Matrix product state methods for excitations

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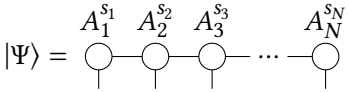
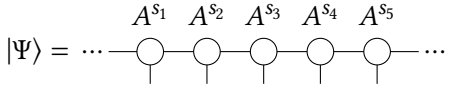
Infinite matrix product states



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

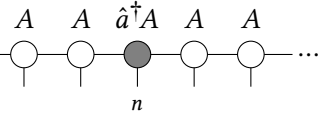


- Observables can be calculated by fixed-point relations
- No finite-size effects: only finite entanglement (bond dimension)
- How to get information about excitations? (Dynamics vs statics)

Single-mode approximation

Given a creation operator $\hat{a}^\dagger$, get an approximate excited state

$$|\Phi_k\rangle = \sum_n e^{ikn} \hat{a}_n^\dagger |\Psi\rangle = \sum_n e^{ikn} \cdots$$

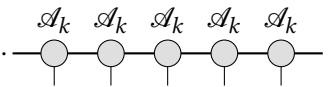


MPO:

$$\hat{W}_k = \begin{pmatrix} e^{ik}\hat{I} & \hat{a}^\dagger \\ 0 & \hat{I} \end{pmatrix}$$

Can write as a block-triangular MPS

$$|\Phi_k\rangle = \cdots, \qquad \mathscr{A}_k = \begin{pmatrix} e^{ik}A & \hat{a}^\dagger A \\ 0 & A \end{pmatrix}$$



MPS excitation ansatz

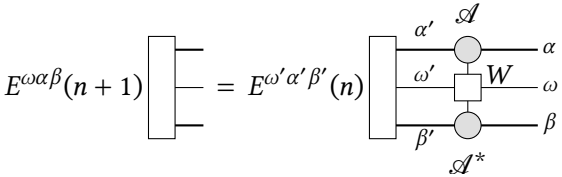
$$|\Phi_k[B]\rangle = \sum_n e^{ikn} \cdots \underset{n}{\overset{A \; A \; B \; \tilde{A} \; \tilde{A}}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc}} \cdots$$

$$= \cdots \overset{\mathscr{A} \; \mathscr{A} \; \mathscr{A} \; \mathscr{A} \; \mathscr{A}}{\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc\!\!-\!\!\bigcirc} \cdots, \qquad \mathscr{A} = \begin{pmatrix} e^{ik}A & B \\ 0 & \tilde{A} \end{pmatrix}$$

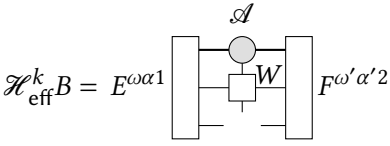
- Generalization of single-mode approximation $B = \hat{a}^\dagger A$
- B can be optimized for each k
- Block-triangular structure: reminiscent of MPOs
- Reuse ground state data instead of starting from scratch
- Non-injective: needed to differentiate excitation from background

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

Excitation ansatz fixed-point equations



- Only need $\omega' \leq \omega, \;\; \alpha' \leq \alpha, \;\; \beta' \leq \beta \quad \Rightarrow \quad$ solve recursively
- Same algorithm as iMPS, but with extra indices α, β

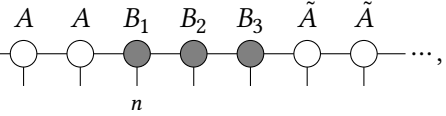


JJO & McCulloch, Phys. Rev. Research **7**, 023018 (2025)
Compare Michel & McCulloch, arXiv:1008.4667

Multi-site windows

For broader excitations, increase size of window:

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

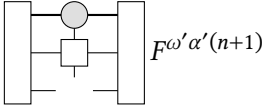


$$\cdots,$$

$$\mathscr{A} = \begin{pmatrix} e^{ik}A & B_1 & & \\ & 0 & B_2 & \\ & & 0 & B_3 \\ & & & \tilde{A} \end{pmatrix}$$

Optimize one tensor at a time (EA DMRG):

$$\mathscr{H}^{n,k}_{\text{eff}} B_n =$$



Compare Vanderstraeten et al., Phys. Rev. B **101**, 115138 (2020)

Expectation values

Expectation values are polynomials in system size L:

$$\langle \hat{H} \rangle = \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle} = \frac{EL^2 + \Delta L}{L} = EL + \Delta$$

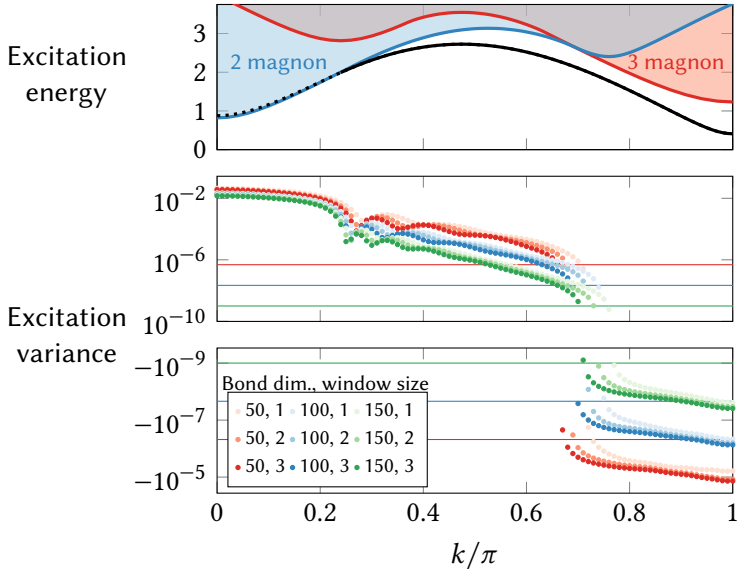
Can calculate the variance:

$$\langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = \sigma_E^2 L + \sigma_\Delta^2$$

Since we only have an approximation to the GS:

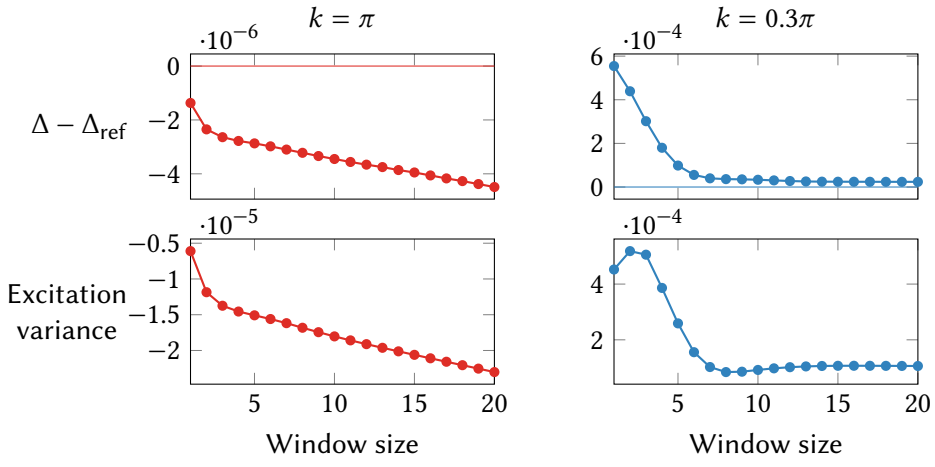
- Δ can be less than the actual value
- σ_Δ^2 can be negative
- Bound by error in GS

Spin-1 Heisenberg model



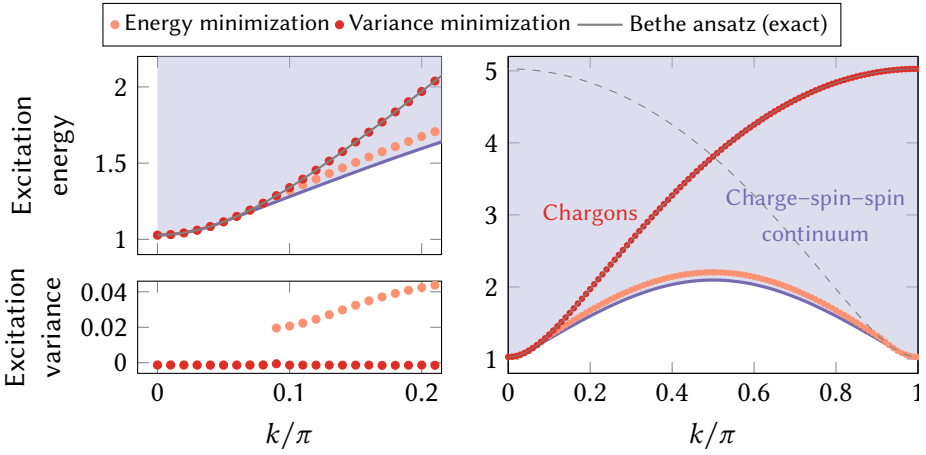
Spin-1 Heisenberg model

Tuning window size (bond dim. 50)



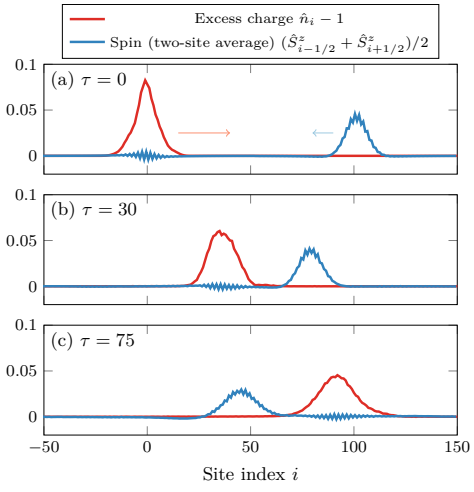
Minimizing energy variance

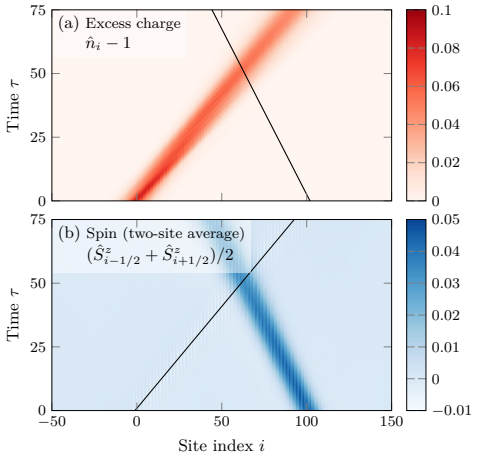
Chargons in the Hubbard model, $U/t = 5$



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

Wave packet preparation: spin–charge separation

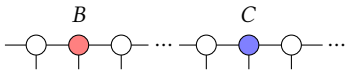




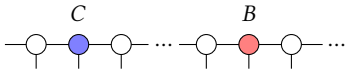
Van Damme et al., Phys. Rev. Research **3**, 013078 (2021)

Multi-particle states

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

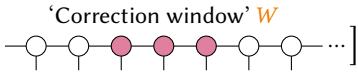


$$+ q_2 \sum_{m<n} e^{i(k_2 m + k_1 n)} \cdots$$



‘Correction window’ W

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



$$\Big],$$

$$\mathscr{A} = \begin{pmatrix} e^{i(k_1+k_2)}A & q_1 B & q_2 C & W \\ & e^{ik_2}A & & C \\ & & e^{ik_1}A & B \\ & & & A \end{pmatrix}$$

Generalizes to ≥ 3 excitations

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

Conclusion

- Excitation ansatz wave functions are triangular MPSs
- Can calculate fixed-point relations recursively
- Works for arbitrary operators; variance minimization
- Directly handles extensions to the EA (multi-site windows, multi-particle states)