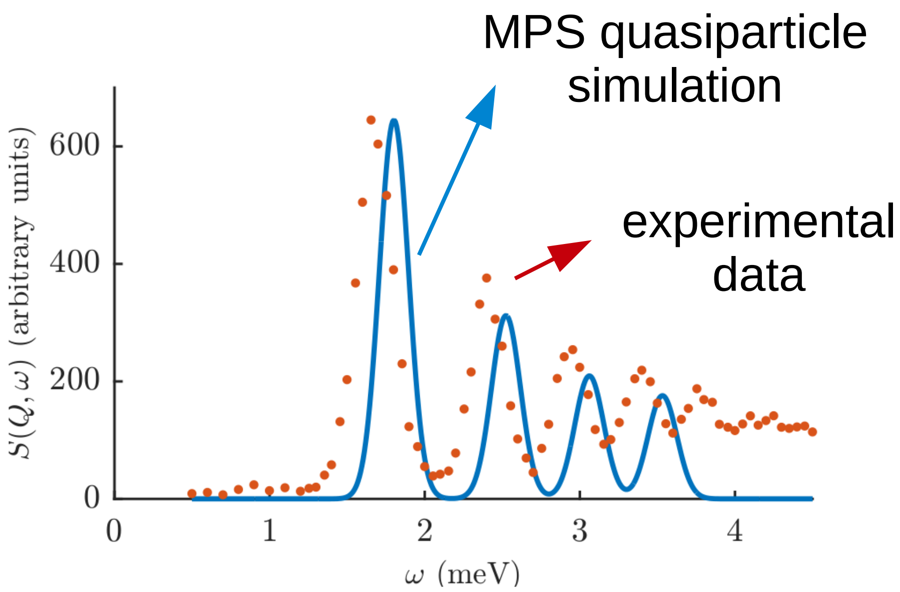

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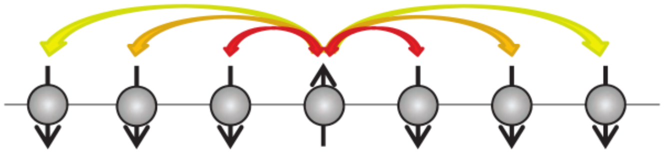

Spin chains with long-range interactions

$$H = -\sum_{i<j} \frac{S_i^z S_j^z}{(j-i)^\alpha} + h \sum_i S_i^x$$

LV, Van Damme, Büchler, Verstraete,
PRL 121, 090603 (2018)

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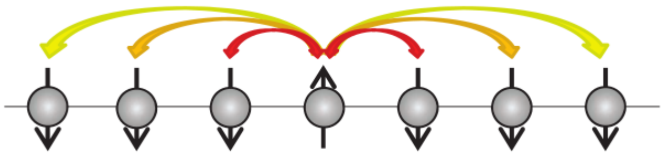

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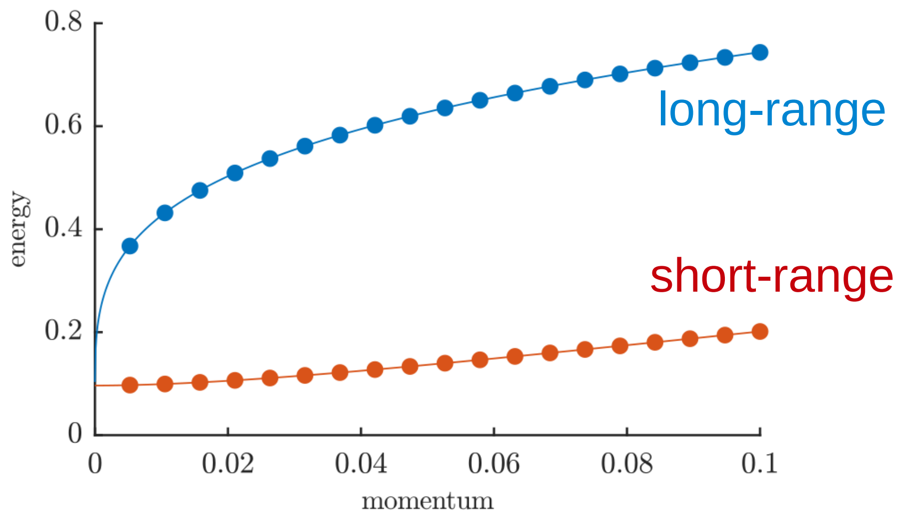

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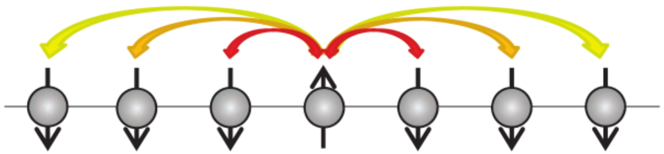

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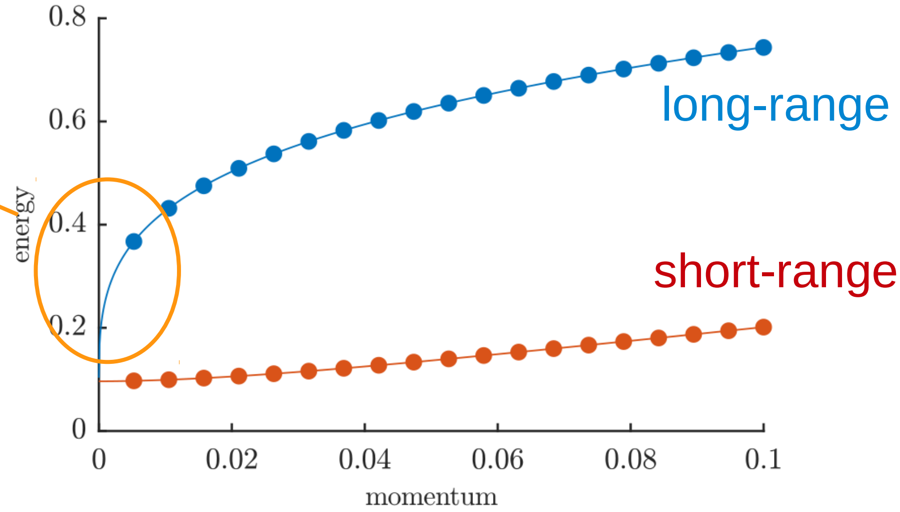
infinite group velocity



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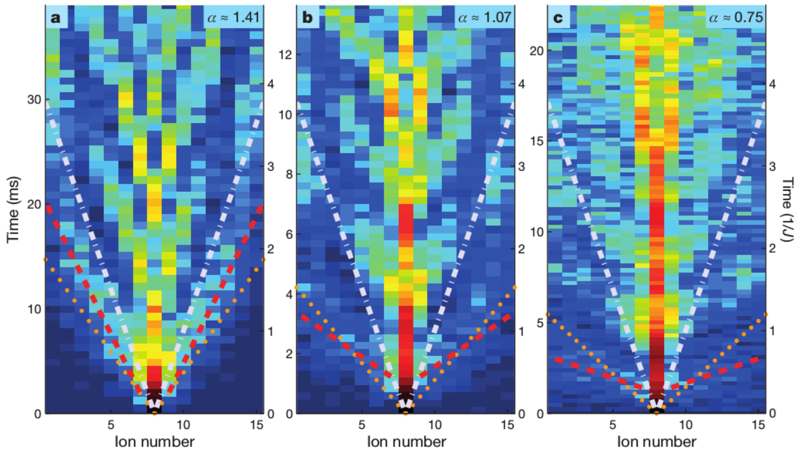

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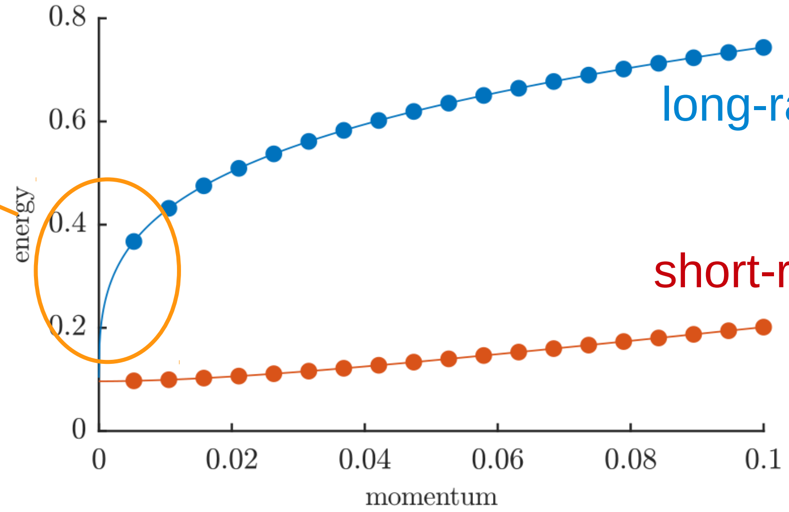

LV, Van Damme, Büchler, Verstraete, PRL 121, 090603 (2018)

The MPS quasiparticle ansatz

Quasiparticles and symmetries

→ by implementing symmetries in the MPS representation, we can fix quantum numbers

→ fractionalization: spinons, chargeons, holons, etc.

Zauner-Stauber, LV, Haegeman, McCulloch, Verstraete, PRB 97, 235155 (2018)

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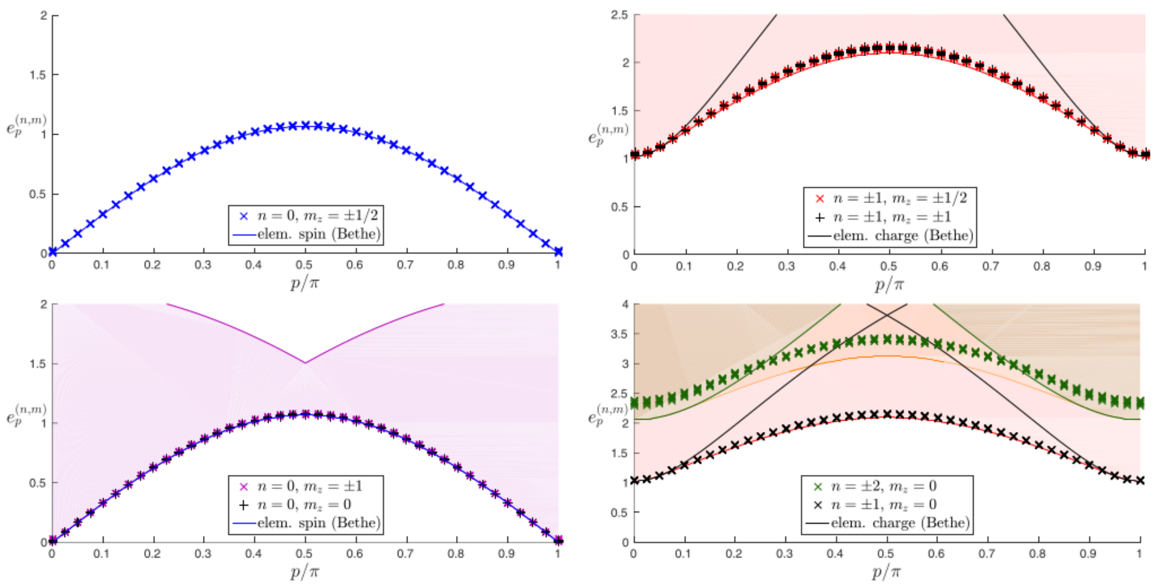

spin excitations　　charge excitations

one-dimensional Hubbard model

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Elementary excitations have a natural interpretation in terms of particles moving against a strongly-correlated background state

→ can we do many-particle physics?

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Stationary scattering theory

→ find two-particle wavefunctions variationally

→ the asymptotic part of the wavefunction contains the two-particle S matrix

LV, Haegeman, Osborne, Verstraete, PRL 112, 257202 (2014)
LV, Verstraete, Haegeman, PRB 92, 125136 (2015)
LV, Haegeman, Verstraete, Poilblanc, PRB 93, 235108 (2016)

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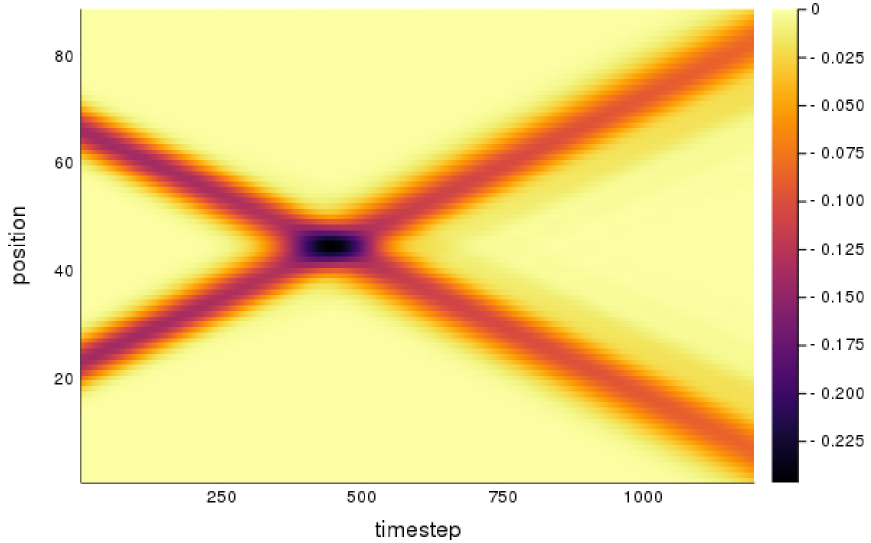
→ can we do many-particle physics?

Dynamical scattering theory



→ determine scattering phase shift?

Van Damme, Haegeman, Verstraete, LV, *in preparation*

Two-particle scattering

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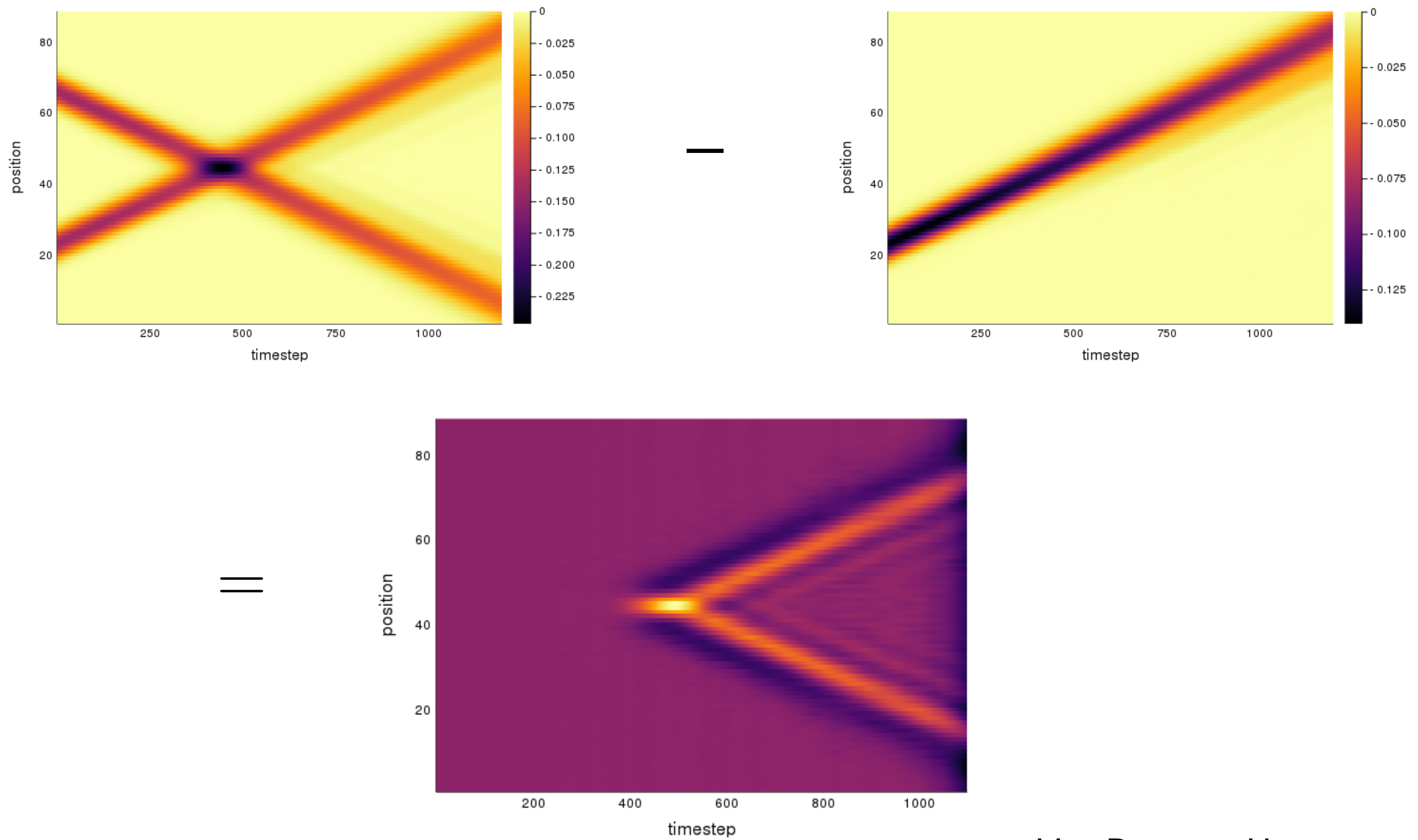

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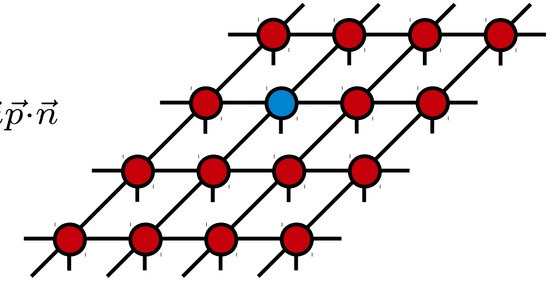
Excitation ansatz can be extended to two dimensions

LV, Mariën, Verstraete, Haegeman, PRB 92, 201111 (2015)
LV, Haegeman, Verstraete, arXiv: 1809.06747 (2018)

The PEPS quasiparticle ansatz

Excitation ansatz can be extended to two dimensions

$$|\Phi_{\vec{p}}(B;A)\rangle = \sum_n \mathrm{e}^{i\vec{p}\cdot\vec{n}}$$

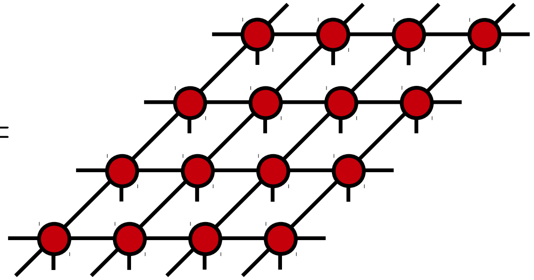


BUT: numerical manipulations are a lot harder

LV, Mariën, Verstraete, Haegeman, PRB 92, 201111 (2015)
LV, Haegeman, Verstraete, arXiv: 1809.06747 (2018)

The PEPS quasiparticle ansatz

Step 1: find an optimal PEPS approximation for the ground state

$|\Psi(A)\rangle =$ 

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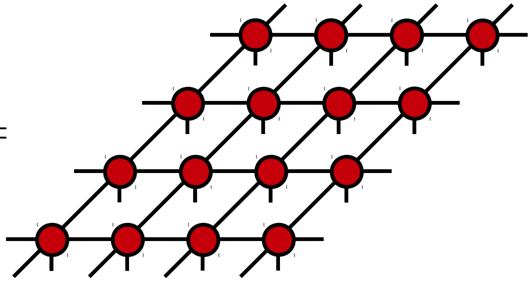
$$|\Psi(A)\rangle =$$ 

Different algorithms

→ simple update

Jiang, Weng, Xiang, PRL 101, 090603 (2008)

→ full update

Jordan, Orús, Vidal, Verstraete, Cirac, PRL 101, 250602 (2008)

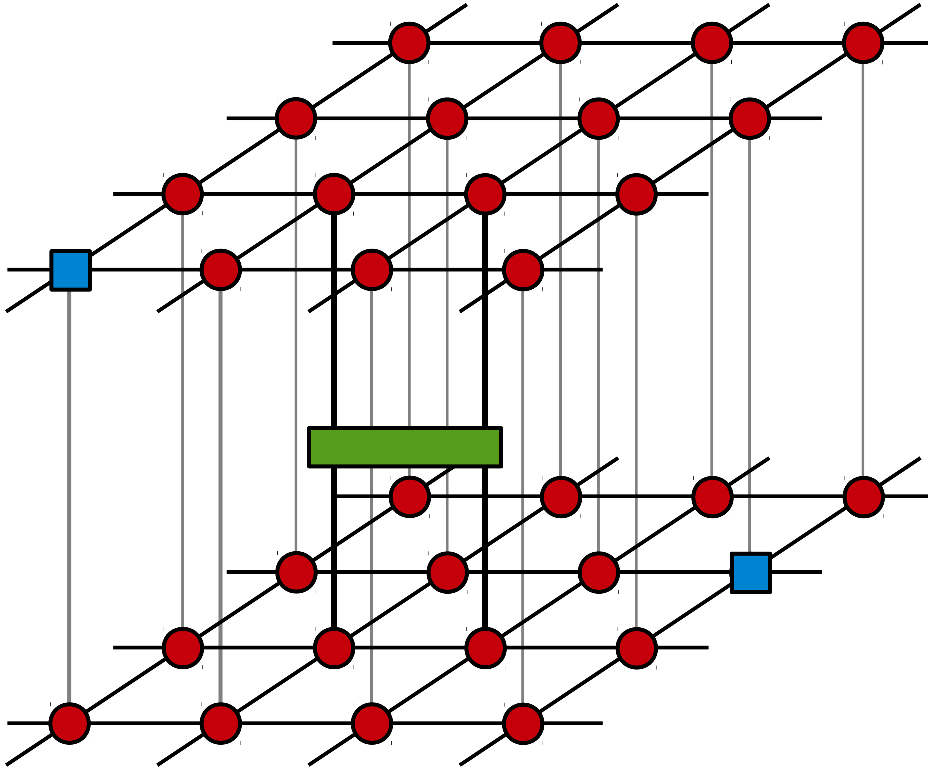
→ variational optimization

Corboz, PRB 94, 035133 (2016)
LV, Haegeman, Corboz, Verstraete PRB 94, 155123 (2016)

The PEPS quasiparticle ansatz

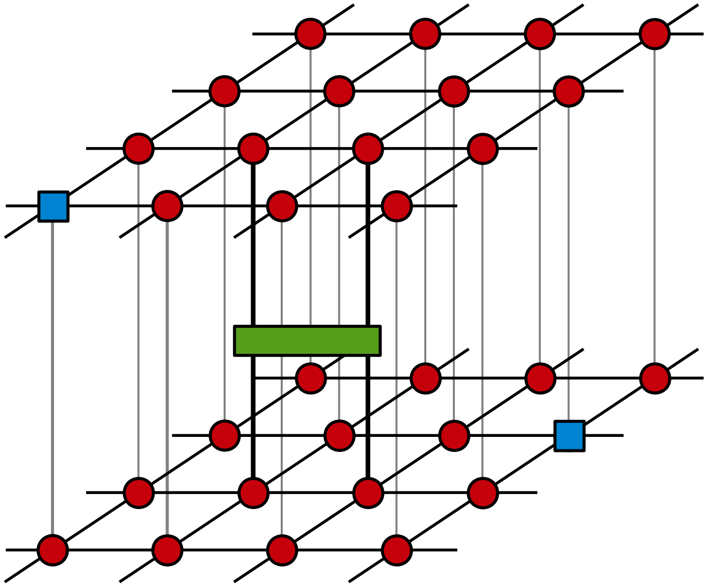
Step 2: evaluation of the energy

$$\langle \Phi_{\vec{p}}(B;A)|\, H \,|\Phi_{\vec{p}}(B;A)\rangle \sim$$



The PEPS quasiparticle ansatz

Evaluation of the energy involves non-trivial contractions



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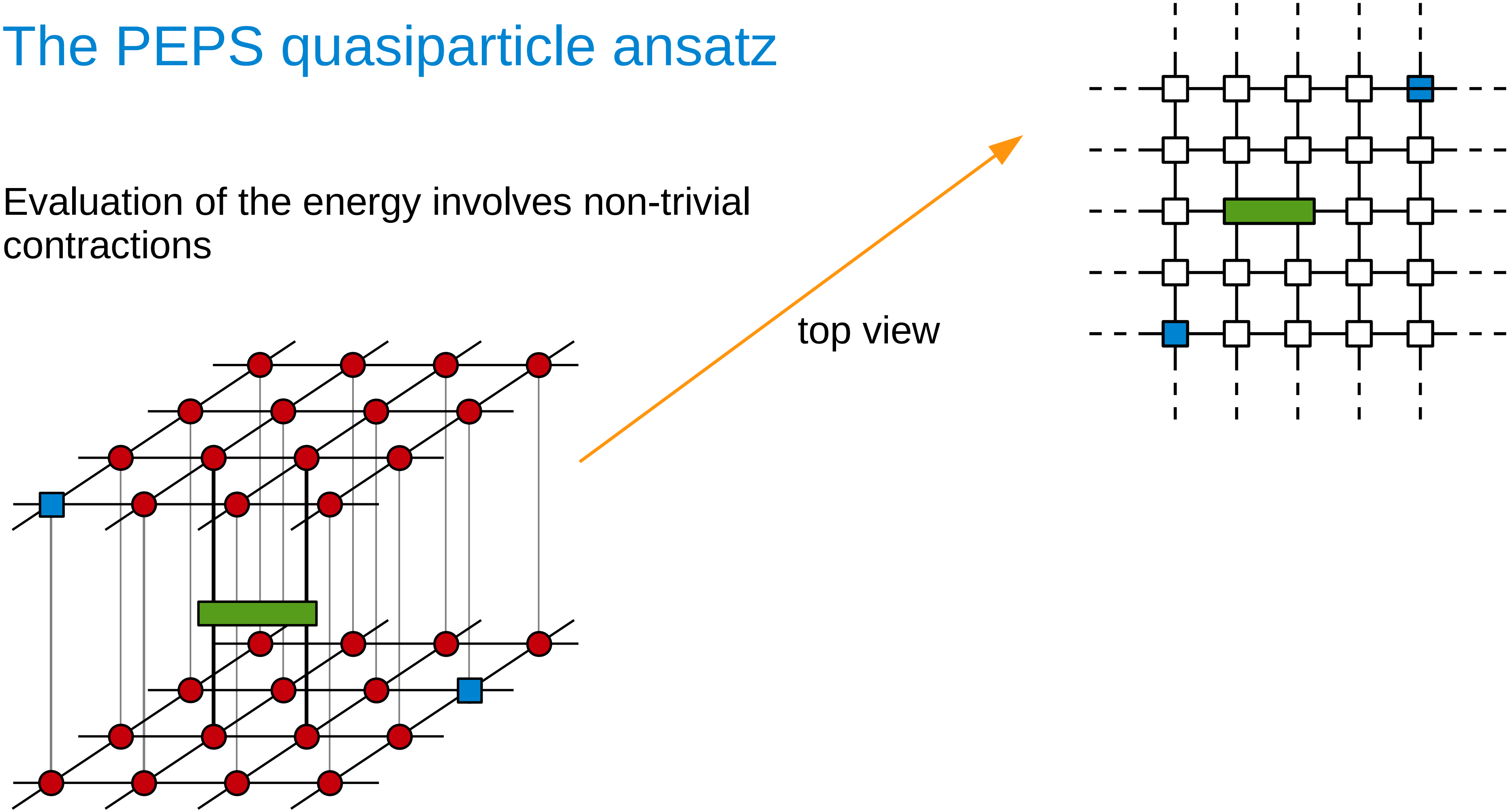

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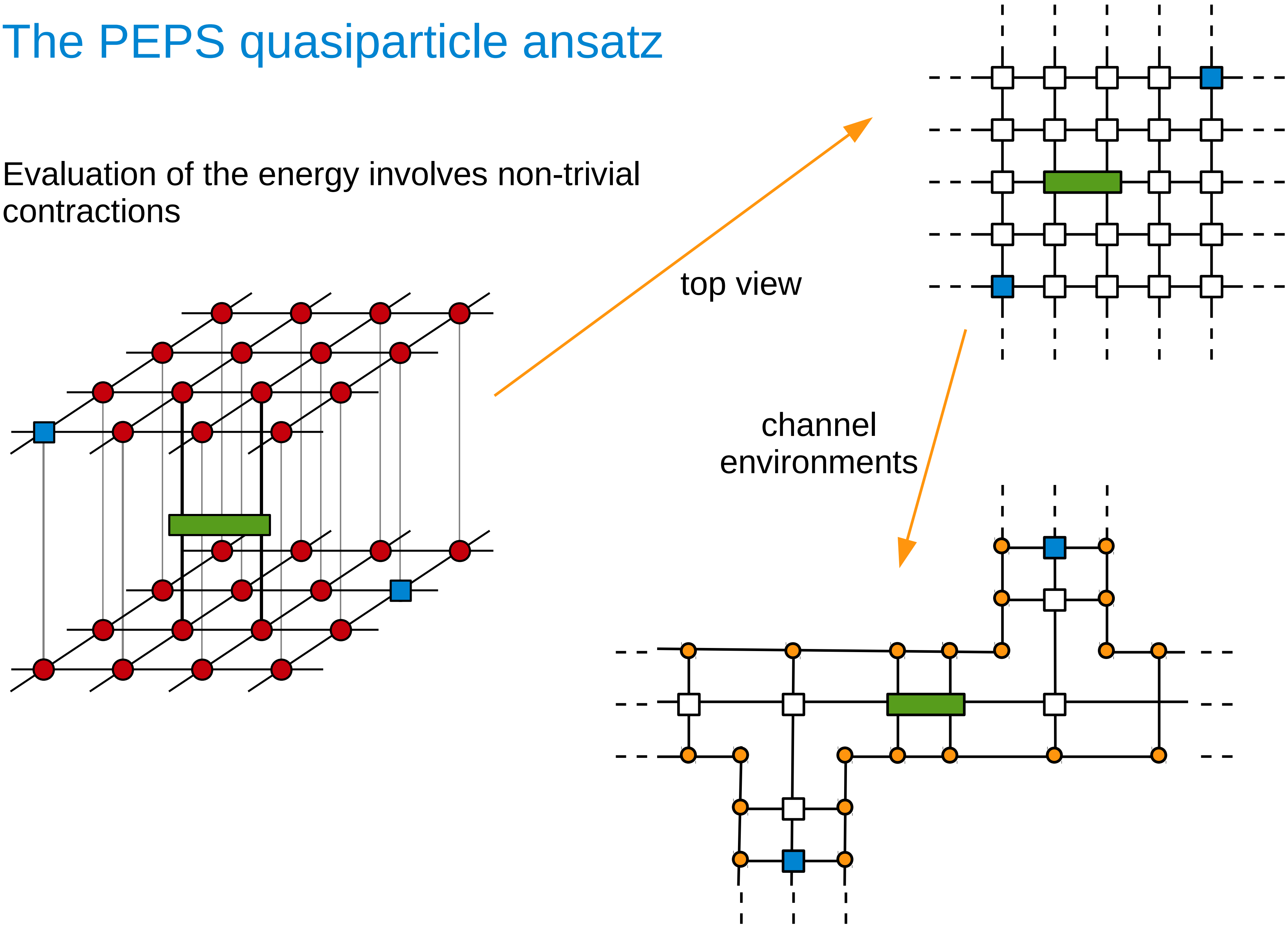

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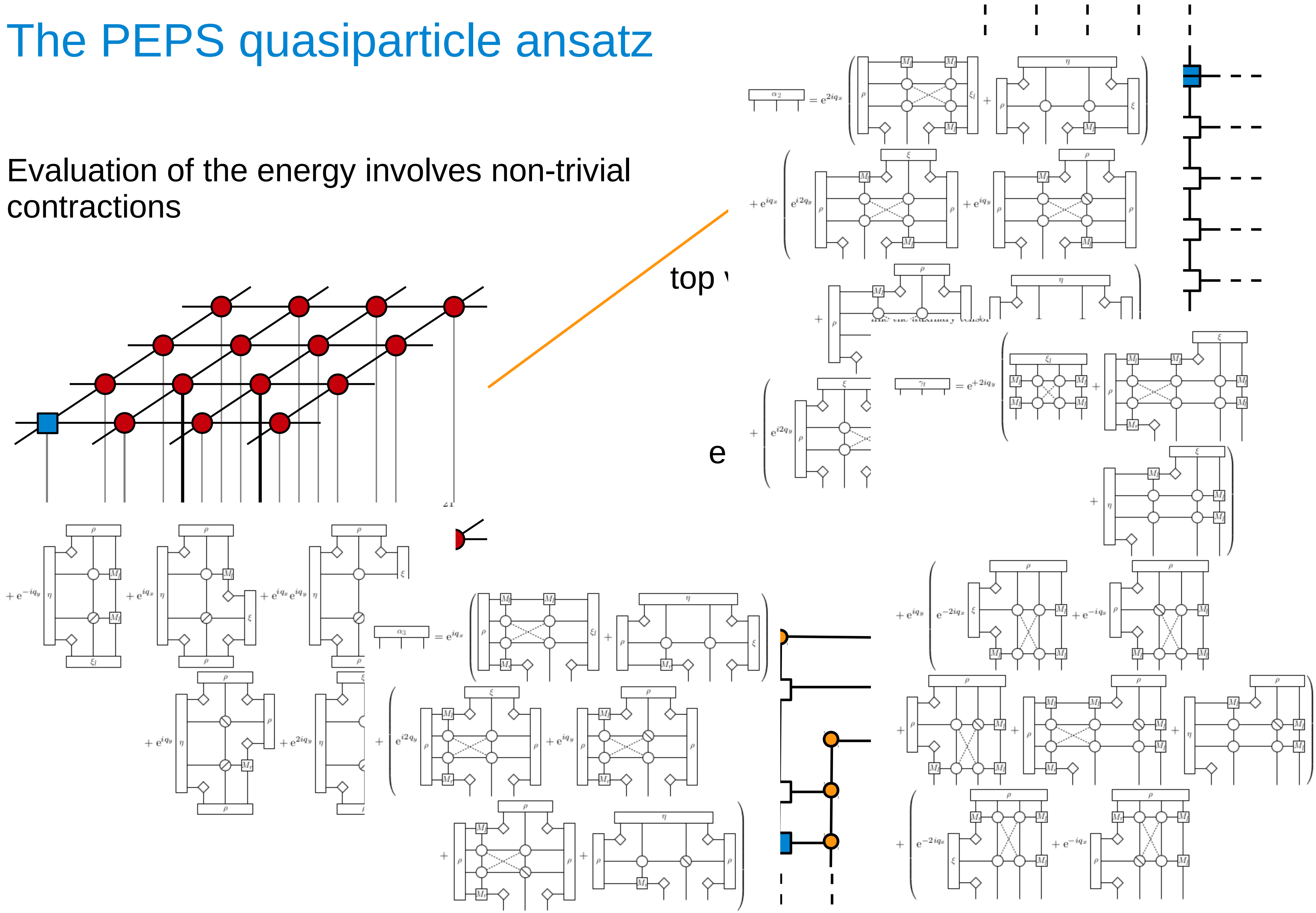

The PEPS quasiparticle ansatz

Benchmark: two-dimensional Ising model on the square lattice

$$H_{\text{Ising}} = -\sum_{\langle ij \rangle} S_i^z S_j^z + \lambda \sum_i S_i^x$$

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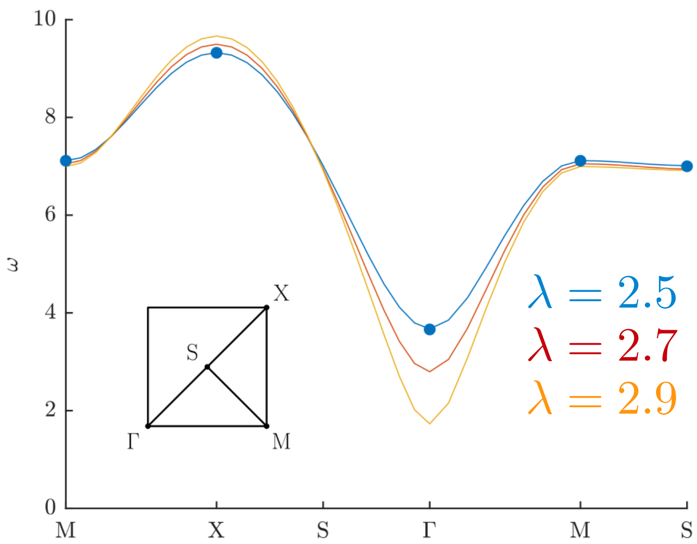
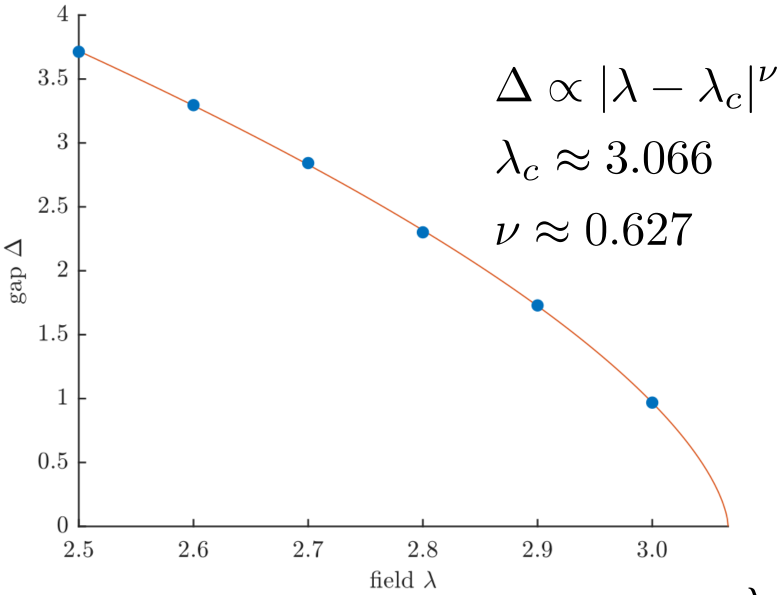
dispersion relation (D=3)



gap as a function of field

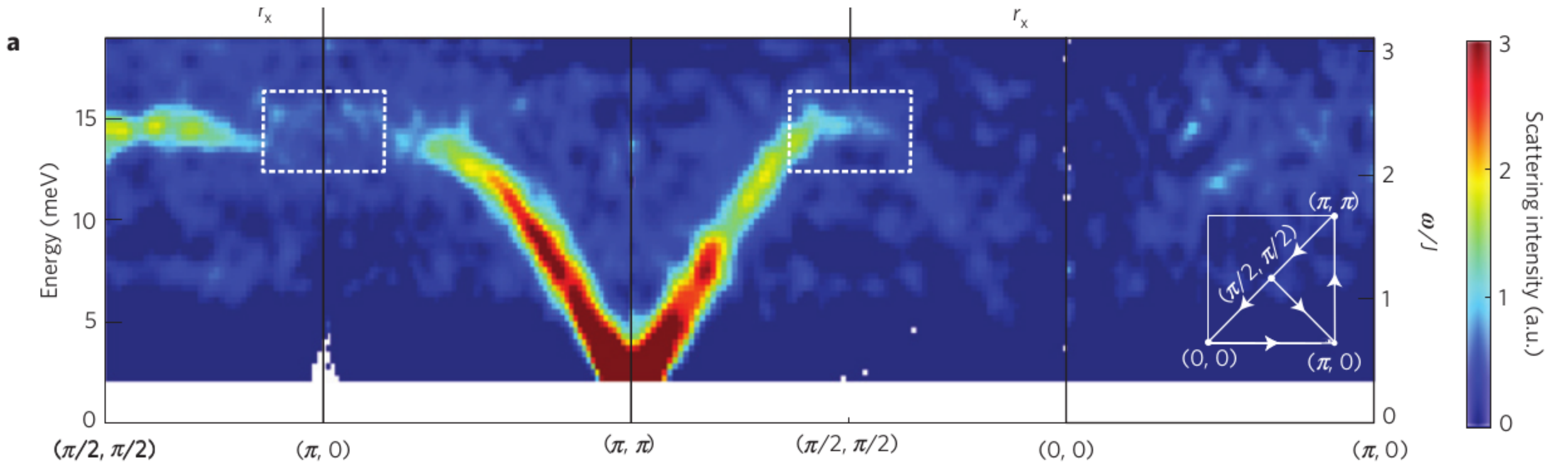


Monte Carlo: $\lambda_c = 3.044$, $\nu = 0.630$

The PEPS quasiparticle ansatz

Application: spin-wave anomaly in square-lattice Heisenberg model

inelastic neutron-scattering experiments have
revealed a drop in the dispersion relation

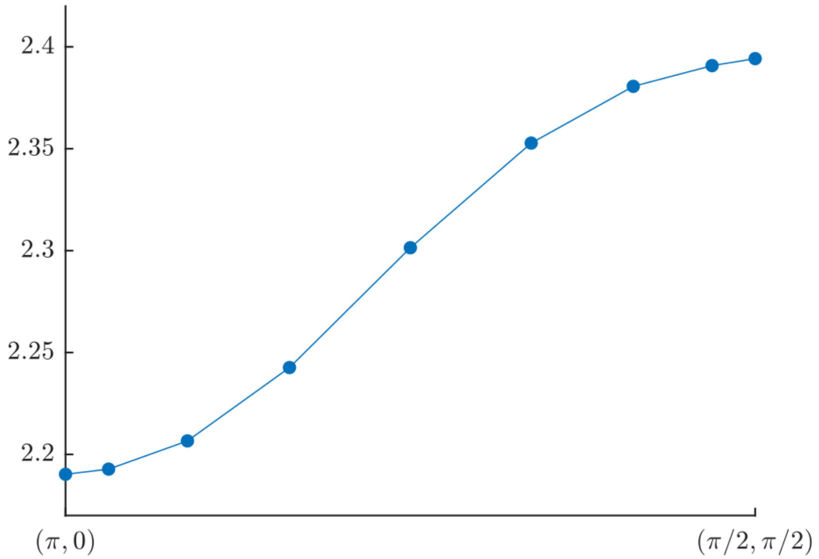


Dalla Piazza, et. al., Nature Physics 11, 62 (2015)

The PEPS quasiparticle ansatz

Example: spin-wave anomaly in square-lattice Heisenberg model

inelastic neutron-scattering experiments have revealed a drop in the dispersion relation



	$(\pi/2, \pi/2)$	$(\pi, 0)$
Quantum Monte Carlo	2.4085	2.13
Perturbation theory	2.375	2.2
Exact diagonalization	2.4144	2.2281
Two-dimensional DMRG	2.40	2.06-2.07
PEPS $D = 4$	2.39	2.19

LV, Haegeman, Verstraete, arXiv: 1809.06747 (2018)

Overview

Quasiparticles in strongly-correlated quantum systems

The MPS quasiparticle ansatz

Two-particle scattering

The PEPS quasiparticle ansatz

Outlook

Outlook

We can create quasiparticle excitations for generic spin systems in one and two dimensions

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We can create quasiparticle excitations for generic spin systems in one and two dimensions

- → electronic systems (Hubbard model)
- → topological excitations in two-dimensional systems (spinons, anyons, etc.)
- → many-particle physics
- → quasiparticles at finite temperature

Thank you!