Studying bound states with the MPS excitation ansatz

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Excitations in the Ising model

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

Elementary excitations are domain walls

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

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

Separation between two domain walls doesn't affect energy

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

$$\Delta = 4J$$

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

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

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

Energy scales linearly with domain wall separation

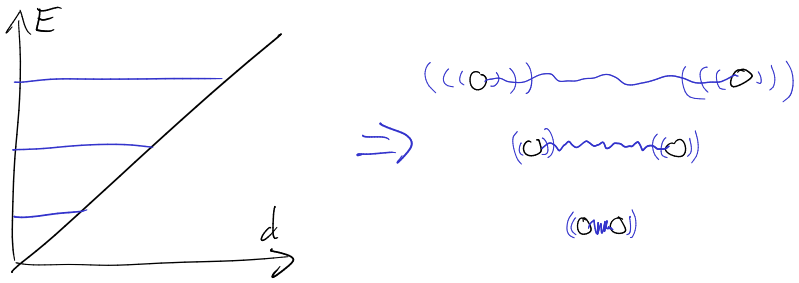
$$\cdots \uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow \cdots \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\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

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

Lowest-energy excitations are bound domain-wall pairs

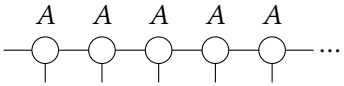
Bound state spectra

Can solve for energy eigenstates in linear potential



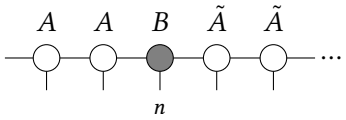
Larger energies correspond to larger separations

Algorithm: MPS excitation ansatz

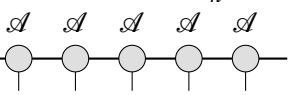
$$|\Psi\rangle = \cdots$$ 

$$\cdots$$

Use to form an ansatz for excitations with momentum k

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

$$\cdots$$

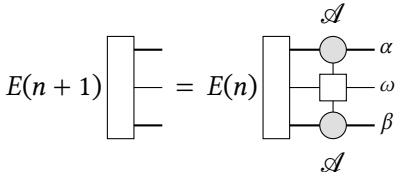
$$= \cdots$$ 

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

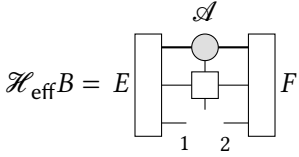
Block-triangular structure: reminiscent of MPOs

Haegeman et al., PRB **85**, 100408(R) (2012)

Excitation ansatz fixed-point equations



- Solve for fixed point recursively in terms of block indices α, β, ω
- Same algorithm as iMPS, but with extra indices α, β
- Can construct effective Hamiltonian to optimize B:

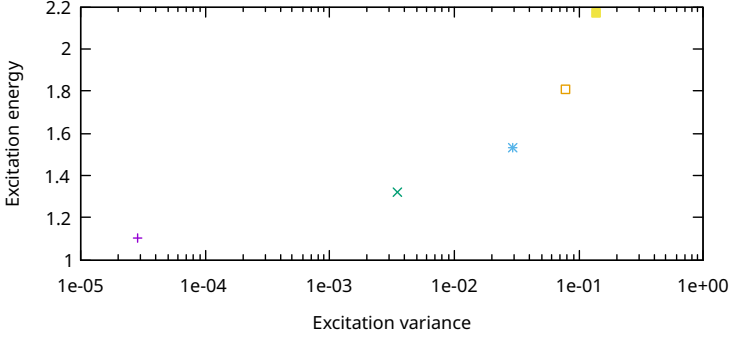


JJO & McCulloch, PRR **7**, 023018 (2025); Michel & McCulloch, arXiv:1008.4667

Example calculation: Ising model

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

Total momentum $k = 0$



Higher-energy excitations have much larger variance: how to improve?

Multi-site windows

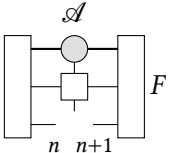
For broader excitations, increase size of window

$$|\Phi_k[\mathbf{B}]\rangle = \sum_n e^{ikn} \cdots \underset{n}{\overset{A\ A\ B_1\ B_2\ B_3\ \tilde{A}\ \tilde{A}}{\text{---○---○---●---●---●---○---○---}}} \cdots,$$

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

Optimize one tensor at a time (EA DMRG)

$$\mathscr{H}^{(n)}_{\text{eff}} B_n =$$



- Can apply environment expansion as well (see Ian's talk on Tuesday)
- Also seems to converge in two half-sweeps?

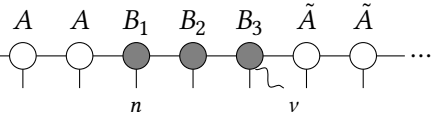
Vanderstraeten et al., PRB **101**, 115138 (2020)

Simultaneous optimization

What if we want multiple eigenstates?

- Project away lower states?
- Our method: optimize multiple levels ν simultaneously

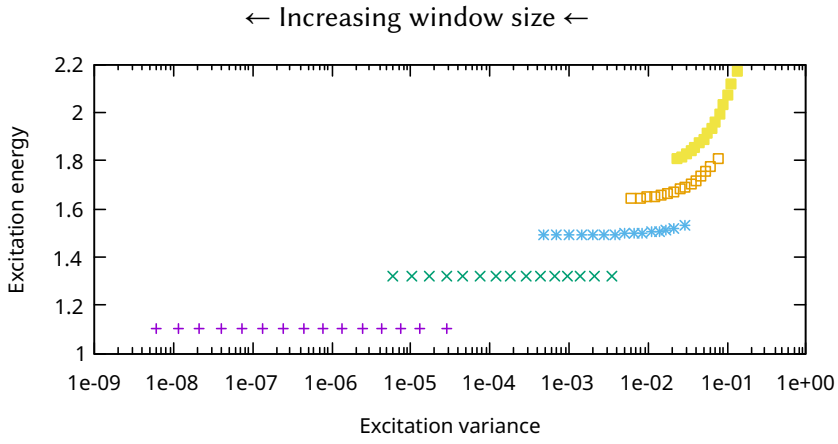
$$|\Phi_k^\nu[\mathbf{B}]\rangle = \sum_n e^{ikn} \cdots$$



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

JJO & McCulloch, in preparation

Example calculation: Ising model

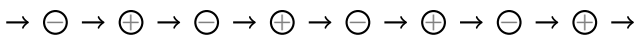


See also Vanderstraeten et al., PRB **101**, 115138 (2020)

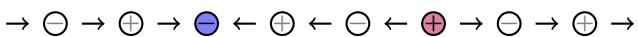
Application: Confinement in the quantum link model

$$\hat{H} = -\frac{\kappa}{2}\sum_j \left(\hat{\phi}_j^\dagger \hat{S}^-_{j,j+1}\hat{\phi}_j + \text{H.c.}\right) + m\sum_j (-1)^j \hat{\phi}_j^\dagger \hat{\phi}_j + \frac{g^2}{2}\sum_j (\hat{S}^z_{j,j+1})^2 - \chi \sum_j \hat{S}^z_{j,j+1}$$

- Staggered fermions
- Represent the gauge fields with spin-S ($= 1/2$ here)

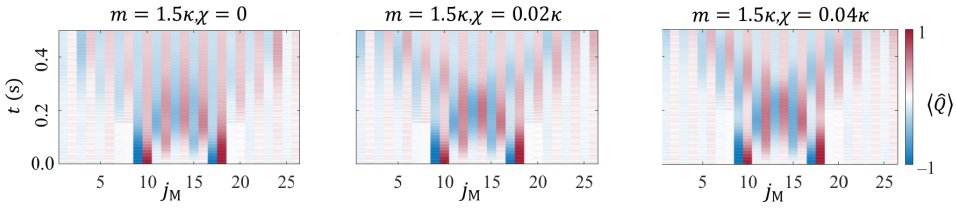


- Flux string between charges

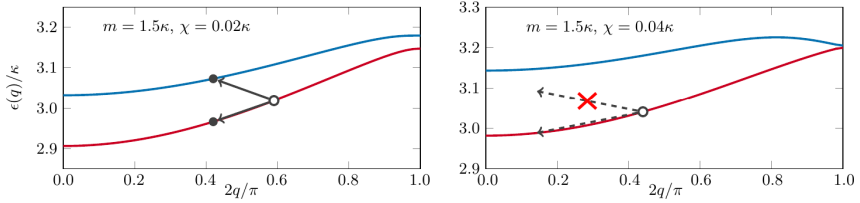


- Confined by external field χ
- 'Meson' bound states

Meson scattering

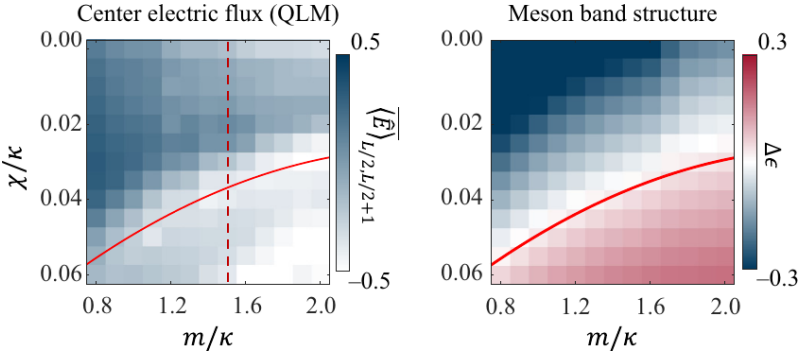


→ Increasing confinement →



Su*, JJO*, Halimeh, PRX Quantum **5**, 040310 (2024)

Band structure determines scattering behaviour



- If wave packets dissociate, central flux stays low after collision
- If they remain coherent, flux goes back to original value (0.5)
- Heuristic measure based on band gap correctly predicts behaviour

Su*, JJO*, Halimeh, PRX Quantum **5**, 040310 (2024)

Unbound states?

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

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

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

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

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

Conclusion

- Excitation ansatz states are block triangular MPSs
- Can extend window size to describe large bound states
- Simultaneous optimization
- Bound state spectrum can determine scattering behaviour