Matrix product state methods for excitations

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Motivation

Many-body problem

- Full diagonalization generally infeasible
- Is there some structure we can use?

Motivation

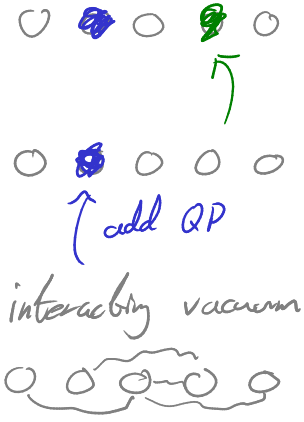
Many-body problem

- Full diagonalization generally infeasible
- Is there some structure we can use?

Quasiparticle picture

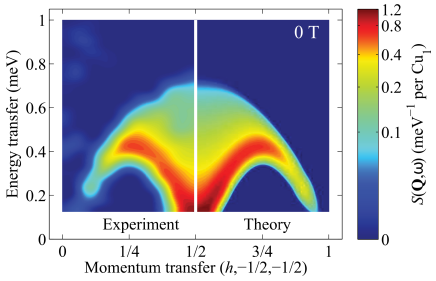
- At $T = 0$, described by ground state
- At low T, described by quasiparticles on top of the ground state

$\rightarrow$ Many-body problem reduced to 'few-body'



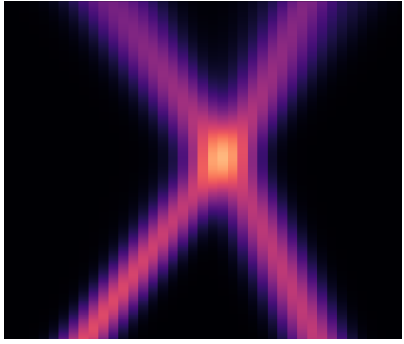
Motivation

- Band structure of materials



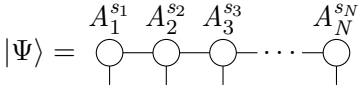
Mourigal et al., Nat. Phys. **9**, 435 (2013)

- Collision simulations



Matrix product states

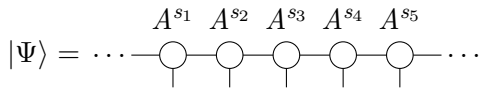
Need an ansatz for the ground state: Matrix product states



- Compress exponential Hilbert space to polynomial
- Area law: 'locally entangled' states
- Energy optimization via DMRG

Infinite matrix product states

Explicitly enforce translation invariance and take $N \to \infty$: Infinite MPS



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

Matrix product operators

Represent operators as (i)MPOs (block triangular)

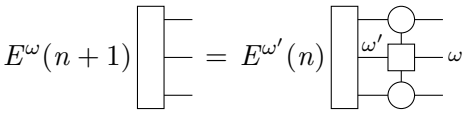
$$H = \cdots - \boxed{W} - \boxed{W} - \boxed{W} - \cdots, \qquad \text{e.g.} \quad W = \begin{pmatrix} I & JS^z & hS^x \\ 0 & 0 & S^z \\ 0 & 0 & I \end{pmatrix}$$

Cannot contract full diagram: define transfer operator

$$\mathcal{T} = \begin{array}{c} A \\ \bigcirc \\ \boxed{W} \\ \bigcirc \\ A \end{array}$$

Transfer operator fixed point

Need to solve fixed-point equation



- Recursive in MPO index ω
- Polynomial in system size n (extensive)

Transfer operator fixed point

Warning: Technical!

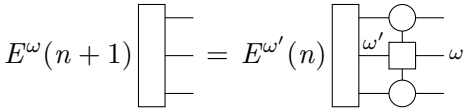
For $\omega \in \{1, \cdots, w\}$:

$$E^{\omega}(n+1) = E^{\omega}(n)\, T^{\omega}_{\omega} + C^{\omega}(n), \qquad C^{\omega}(n) \equiv \sum_{\omega' < \omega} E^{\omega'}(n)\, T^{\omega}_{\omega'}$$

- $C^{\omega}(n)$ can be evaluated directly
- Each case depend on diagonal component T^{ω}_{ω}

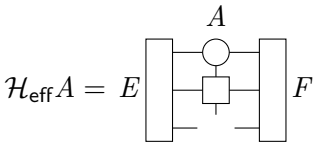
Michel & McCulloch, arXiv:1008.4667

Transfer operator fixed point



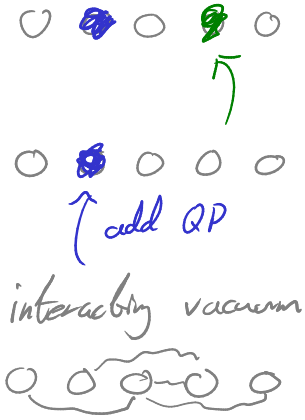
- Once we have final element $E^{w}(n)$, expectation value can be read off

Local iDMRG/VUMPS updates via effective Hamiltonian



Excitations

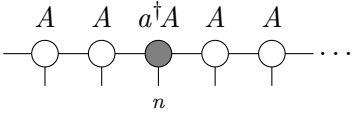
- Now that we have an ansatz for the ground state, want to find excitations
- Could use DMRG, but orthogonalize against GS
- Inefficient: Build upon GS



Single-mode approximation

Suppose we have an approximation for the excitation creation operator $a^\dagger$
$\rightarrow$ Construct excitation with momentum k

$$|\Phi_k\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} a_n^\dagger |\Psi\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots$$



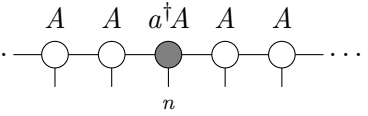
MPO:

$$W_k = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} I & a^\dagger \\ 0 & I \end{pmatrix}$$

Single-mode approximation

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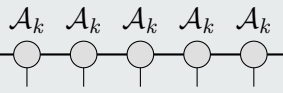


MPO:

$$W_k = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} I & a^\dagger \\ 0 & I \end{pmatrix}$$

Can write in a translation invariant form with block-triangular MPS

$$|\Phi_k\rangle = \cdots$$

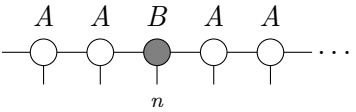


$$\cdots, \qquad \mathcal{A}_k = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} A & a^\dagger A \\ 0 & A \end{pmatrix}$$

MPS excitation ansatz

- Need to optimize $a^\dagger$ for each k (dressed creation operator)
- Or just optimize the perturbation to the MPS (excitation ansatz)

$$|\Phi_k[B]\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots$$



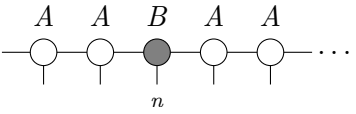
$\cdots$

Haegeman et al., Phys. Rev. B **85**, 100408(R) (2012)
JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

MPS excitation ansatz

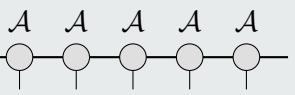
- Need to optimize $a^\dagger$ for each k (dressed creation operator)
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$$|\Phi_k[B]\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots A\ A\ B\ A\ A \cdots$$



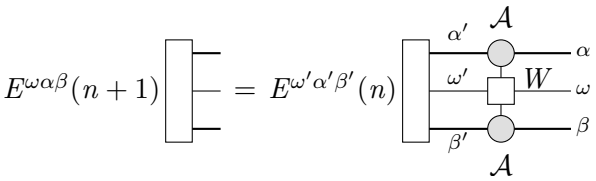
Also has block-triangular form

$$|\Phi_k[B]\rangle = \cdots \mathcal{A}\ \mathcal{A}\ \mathcal{A}\ \mathcal{A}\ \mathcal{A} \cdots, \qquad \mathcal{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k}A & B \\ 0 & A \end{pmatrix}$$



Haegeman et al., Phys. Rev. B **85**, 100408(R) (2012)
JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

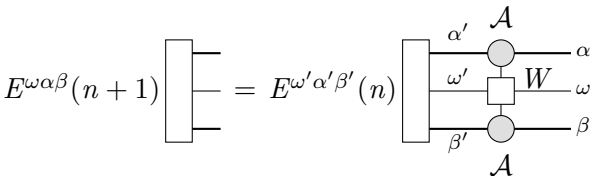
Excitation ansatz fixed-point equations



- Same algorithm as for iMPO, but with extra indices α, β

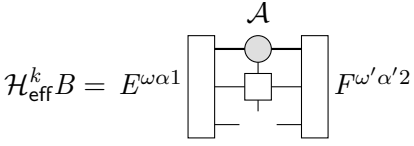
JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

Excitation ansatz fixed-point equations



- Same algorithm as for iMPO, but with extra indices α, β

Optimize via

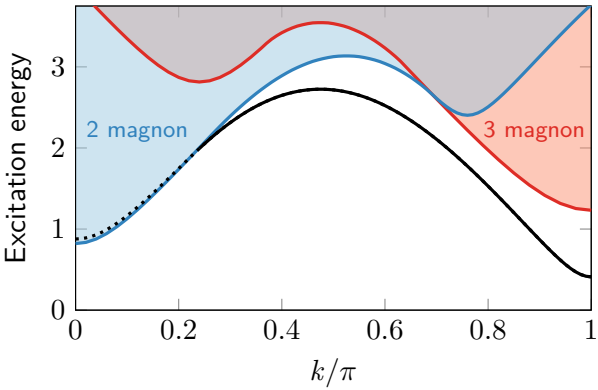


JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

Spin-1 Heisenberg model

$$H = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

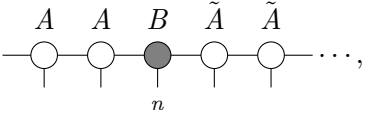
- Elementary excitations gapped magnons
- Multi-magnon energies can be obtained by summing single-magnon energies



Topologically nontrivial excitations

Can handle by using two different boundarys

$$|\Phi_k[B]\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots$$



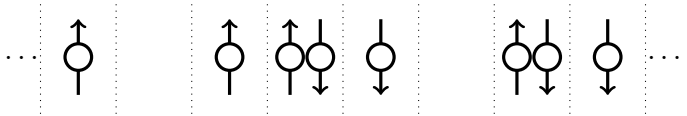
$$\cdots, \qquad \mathcal{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k}A & B \\ 0 & \tilde{A} \end{pmatrix}$$

For example

- Domain wall excitations $\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow$
- Shifted quantum numbers

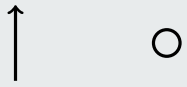
Zauner-Stauber et al., Phys. Rev. B **97**, 235155 (2018)

Hubbard model



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

Elementary excitations are isolated spin and charge (fractionalization)



Hubbard model GS MPS

We use a symmetric MPS with conserved particle number and spin projection (N, S^z)

An unpolarized state at half filling needs a unit cell of two sites

$$|\Psi\rangle = \cdots \underset{A_1}{\bigcirc} - \underset{A_2}{\bigcirc} - \underset{A_1}{\bigcirc} - \underset{A_2}{\bigcirc} - \underset{A_1}{\bigcirc} - \underset{A_2}{\bigcirc} \cdots$$

The reason is purely numeric:

- Spin-1/2 particles have QN $(1, \pm 0.5)$
- We need QN $(1, 0)$ per site

$\rightarrow$ Numerical breaking of translation symmetry

Fractionalized excitations

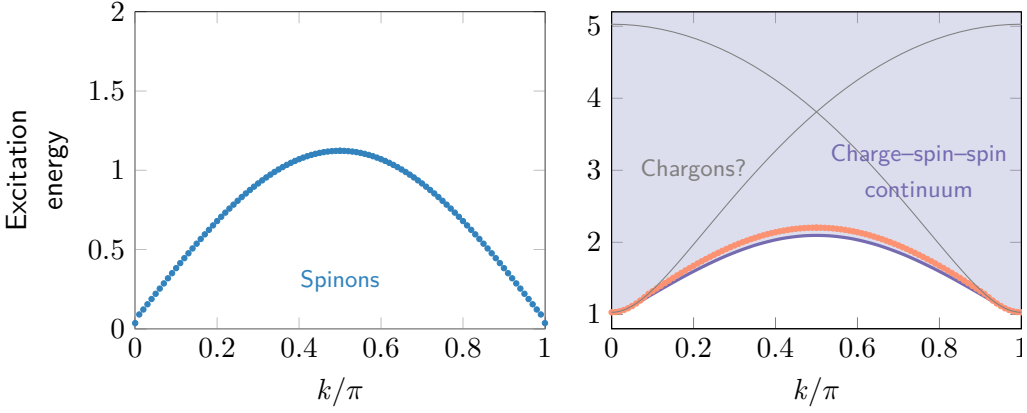
To represent excitations with fractional QNs, need to shift right unit cell

$$|\Phi\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \Big[\cdots \underset{n}{\overset{A_1\ A_2\ B_1\ A_1\ A_2\ A_1}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bullet\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc}} \cdots$$

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

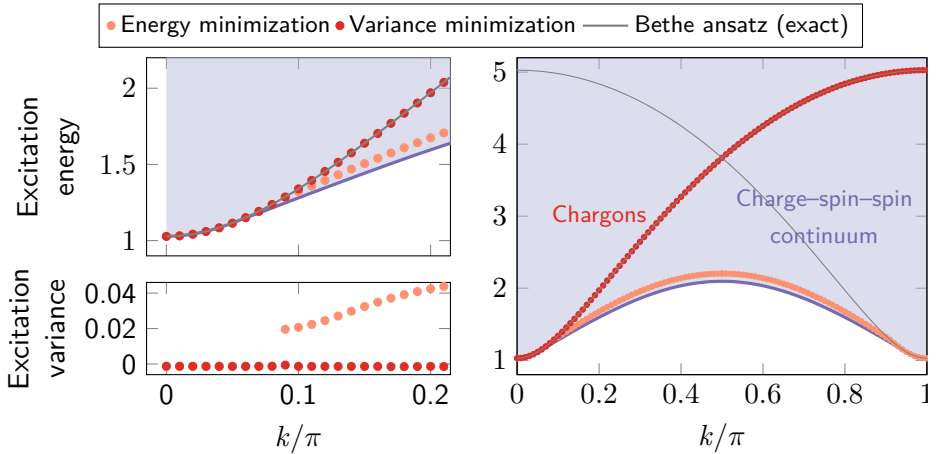
V. Zauner-Stauber et al., Phys. Rev. B **97**, 235155 (2018)

Excitation spectra ($U/t = 5$)



→ Chargon spectra blocked by continuum from gapless spinons

Minimizing energy variance



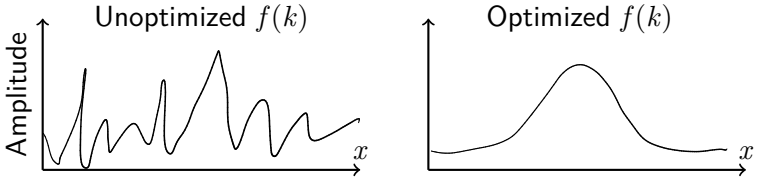
JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

Real-space wave packets

Construct real-space wave packets

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

$\rightarrow$ Optimize $f(k)$ to localize wave packet



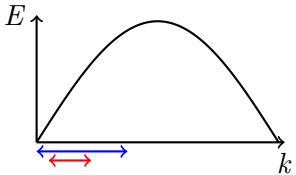
Van Damme et al., Phys. Rev. Research **3**, 013078 (2021)

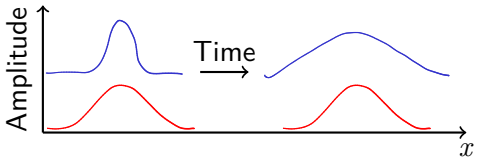
Coherent wave packets

Sample components around a certain momentum

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

$\to$ Group velocity is proportional to slope of dispersion relation

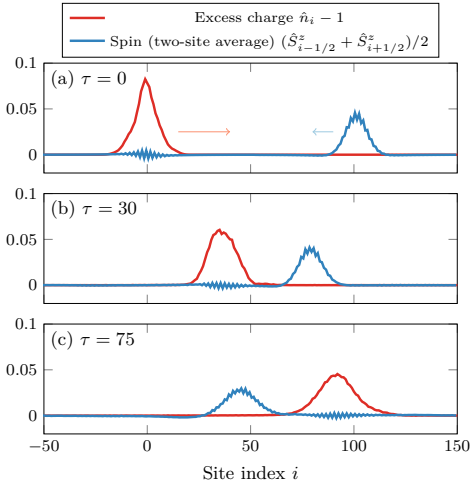


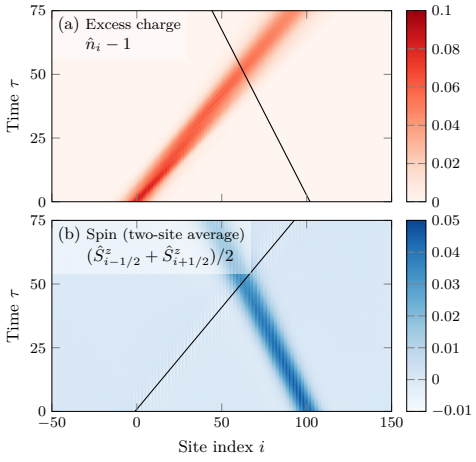


Need to balance wave packet size and dispersion over time (uncertainty principle)

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

Spin–charge separation in the Hubbard model





JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)

Multi-site windows

For broader excitations, increase size of window

$$|\Phi_k[\mathbf{B}]\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots \underset{n}{\overset{A \quad A \quad B_1 \quad B_2 \quad B_3 \quad \tilde{A} \quad \tilde{A}}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bullet\!\!-\!\!\bullet\!\!-\!\!\bullet\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc}} \cdots, \qquad \mathcal{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k}A & B_1 & & \\ & 0 & B_2 & \\ & & 0 & B_3 \\ & & & \tilde{A} \end{pmatrix}$$

Good for spatially broad excitations, e.g. bound states

Optimize one tensor at a time (EA DMRG)

$$\mathcal{H}^{(n)}_{\text{eff}} B_n = E \quad \overset{\mathcal{A}}{\underset{n \;\; n+1}{\square}} \quad F$$

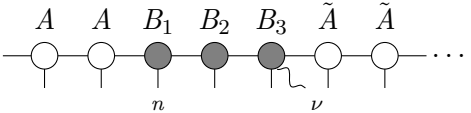
Vanderstraeten et al., PRB **101**, 115138 (2020)

Simultaneous optimization

What if we want multiple eigenstates?

- Project away lower states?
- Alternatively: Optimize multiple levels ν simultaneously

$$|\Phi_k^\nu[\mathbf{B}]\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} \cdots$$



Similar in spirit to 'multi-target' MPS [Li et al., PRB **109**, 045115 (2024)]

Excitations in the Ising model

$$\hat{H} = -J \sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z$$

Elementary excitations are domain walls

$$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow \cdots$$

$$\Delta = E - E_{\mathsf{GS}} = 2J$$

Separation between two domain walls doesnt affect energy

$$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow \cdots$$

$$\Delta = 4J$$

Excitations in the Ising model with a longitudinal field

$$\hat{H} = -J \sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + h_\parallel \sum_j \hat{\sigma}_j^z$$

Domain wall excitations have an extensive energy

$$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow \cdots$$

$$\Delta = 2J + 2h_\parallel N_\downarrow$$

Energy scales linearly with domain wall separation

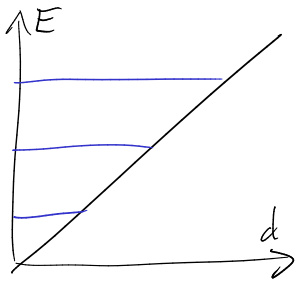
$$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow \cdots$$

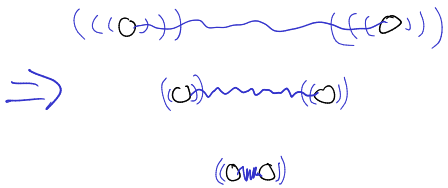
$$\Delta \approx 4J + 2h_\parallel \qquad \Delta \approx 4J + 10h_\parallel \qquad \Delta \approx 4J + 18h_\parallel$$

Lowest-energy excitations are bound domain-wall pairs

Bound state spectra

Can solve for energy eigenstates in linear potential



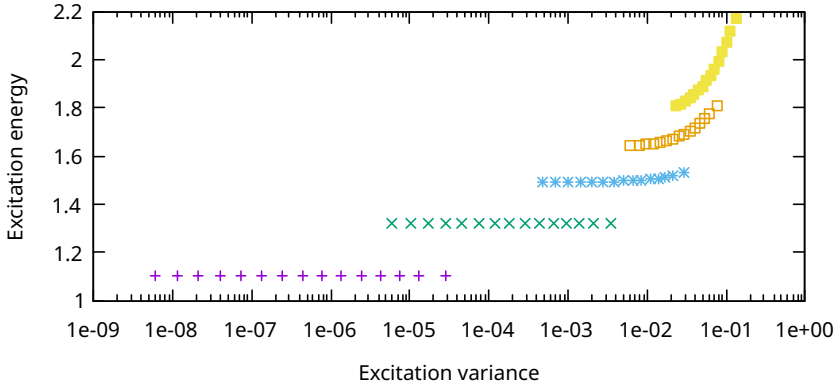


Larger energies correspond to larger separations

Ising model excitation spectrum ($k = 0$)

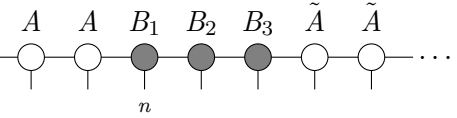
$$\hat{H} = -\sum_j \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z + 0.8 \sum_j \hat{\sigma}_j^x + 0.01 \sum_j \hat{\sigma}_j^z$$

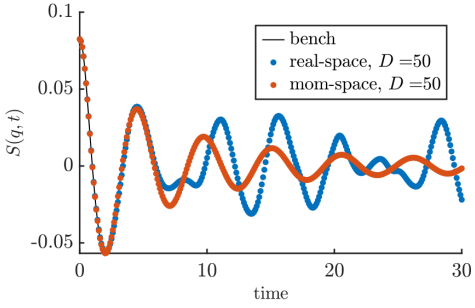
← Increasing window size ←



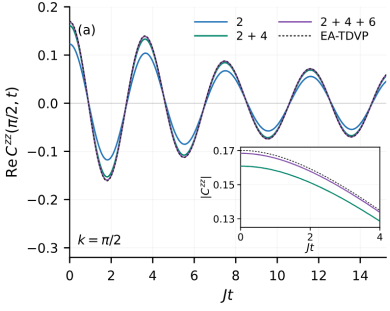
Momentum-resolved time evolution

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





Van Damme and Vanderstraeten, PRB **105**, 205130 (2022)



JJO and McCulloch, arXiv:2610.42127

Scattering states?

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

$$+ q_2 \sum_{m<n} \mathrm{e}^{\mathrm{i}(k_2 m + k_1 n)} \cdots \underset{m}{C} \cdots \underset{n}{B} \cdots$$

$$+ \mathrm{e}^{\mathrm{i}(k_1+k_2)n} \cdots \underset{n}{\text{`Correction window' } W} \cdots \Big],$$

$$\mathcal{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}(k_1+k_2)} A & q_1 B & q_2 C & W \\ & \mathrm{e}^{\mathrm{i}k_2} A & & C \\ & & \mathrm{e}^{\mathrm{i}k_1} A & B \\ & & & A \end{pmatrix}$$

Cf. Vanderstraeten et al., PRB **92**, 125136 (2015)

Conclusion

- Excitation ansatz states are block triangular MPSs
- Topological excitations via different boundaries
- Wave packet creation
- Extend window size to describe large bound states
- Momentum-resolved evolution
- Outlook: Scattering states