Matrix Product State Methods for Excitations

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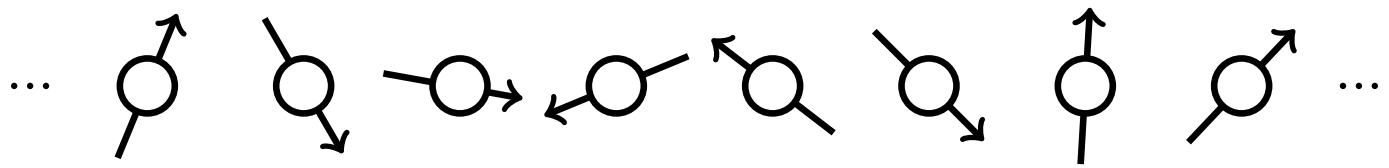
Introduction: Quantum many-body physics

Consider an N-body system:



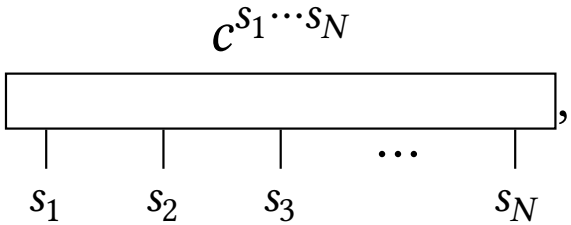
Classical: $\mathcal{O}(N)$ DOFs.

Quantum: $\mathcal{O}(\exp N)$ DOFs.

Introduction: Matrix product states

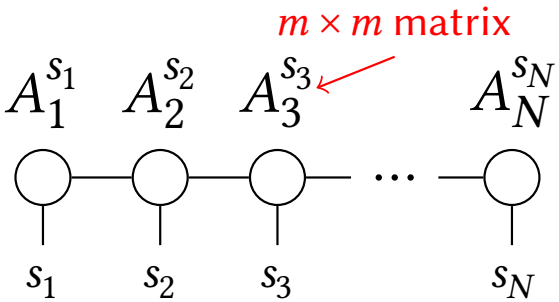
General pure state:

$$|\Psi\rangle = \sum_{s_1 \cdots s_N} c^{s_1 \cdots s_N} |s_1 s_2 s_3 \cdots s_N\rangle, \qquad \mathcal{O}(\exp N) \text{ DOFs.}$$



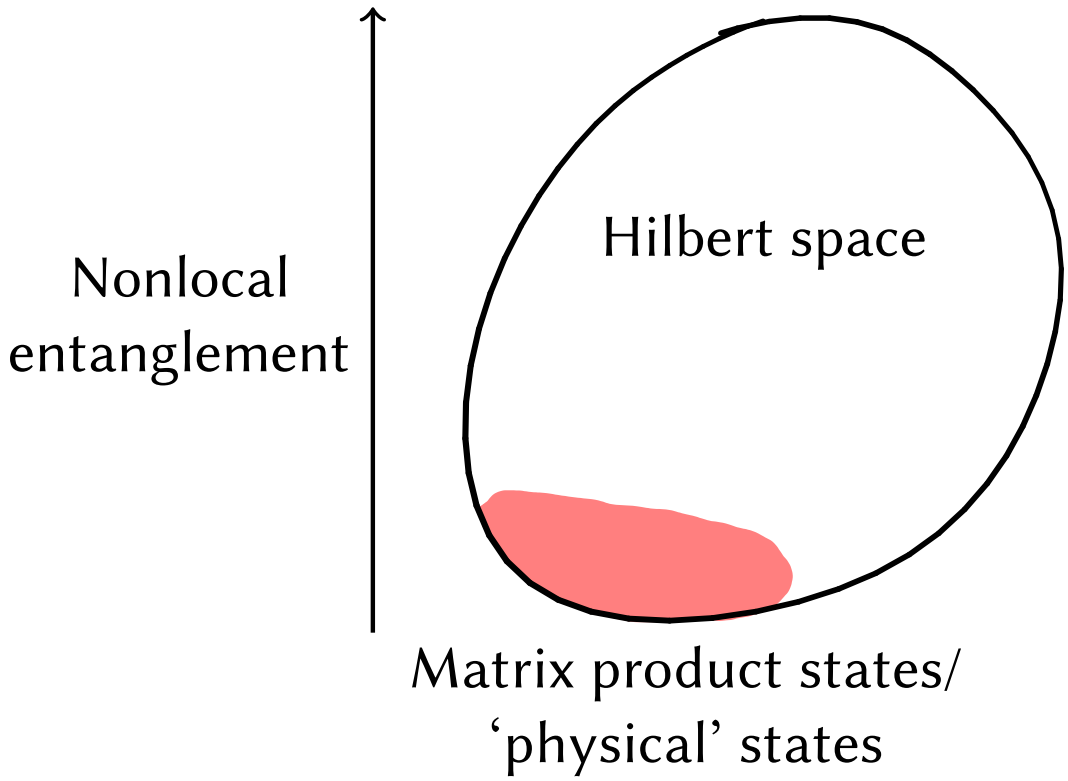
Compress as a **matrix product state**:

$$|\Psi\rangle = \sum_{s_1 \cdots s_N} A_1^{s_1} A_2^{s_2} A_3^{s_3} \cdots A_N^{s_N} |s_1 s_2 s_3 \cdots s_N\rangle, \qquad \mathcal{O}(Nm^2) \text{ DOFs.}$$

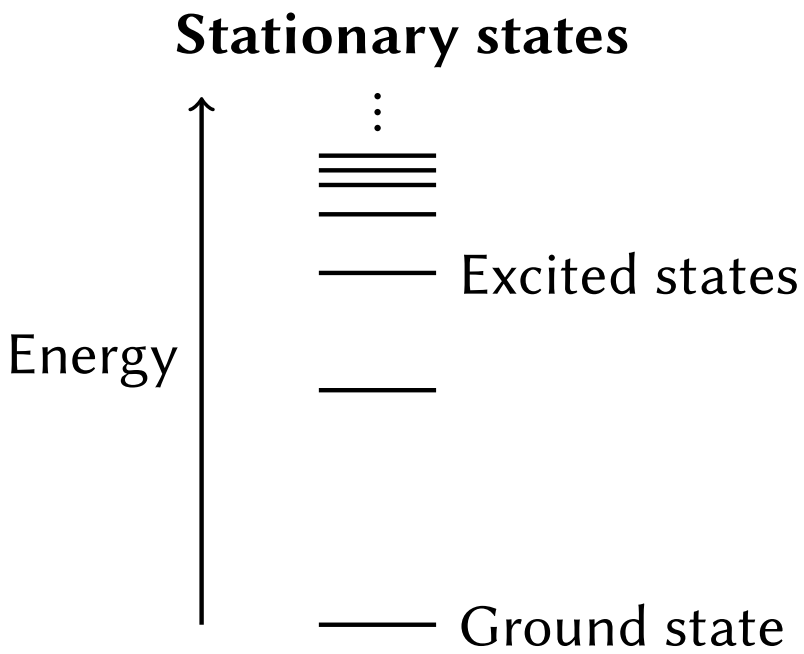


Good at representing locally-entangled ('physical') states.
Controlled by m.

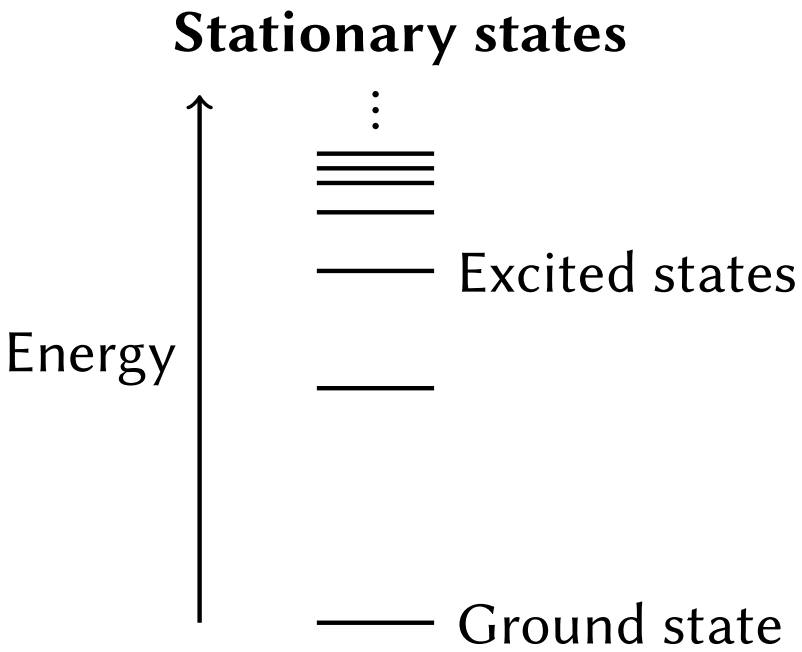
Introduction: ‘Local entanglement’



Low-temperature/energy physics

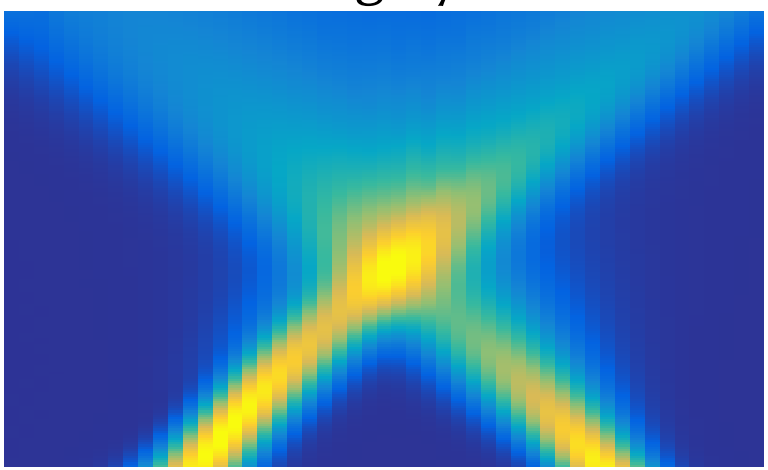


Low-temperature/energy physics



Time evolution

Scattering dynamics

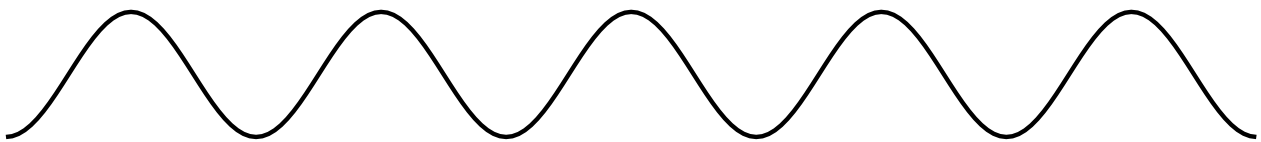


Static vs dynamic methods

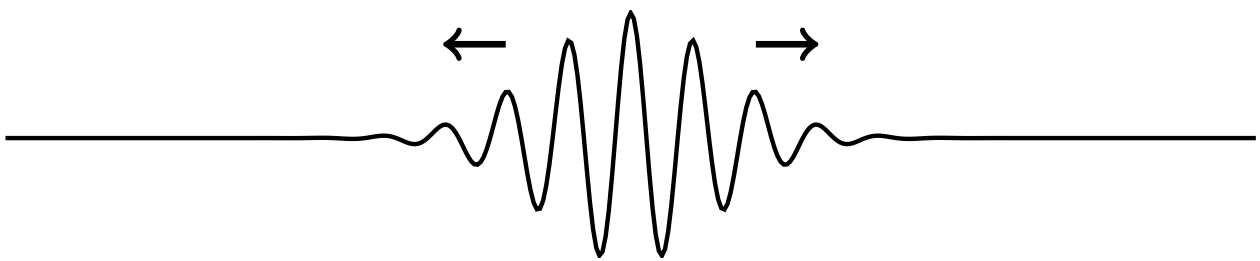
Obtain ground states using standard methods (e.g. DMRG).

Two methods for analysing excitations:

1. **Static**: Solve for the stationary states of the excitations.

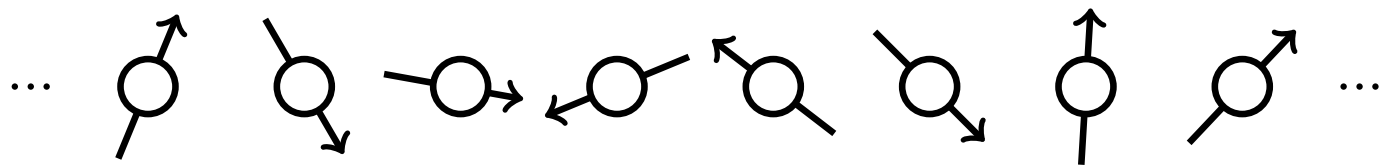


2. **Dynamic**: Time evolution of non-stationary excitations.

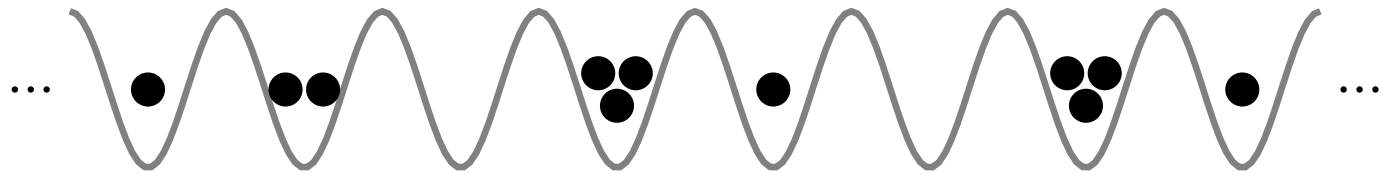


Versatility: Lattice models

- Spin chains

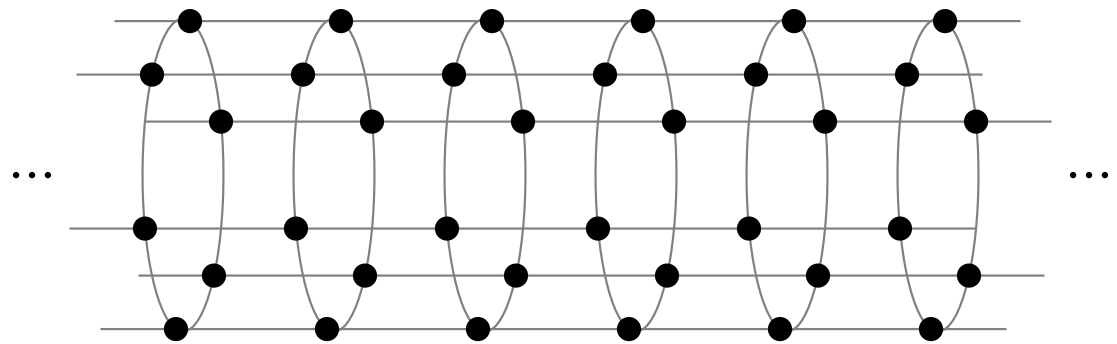


- Bose–Hubbard models



- Lattice gauge theories

2D models?

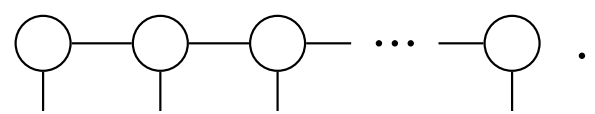


We can also also study 2D models by wrapping them on a cylinder.

Limited to small circumferences ($\lesssim 10$ sites).

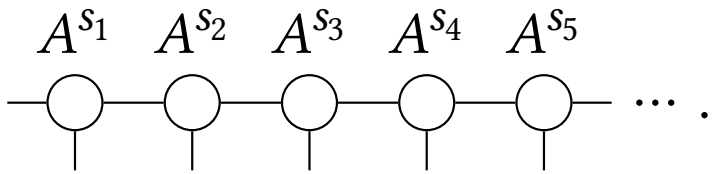
Infinite matrix product states

$$|\Psi\rangle = \quad A_1^{s_1} \quad A_2^{s_2} \quad A_3^{s_3} \qquad\qquad A_N^{s_N}$$



Enforce translation invariance and take $N \to \infty$,

$$|\Psi\rangle = \quad \cdots \quad A^{s_1} \quad A^{s_2} \quad A^{s_3} \quad A^{s_4} \quad A^{s_5} \quad \cdots$$

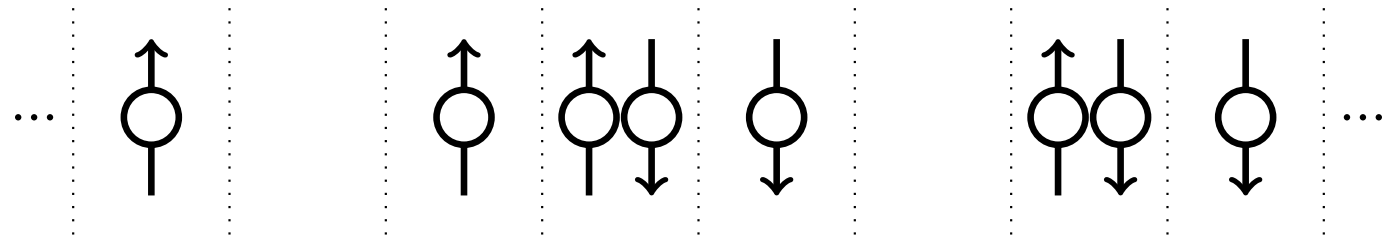


Local/global observables can be calculated by fixed-point relations.

No finite-size effects: only finite entanglement (bond dimension).

I. P. McCulloch, arXiv:0804.2509.

(Fermi–)Hubbard model

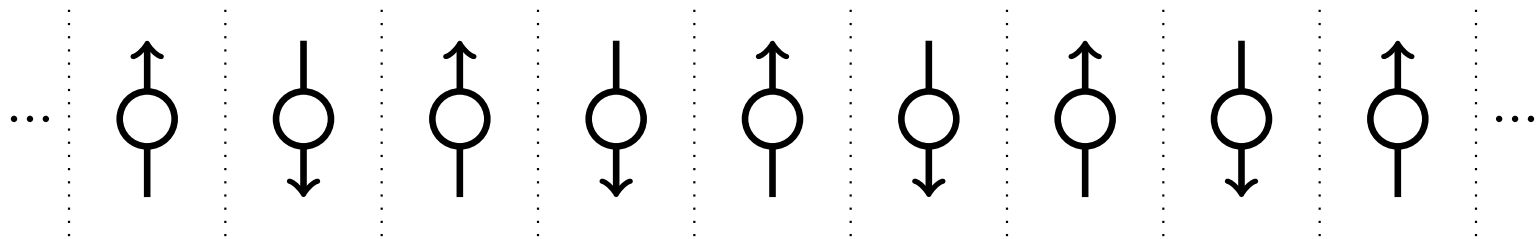


$$H = -t \sum_{\sigma,j} \left(c_{\sigma,j} c^{\dagger}_{\sigma,j+1} + \text{H.c.} \right) + U \sum_{j} n_{\uparrow,j} n_{\downarrow,j}.$$

Exactly solvable using the Bethe ansatz.

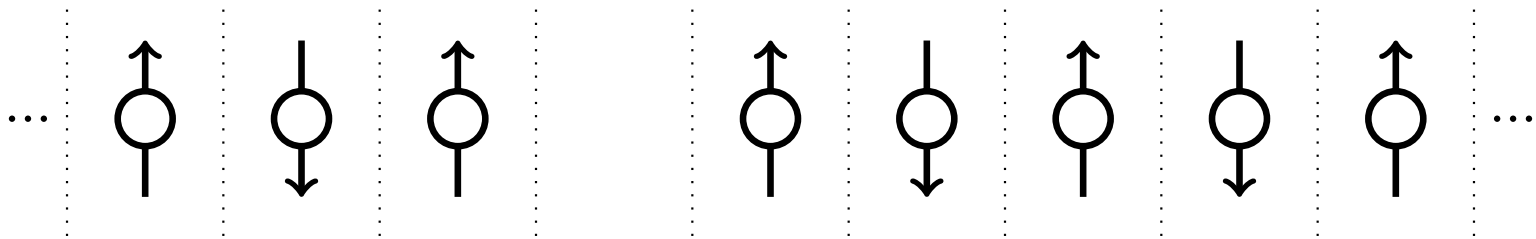
Hubbard model: Spin–charge separation

We look at the unpolarised state at half filling:



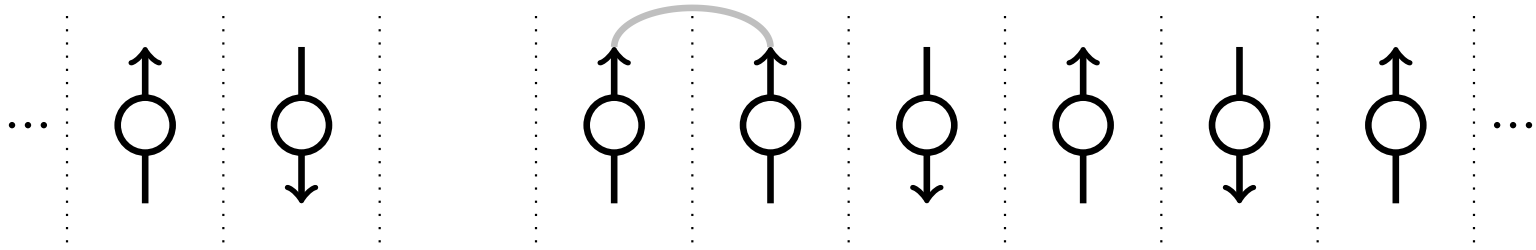
Hubbard model: Spin–charge separation

Remove a fermion from the lattice:



Hubbard model: Spin–charge separation

Move hole left: spin domain wall remains fixed.



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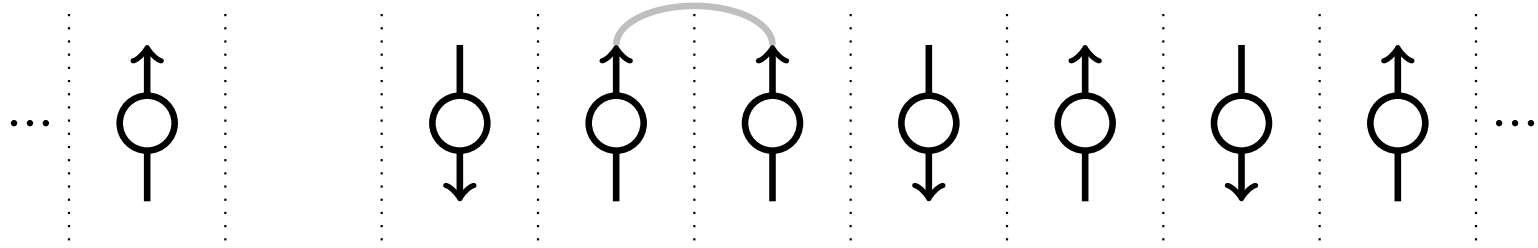

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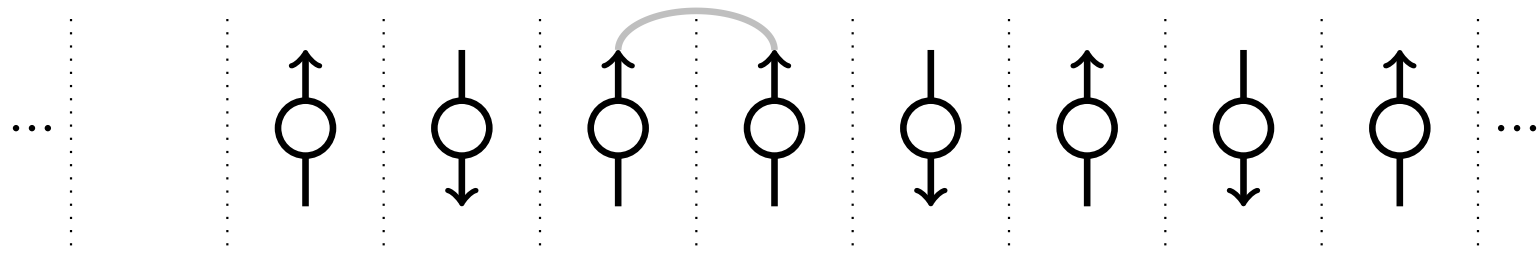
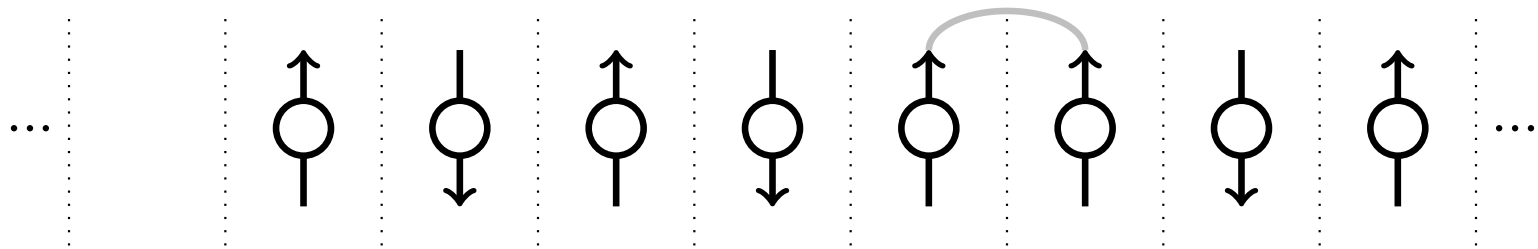


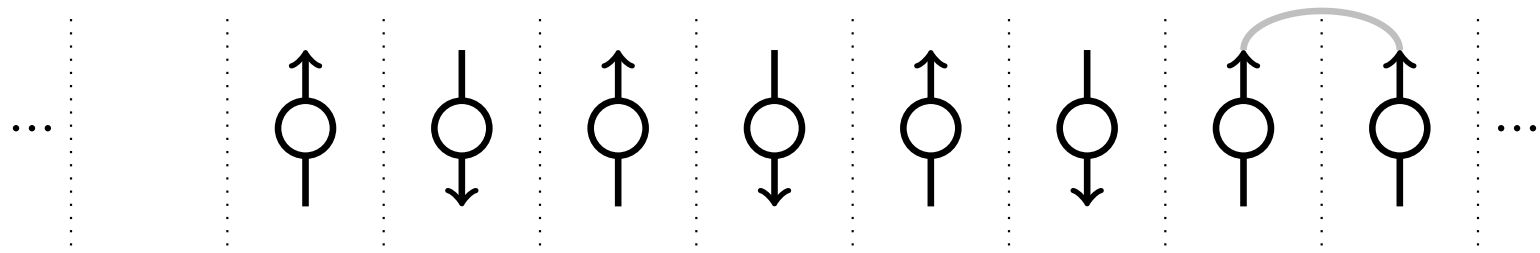
Hubbard model: Spin–charge separation

Move the domain wall right by spin exchange.



Hubbard model: Spin–charge separation

Move the domain wall right by spin exchange.



Hubbard model: Spin–charge separation

Elementary excitations are isolated spin and charge DOFs.

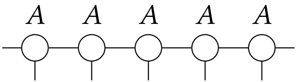
Example of **fractionalisation**.

Related to topological order and anyons (fractionalised statistics).

Static method: Excitation ansatz

Start with a translation-invariant infinite MPS of the ground state:

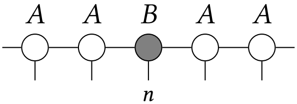
$$|\Psi\rangle = \cdots$$



$$\cdots .$$

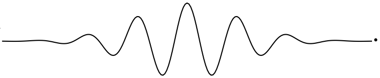
Form a Bloch wave with momentum k:

$$|\Phi_k[B]\rangle = \sum_n e^{ikn} \cdots$$



$$\cdots$$

$$= \sum_n e^{ikn}$$



Optimisation of B for each k gives the low-lying excitation spectrum.
Can specify the quantum numbers of B (spin projection, particle no).

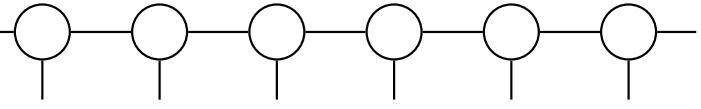
J. Haegeman et al., Phys. Rev. B **85**, 100408(R) (2012).

Aside: Topologically nontrivial excitations

We use a symmetric MPS with fixed particle no and spin projection.

The unpolarised state at half filling needs a unit cell of two sites:

$$|\Psi\rangle = \cdots \; A_1 \; A_2 \; A_1 \; A_2 \; A_1 \; A_2 \; \cdots \; .$$



The reason is purely numeric:

- Spin-1/2 particles have a particle QN 1 and spin proj. QN ± 0.5.
- We need a particle QN 1 and spin proj. QN 0 per site.

This leads to numerical breaking of translation symmetry.

Aside: Topologically nontrivial excitations

Topologically trivial excitations:

$$|\Phi\rangle = \sum_n e^{ikn} \Bigg[\cdots \underset{n}{\overset{A_1\ A_2\ B_1\ A_2\ A_1\ A_2}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bullet\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc}} \cdots$$

$$+ \cdots \underset{n}{\overset{A_1\ A_2\ A_1\ B_2\ A_1\ A_2}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bullet\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc}} \cdots \Bigg].$$

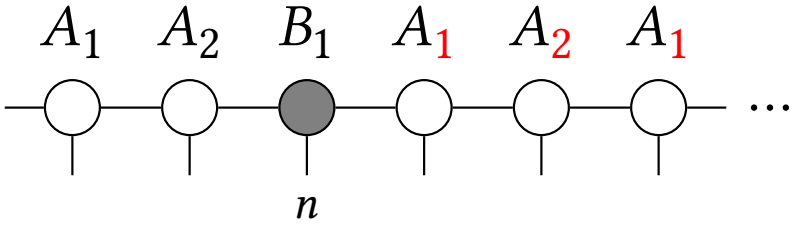
Can only have integer combinations of underlying particle QNs.

V. Zauner-Stauber et al., Phys. Rev. B **97**, 235155 (2018).

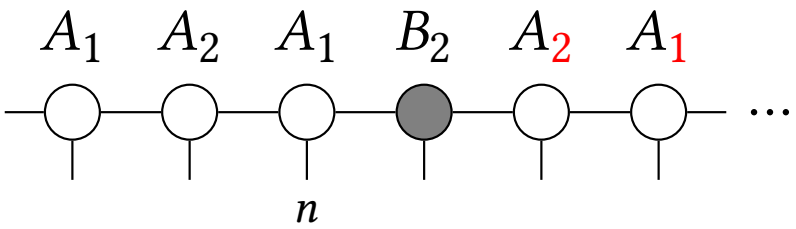
Aside: Topologically nontrivial excitations

Topologically **non**trivial excitations:

$$|\Phi\rangle = \sum_n e^{ikn} \Big[\cdots$$



$$+ \cdots$$



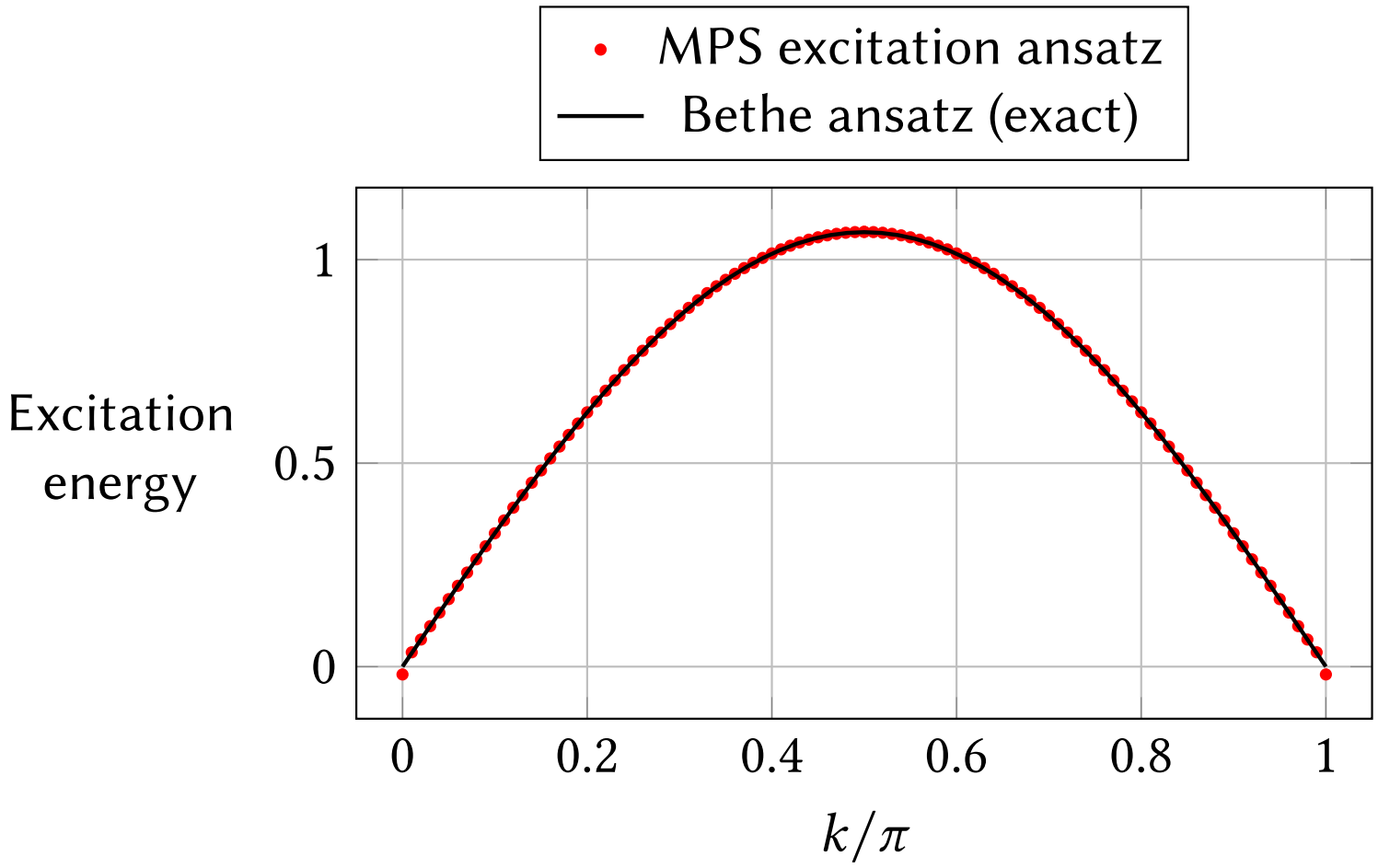
$$\cdots \Big].$$

We can now represent fractional excitations (i.e. spinons, chargons).

V. Zauner-Stauber et al., Phys. Rev. B **97**, 235155 (2018).

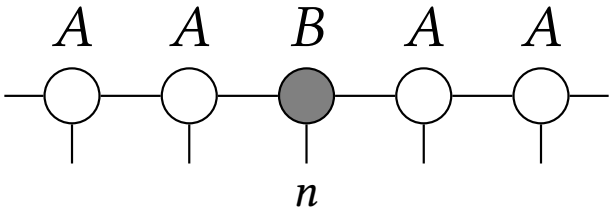
Hubbard model: Spin energies

Using $t = 1, U = 5$



Compare V. Zauner-Stauber et al., Phys. Rev. B **97**, 235155 (2018).

Aside: Expectation values of the excitation ansatz

$$|\Phi\rangle = \sum_n e^{ikn} \cdots$$ 

$$\cdots .$$

For system size L:

$$\langle\Phi|\Phi\rangle = L, \qquad \langle\Phi|H|\Phi\rangle = EL^2 + \Delta L$$

$$\Rightarrow \qquad \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} = EL + \Delta.$$

(E: background state energy density, Δ: excitation energy.)

Aside: Expectation values of the excitation ansatz

Can also apply to higher powers:

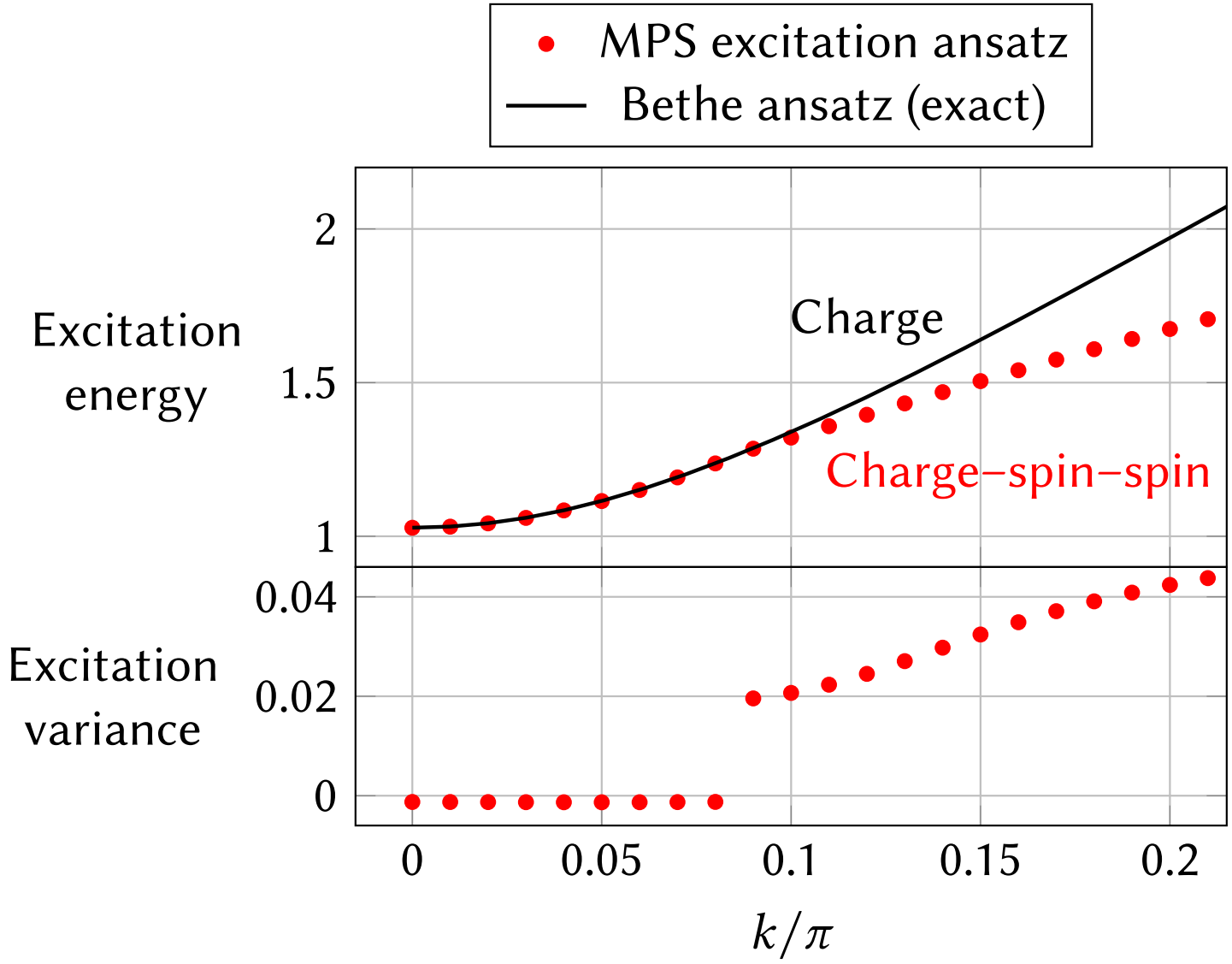
$$\frac{\langle\Phi|H^2|\Phi\rangle - \langle\Phi|H|\Phi\rangle^2}{\langle\Phi|\Phi\rangle} = \sigma_E^2 L + \sigma_\Delta^2.$$

(σ_E^2: background state variance density, σ_Δ^2: excitation variance.)

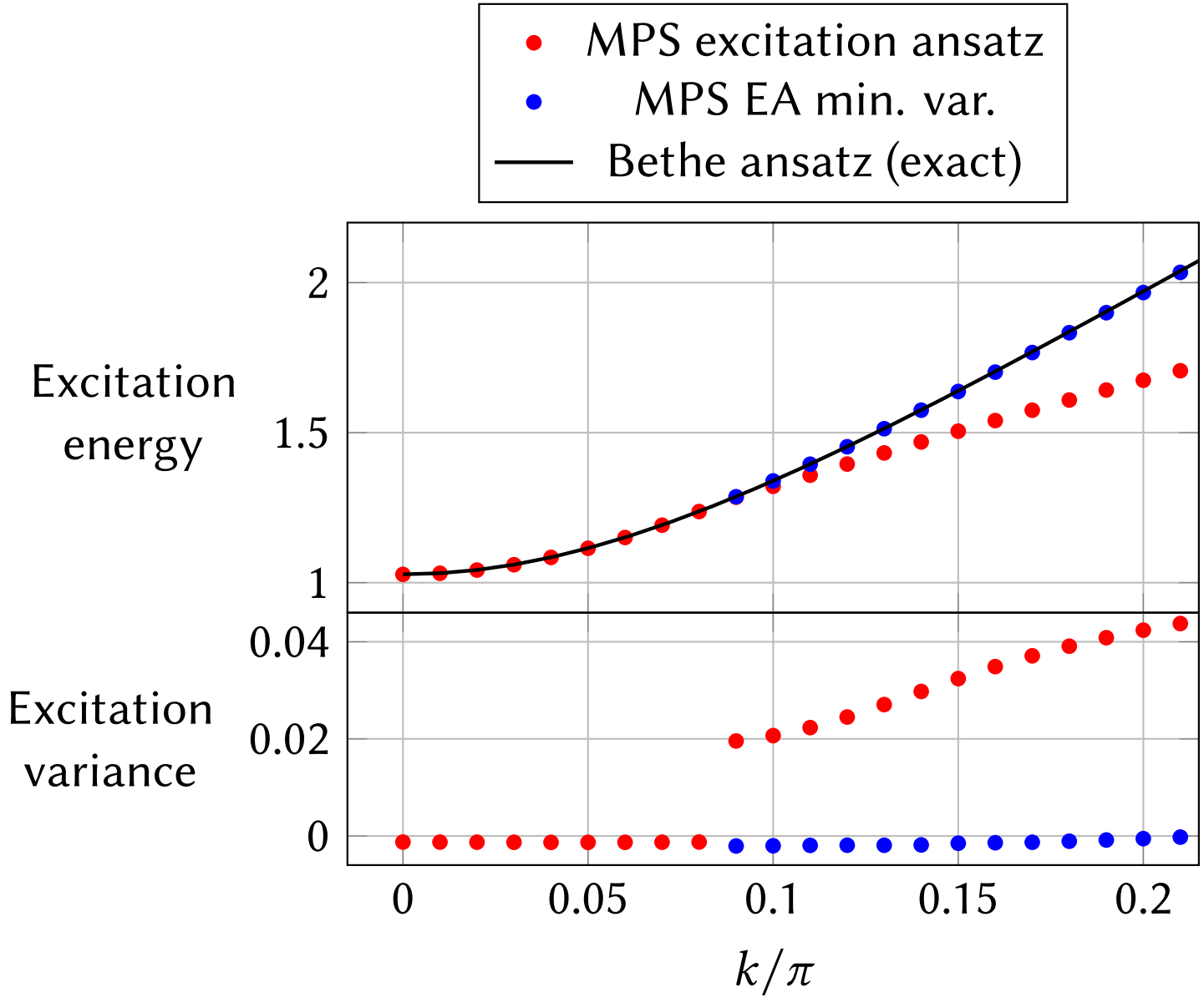
The excitation ansatz is *not* a variational ansatz:

- The excitation energy Δ may be smaller than the true value.
- The excitation variance σ_Δ^2 can be negative!

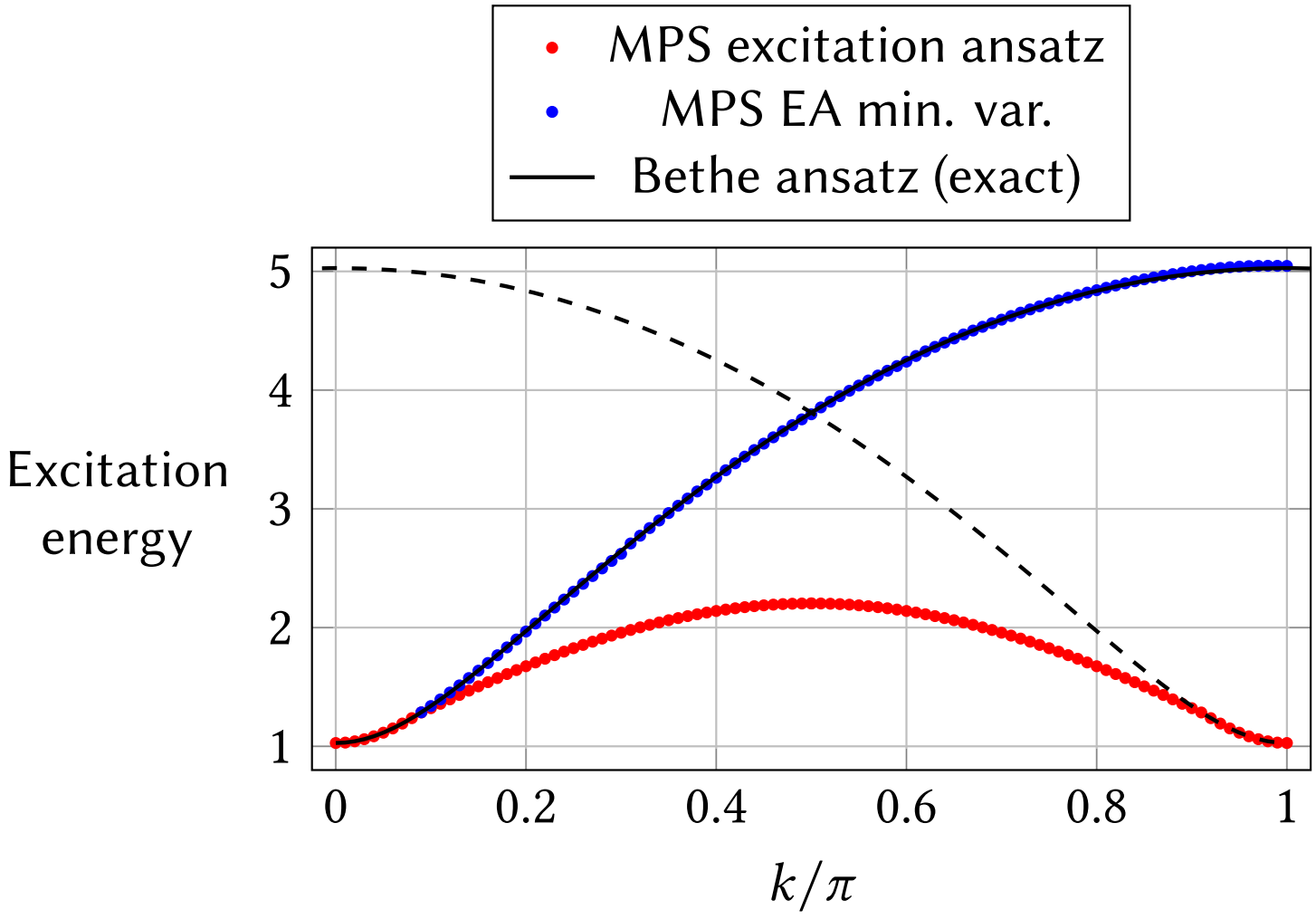
Hubbard model: Charge energies



Minimising energy variance



Minimising energy variance

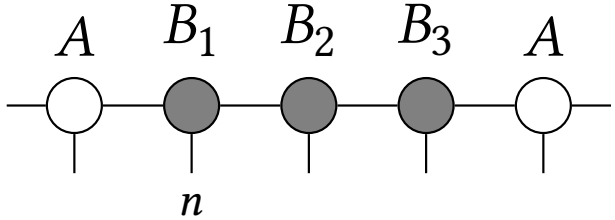


Increasing accuracy

There are two main factors which affect the accuracy of the EA:

1. The accuracy of the background wavefunction.
   Can be improved by using a larger bond dimension.
2. The size of the 'window':

$$|\Phi_k[\mathbf{B}]\rangle = \sum_n e^{ikn} \cdots$$



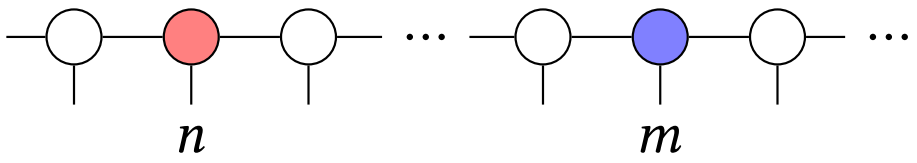
$$\cdots .$$

We can optimise the window one site at a time, like DMRG.

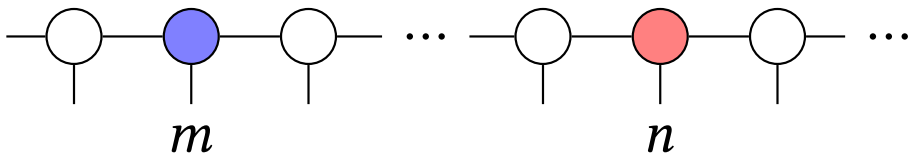
Usually (1) will be the limiting factor, and a 1-site window is enough (unless the excitation is 'broader' than the correlation length).

Multi-particle stationary states?

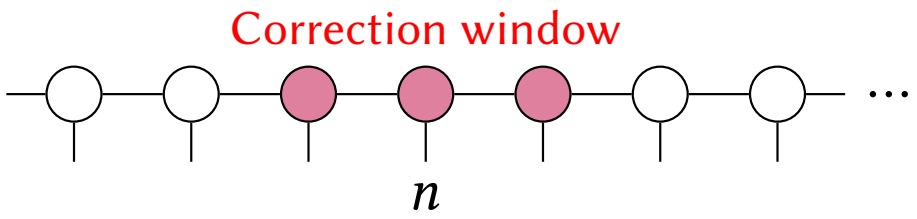
$$|\Upsilon_{k_1,k_2}\rangle = \sum_n \Big[q_1 \sum_{m>n} e^{i(k_1 n + k_2 m)} \ldots$$



$$+ q_2 \sum_{m<n} e^{i(k_2 m + k_1 n)} \ldots$$



$$+ e^{i(k_1+k_2)n} \ldots$$

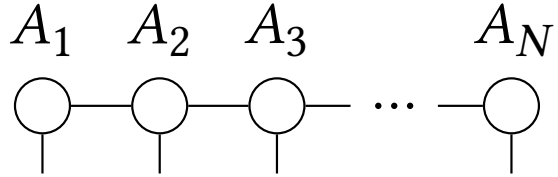


$\Big]$.

Need to solve for q_1, q_2 and the correction window.

L. Vanderstraeten et al., Phys. Rev. B **92**, 125136 (2015).

Time evolution

$|\Psi\rangle =$ 

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Time evolution is described by Schrödinger's equation

$$\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = -\mathrm{i}H|\Psi(t)\rangle\,.$$

Approximate using time-dependent variational principle (TDVP)

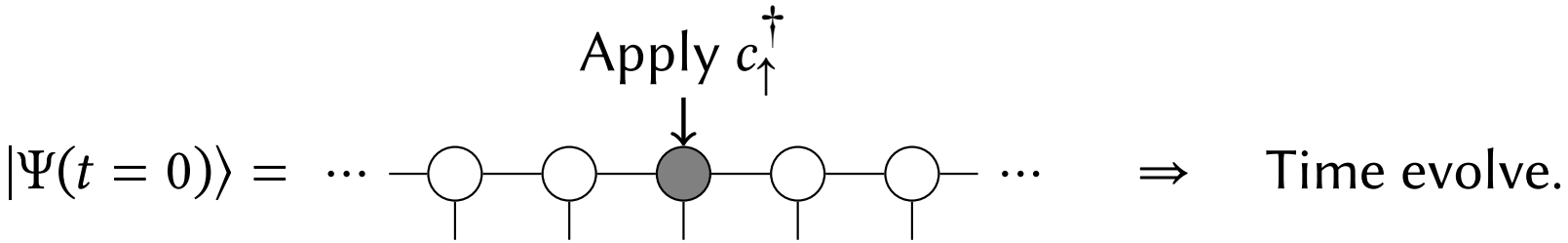
$$\frac{\mathrm{d}}{\mathrm{d}t}A_n(t) = -\mathrm{i}H_n^{\mathrm{eff}}A_n(t), \qquad n = 1, \ldots, N.$$

Sweep across evolving each A-matrix at a time: similar to DMRG.

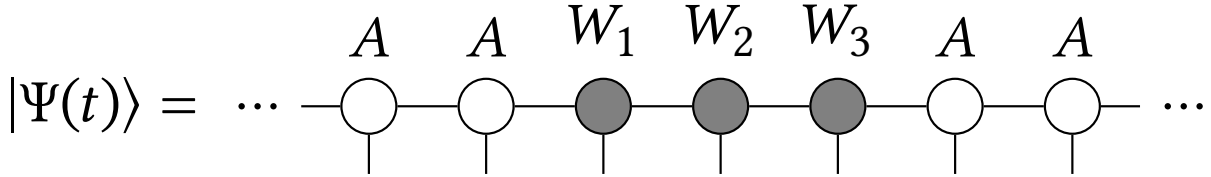
J. Haegeman et al., Phys. Rev. B **94**, 165116 (2016).

Infinite boundary conditions

Usual procedure:



Breaks translation invariance.
We could use a finite system size.
Or we can use a finite window with **infinite boundary conditions**.

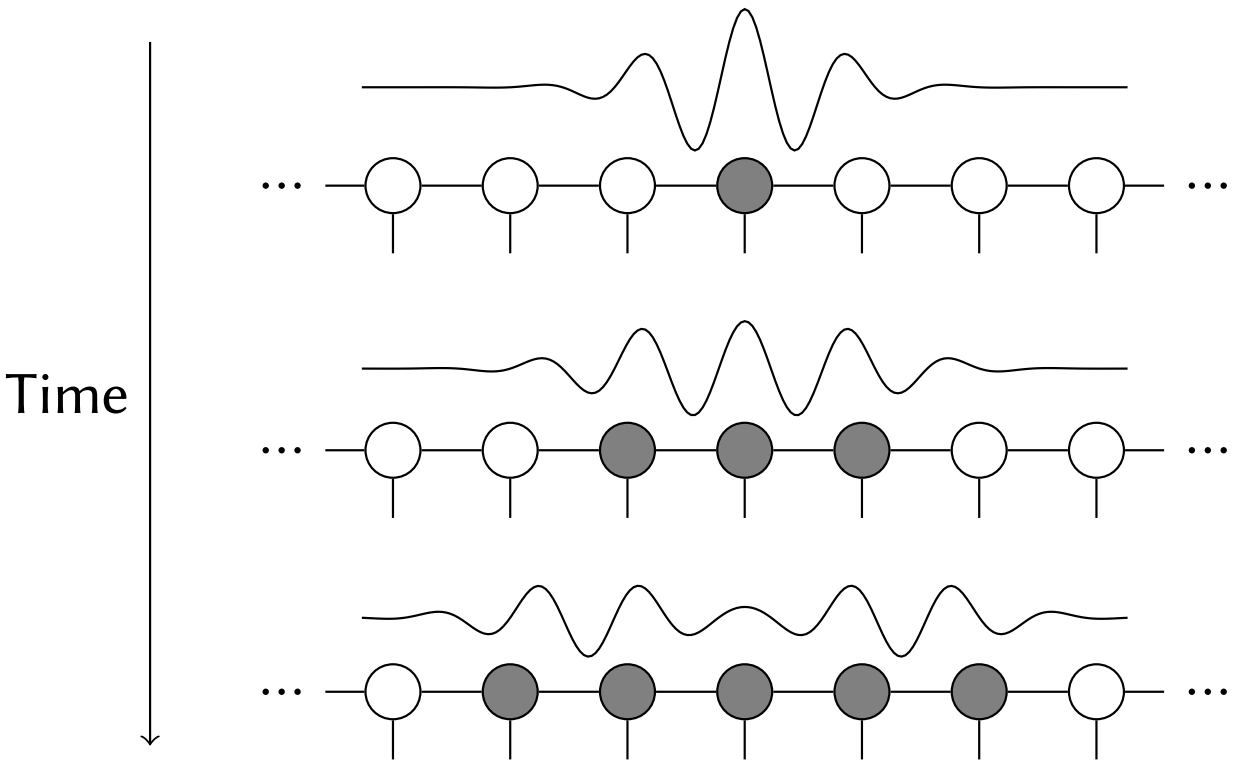


Only evolve the window: the boundaries remain fixed.

H. N. Phien et al., Phys. Rev. B **86**, 245107 (2012).

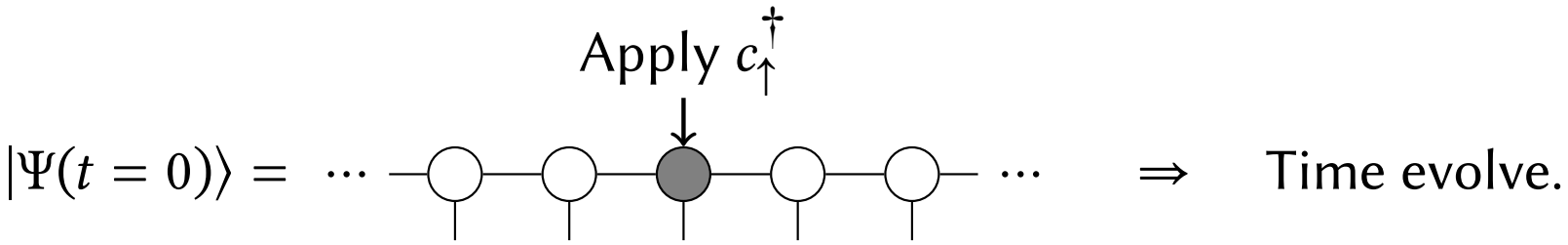
Dynamical window expansion

We can expand the window as the wavefront spreads out:



H. N. Phien et al., Phys. Rev. B **88**, 035103 (2013).

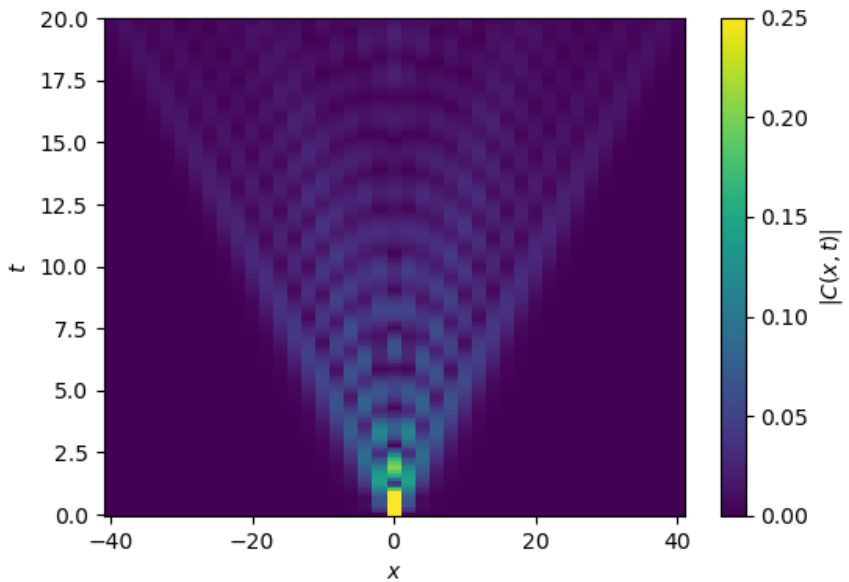
Two-point correlation functions



Can obtain two-point correlation function:

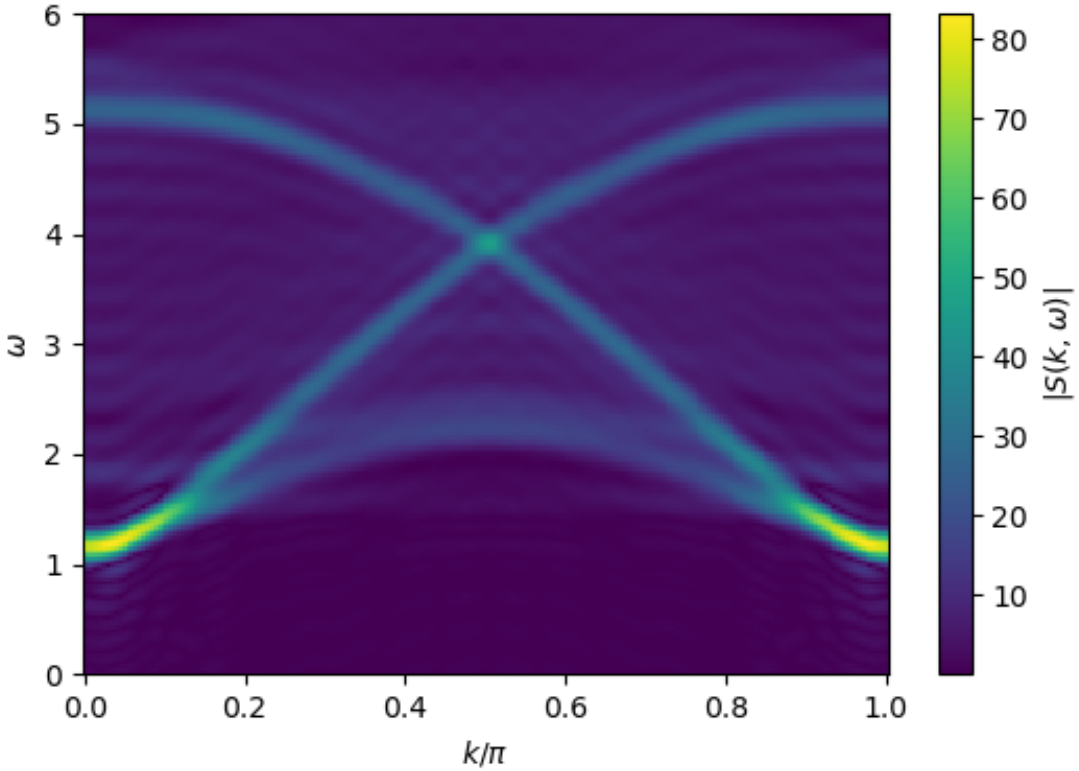
$$C(x,t) = \langle \Psi | c_{\uparrow,x} \mathrm{e}^{-\mathrm{i}Ht} c_{\uparrow,0}^\dagger | \Psi \rangle = \langle \Psi(0) | T^{-x} | \Psi(t) \rangle \,.$$

(T^x: translation operator by x sites.)



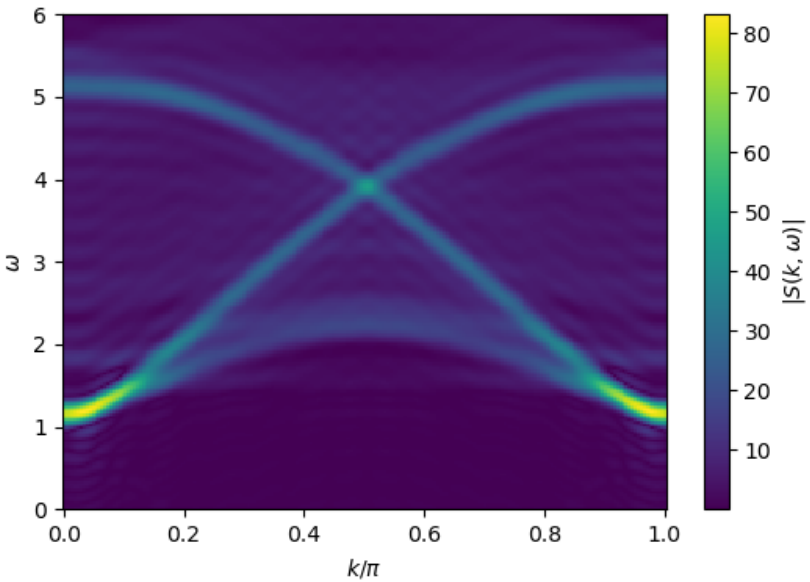
Spectral functions

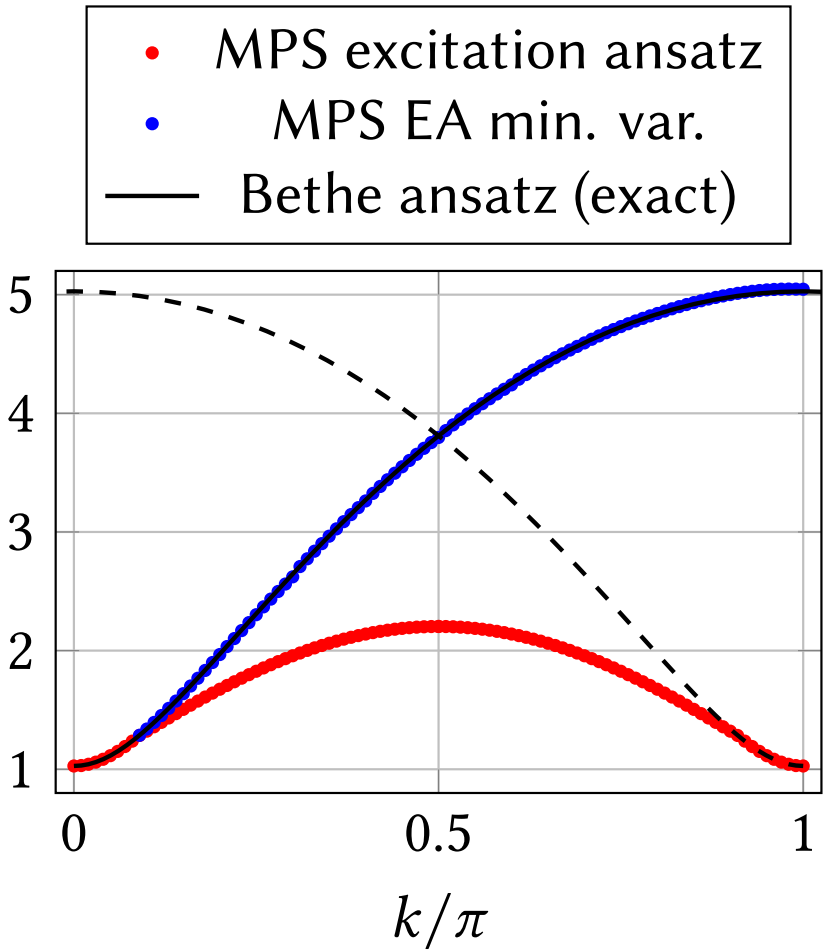
$$C(x,t) \xrightarrow{\text{Fourier transform}} S(k,\omega).$$



(Can use smoothing/extrapolation to reduce finite-time effects.)

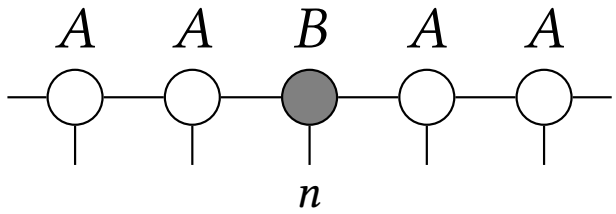
Spectral function vs excitation ansatz





Real-space wavepackets

$$|\Phi_k[B_k]\rangle = \sum_n e^{ikn} \cdots$$

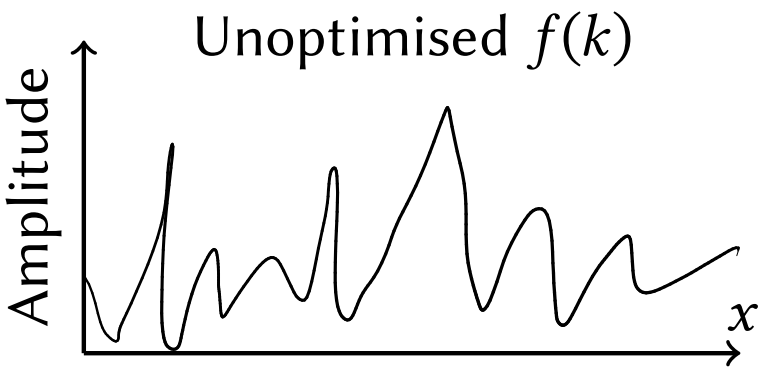


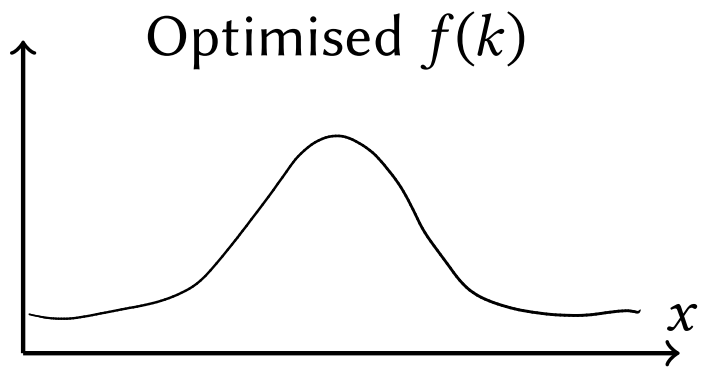
$$\cdots .$$

Form real-space wavepackets:

$$|\Psi\rangle = \int_0^{2\pi} f(k)\,|\Phi_k(B_k)\rangle\,\mathrm{d}k.$$

Optimise $f(k)$ to localise wavepacket.





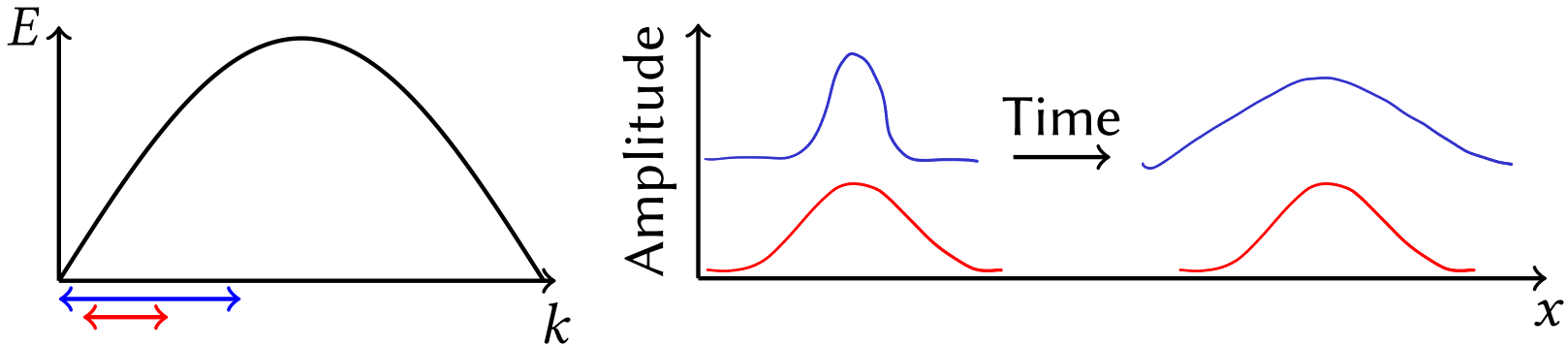
M. Van Damme et al., Phys. Rev. Research **3**, 013078 (2021).

Coherent wavepackets

Sample components around a certain momentum:

$$f(k) \to \mathrm{e}^{-(k-k_0)/2\sigma^2} f(k).$$

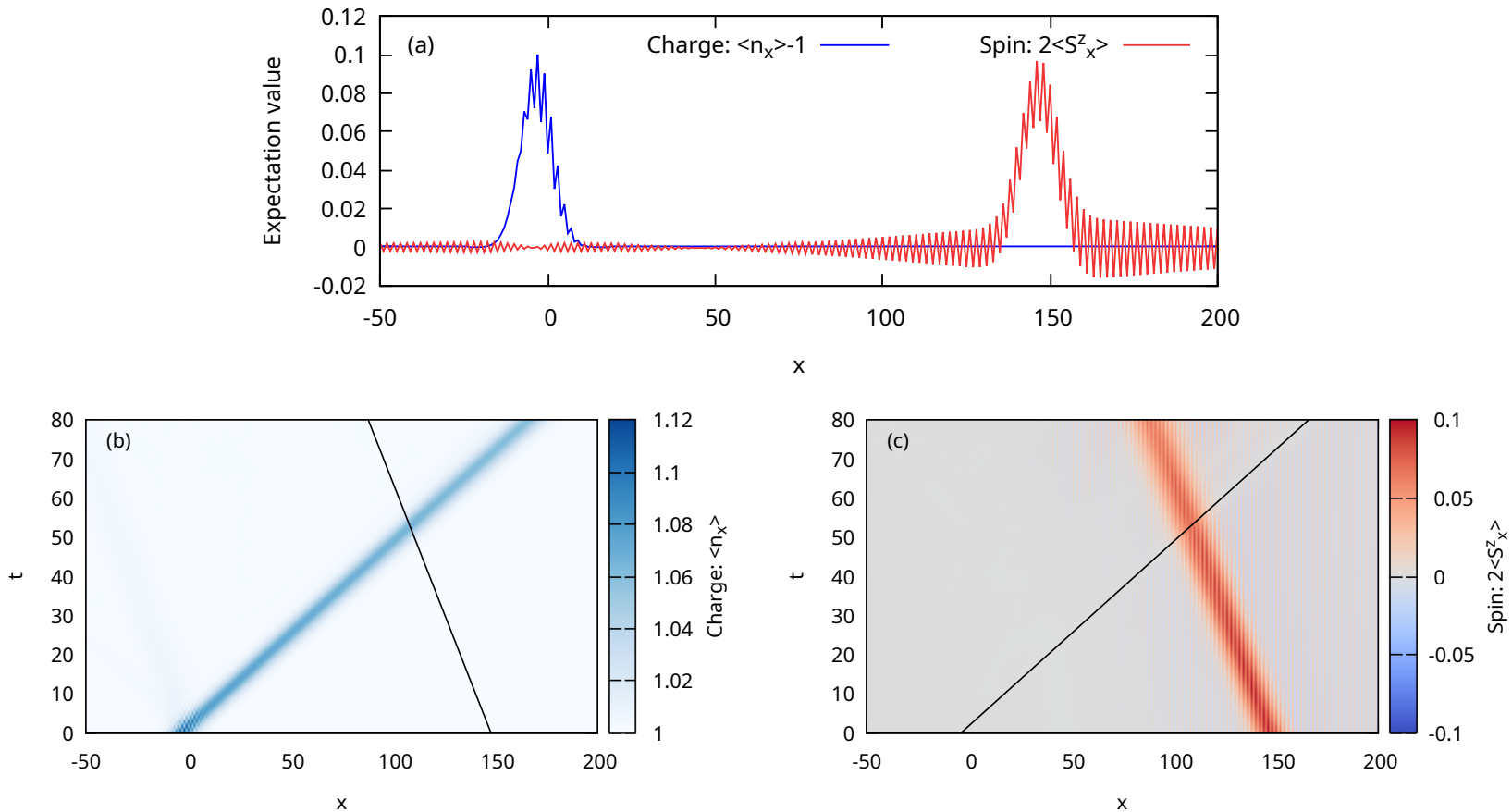
Group velocity is proportional to slope of dispersion relation.



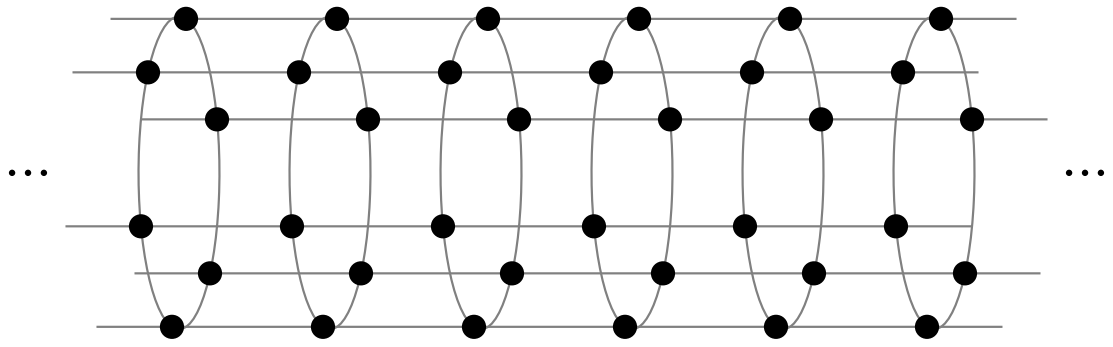
Need to balance wavepacket size and dispersion over time (uncertainty principle).

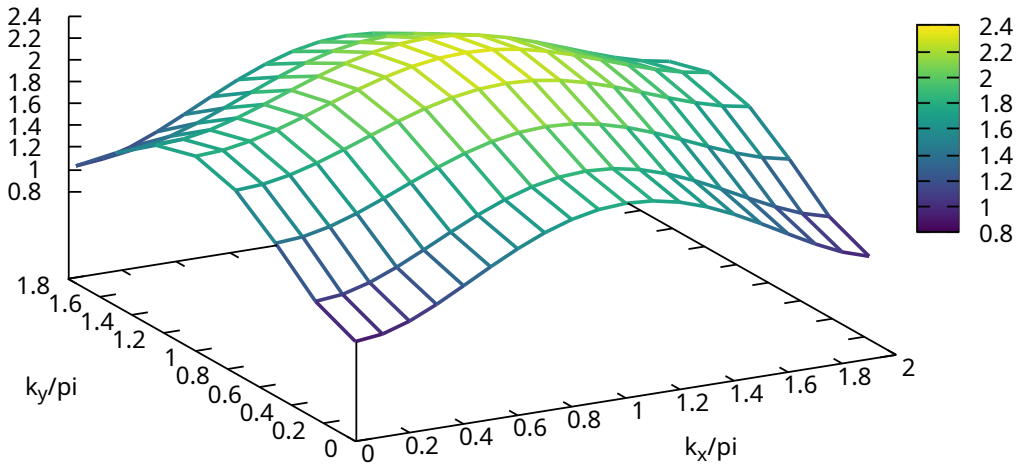
M. Van Damme et al., Phys. Rev. Research **3**, 013078 (2021).

Real-space wavepackets: Hubbard model



What about 2D?





(Transverse-field Ising model, width 8.)

Conclusion

Static methods:

- Directly target momentum-eigenstates.
- Fractional excitations.

Dynamic methods:

- Free excitation of single excitations.
- Scattering of multiple wavepackets.

Code available: `https://github.com/mptoolkit`.
Documentation: `https://mptoolkit.qusim.net`.