Matrix Product State Methods for Excitations

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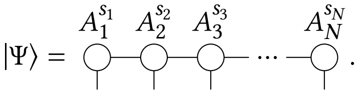
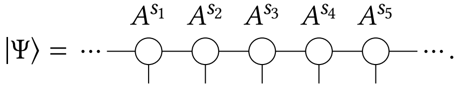
Infinite matrix product states



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

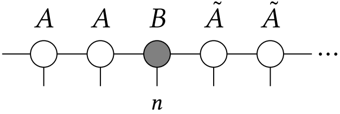


- Observables can be calculated by fixed-point relations.
- No finite-size effects: only finite entanglement (bond dim.).
- How to get information about excitations?
  (Dynamics vs statics.)

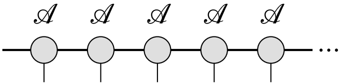
I. P. McCulloch, arXiv:0804.2509, L. Michel and I. P. McCulloch, arXiv:1008.4667.

MPS excitation ansatz

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



$$= \cdots$$

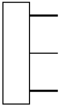
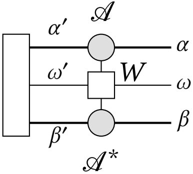


$$\mathscr{A} = \begin{pmatrix} \mathrm{e}^{\mathrm{i}k} A & B \\ 0 & \tilde{A} \end{pmatrix}.$$

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

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

EA fixed point equations

$E^{\omega\alpha\beta}(n+1)$  $= E^{\omega'\alpha'\beta'}(n)$ 

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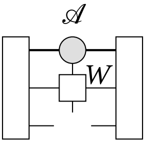
- Only need $\omega' \leq \omega, \;\; \alpha' \leq \alpha, \;\; \beta' \leq \beta \quad \Rightarrow \quad$ Solve recursively.
- Same algorithm as iMPS, but with extra indices α, β.

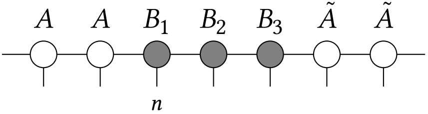
$\mathscr{H}^k_{\text{eff}} B = E^{\omega\alpha 1}$ 

$F^{\omega'\alpha' 2}$.

JO and I. P. McCulloch, in preparation.
Cf. L. Michel and I. P. McCulloch, arXiv:1008.4667.

Multi-site windows

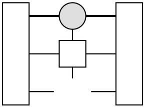
For broader excitations, increase size of window:

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

$\cdots,$

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

Optimise one tensor at a time (EA DMRG):

$$\mathscr{H}_{\mathrm{eff}}^{n,k} B_n = E^{\omega\alpha n}$$  $$F^{\omega'\alpha'(n+1)}.$$

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

Expectation values

Expectation values are polynomials in system size L:

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

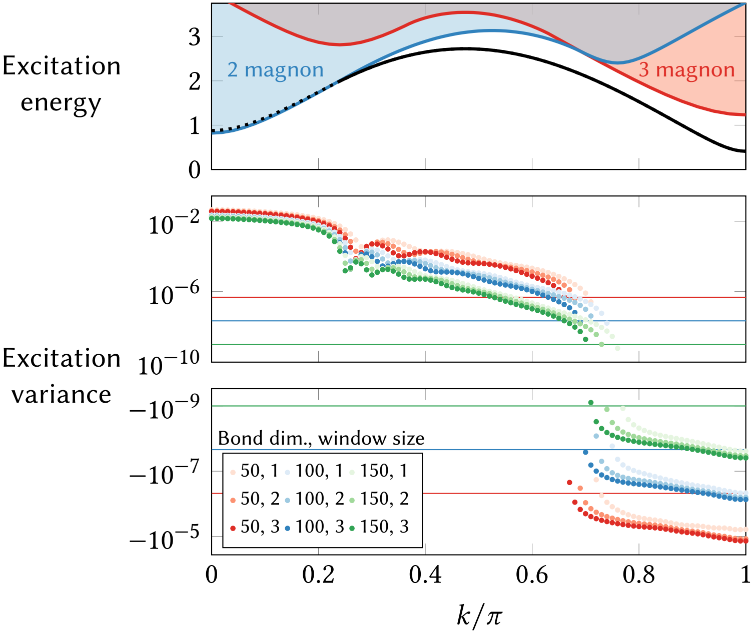
Can calculate the variance:

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

Since we only have an approximation to the GS:

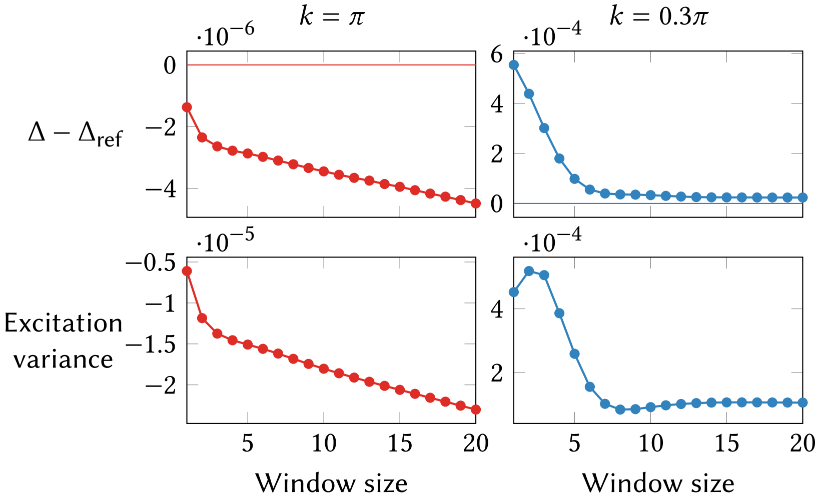
- Δ can be less than the actual value.
- σ_Δ^2 can be negative.
- Bound by error in GS.

Spin-1 Heisenberg model



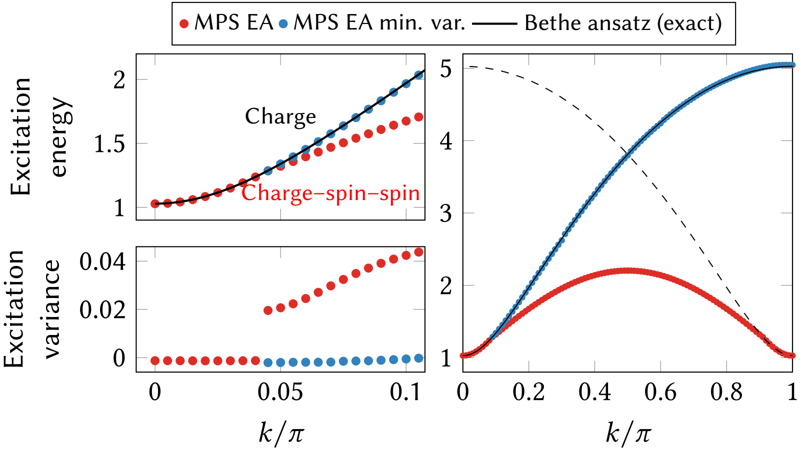
Spin-1 Heisenberg model

Tuning window size (bond dim. 50)



Minimising energy variance

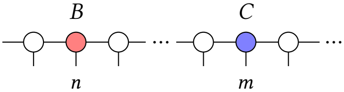
Hubbard model chargons, $U/t = 5$



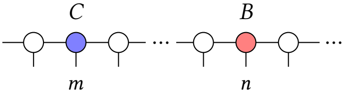
Compare V. Zauner–Stauber et al., Phys. Rev. B **97**, 235155 (2018).

Multi-particle states

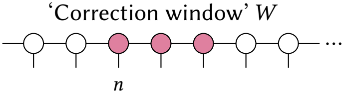
$$|\Upsilon_{k_1,k_2}\rangle = \sum_n \Big[q_1 \sum_{m>n} \mathrm{e}^{\mathrm{i}(k_1 n + k_2 m)} \dots$$



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



$$+ \, \mathrm{e}^{\mathrm{i}(k_1+k_2)n} \dots$$



$$\dots \Big],$$

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

Generalises to ≥ 3 excitations.

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

Conclusion

- Excitation ansatz wavefunctions are triangular MPSs.
- Can calculate fixed point relations recursively.

Thanks to:

- Ian McCulloch (NTHU).

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