APS March Meeting

Large-Scale VQE Simulations with Tensor Networks

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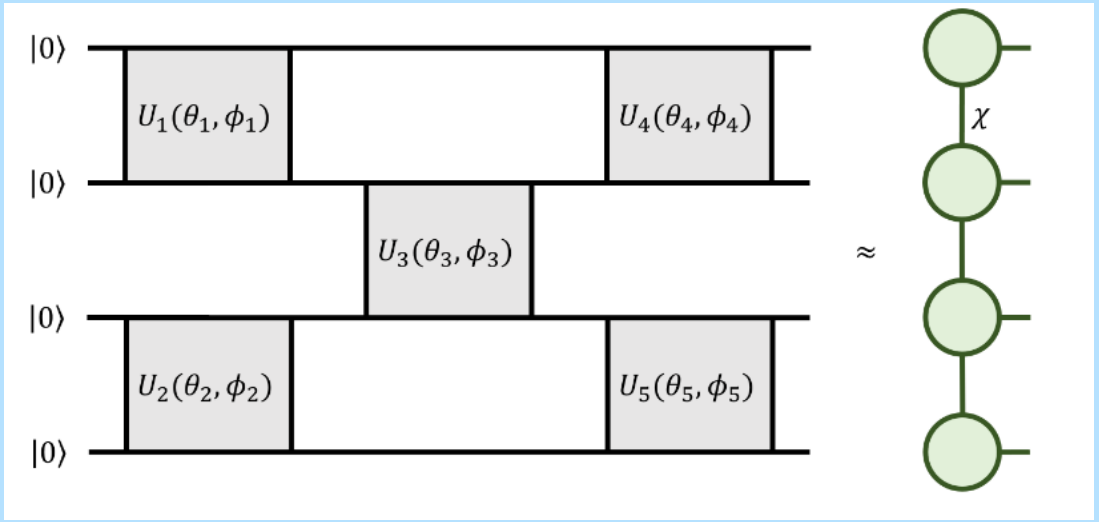
Tensor Networks and VQE

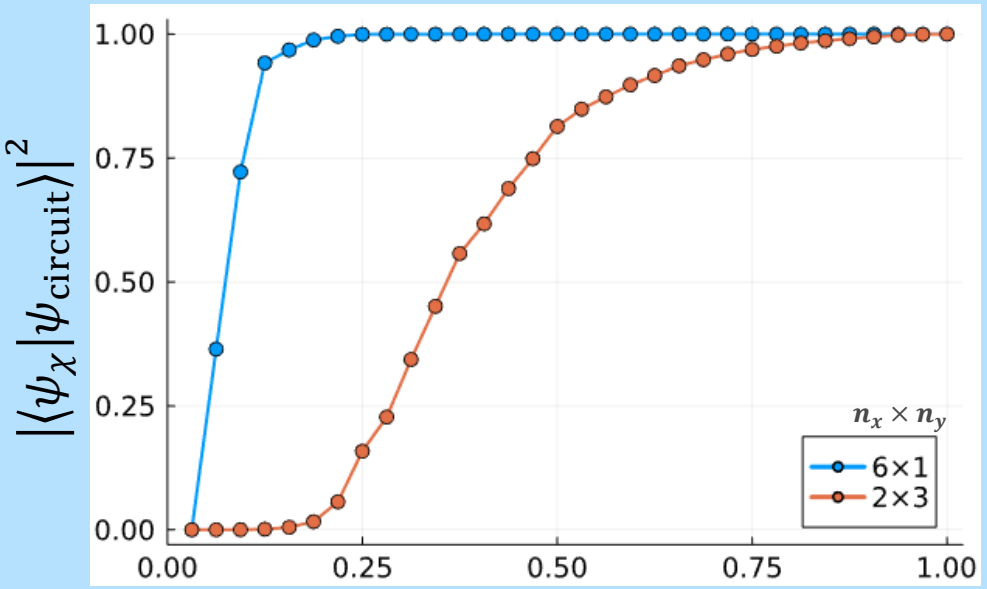
- It's hard to do large-scale circuit optimization
- Use Tensor Networks to approximate parameterized Quantum Circuits

Variational Circuit
$|\psi_{\text{circuit}}\rangle = U(\theta)|0\rangle$

MPS
$|\psi_\chi(\theta)\rangle$



Ground State Hubbard Model

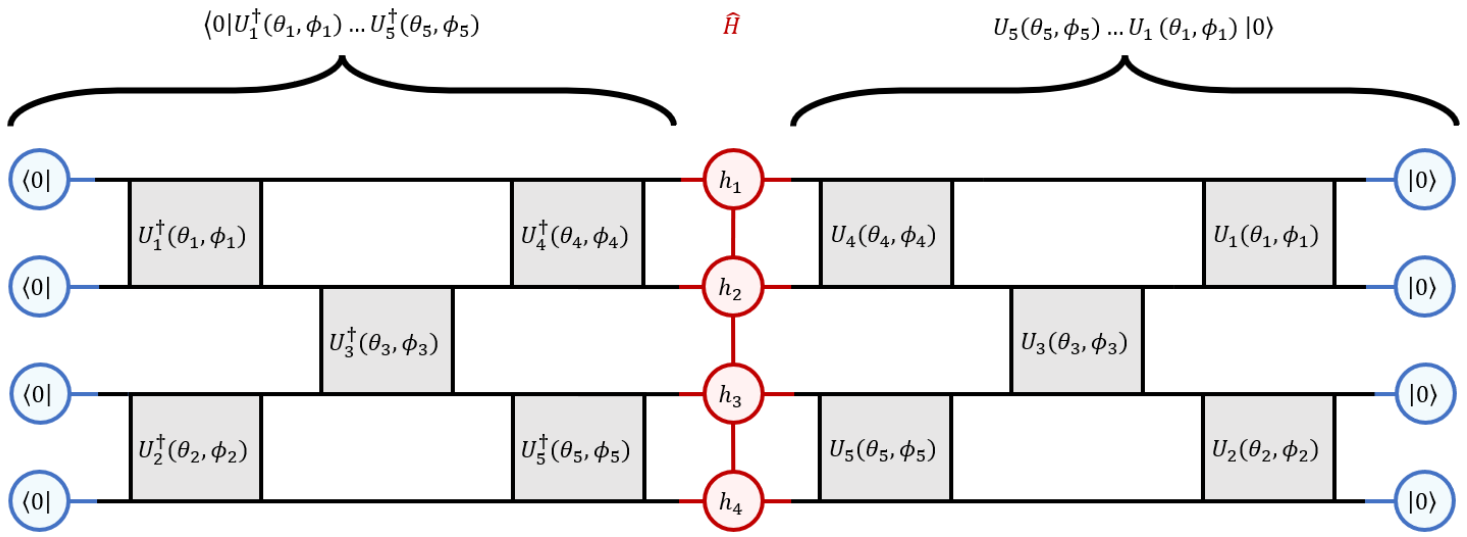


The Goal

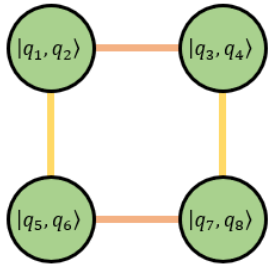
- Perform VQE simulations with many qubits
  - Approximate parameterized quantum circuit as an MPS
  - Observe the performance as we tune the MPS bond dimension

minimize

$$E_\chi(\vec{\theta}) = \left\langle \psi_\chi(\vec{\theta}) \right| H \left| \psi_\chi(\vec{\theta}) \right\rangle \approx$$



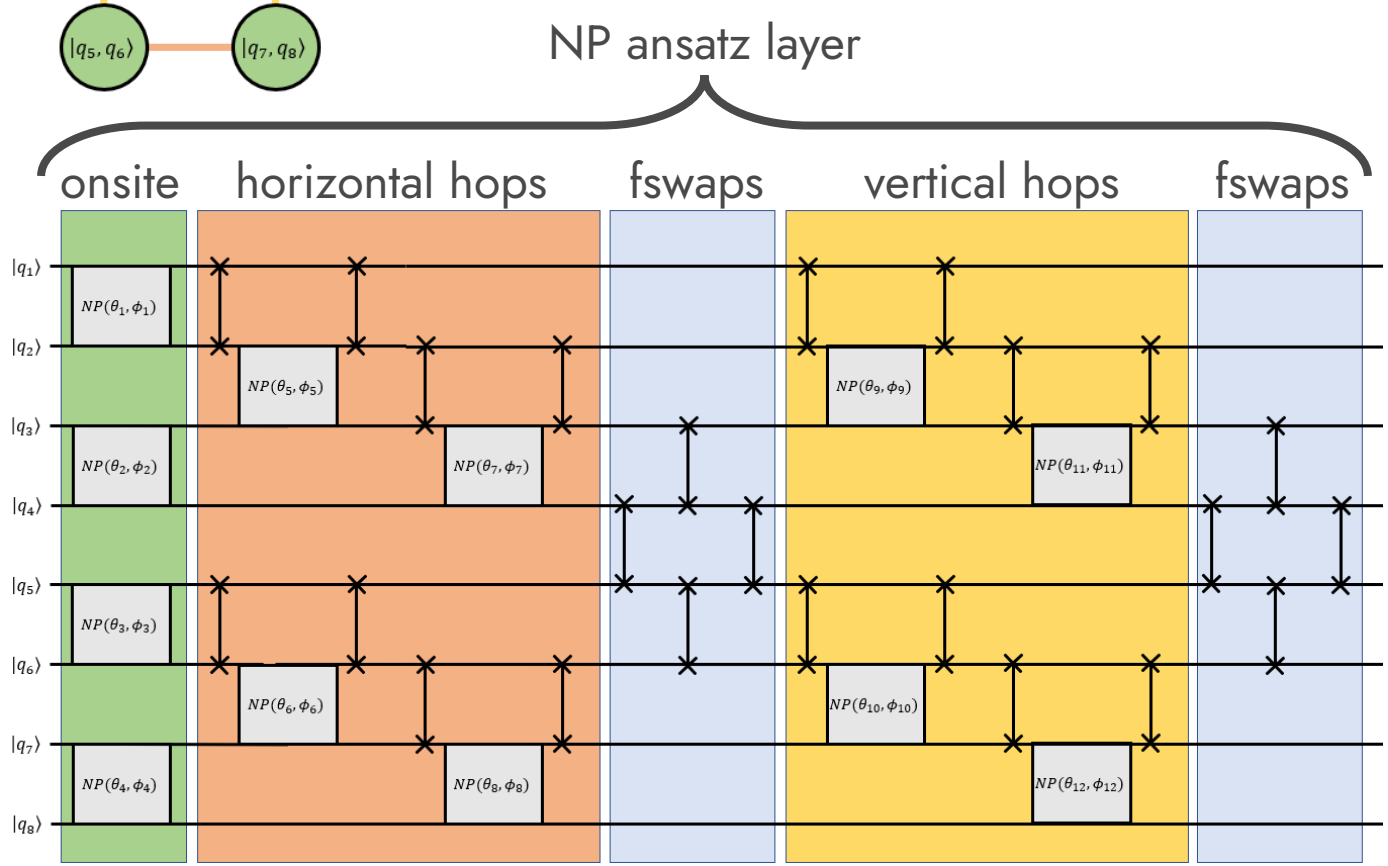
Model and Ansatz



Fermi-Hubbard model with no Boundary Conditions at half filling

$$H = -t \sum_{\langle i,j\rangle,\sigma\in\{\uparrow,\downarrow\}} (a_{i\sigma}^{\dagger} a_{j\sigma} + a_{j\sigma}^{\dagger} a_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (t, U) = (1,2)$$

$$n_q = 2n_x n_y$$



$$NP(\theta, \phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & i\ \sin\theta & 0 \\ 0 & i\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}$$

$$\text{fswap} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

For an $n_x \times n_y$ grid, one layer of the NP ansatz requires $\mathbf{10}\boldsymbol{n_x}\,\boldsymbol{n_y} - \mathbf{4}\boldsymbol{n_x} - \mathbf{4}\boldsymbol{n_y}$ parameters

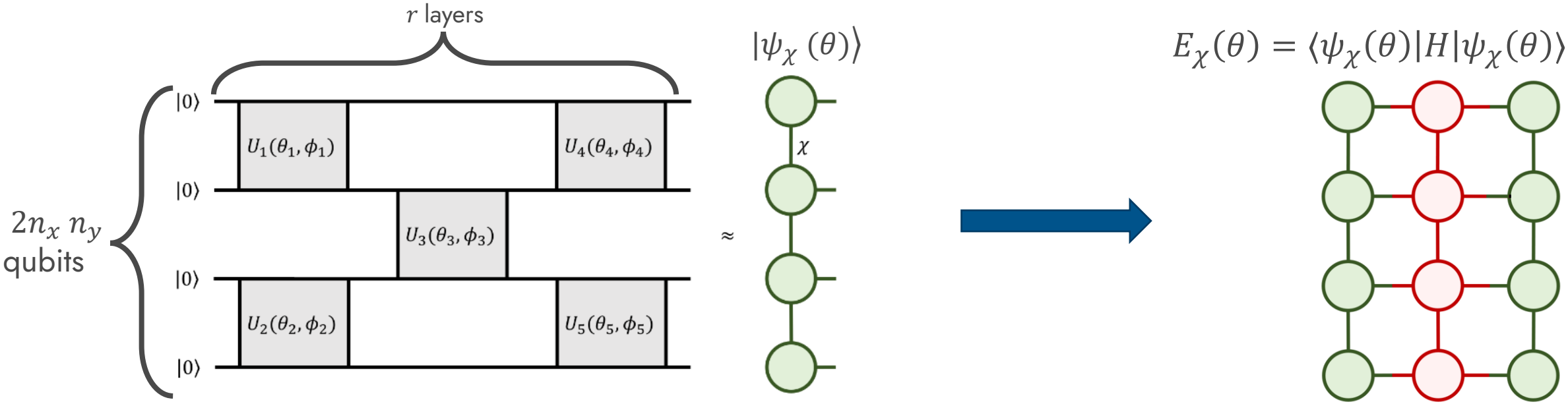
[Cade et al. 2020]

Optimization

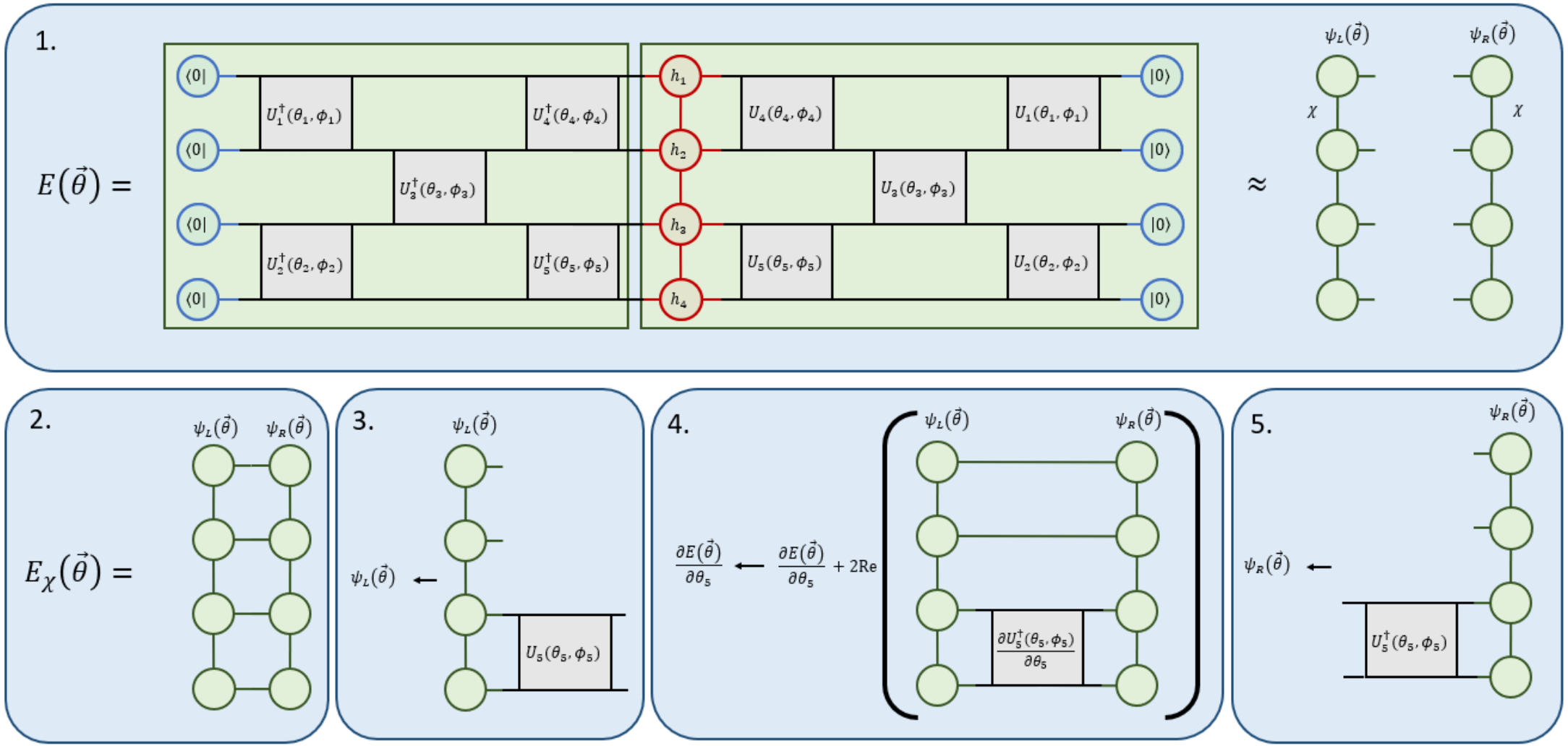
Given a system size $n_x \times n_y$ and r layers of the NP ansatz:

1. Choose a bond dimension χ
2. Minimize $E_\chi(\theta) = \langle\psi_\chi(\theta)|H|\psi_\chi(\theta)\rangle$ with tensor network backend
   - Gradients can be computed using automatic differentiation
   - Optimized with BFGS
   - Optimization terminates when $E_\chi\left(\theta^{(t+1)}\right) - E_\chi\left(\theta^{(t)}\right) < 10^{-7}$
3. Obtain the optimized parameters θ^*_χ

ITensor

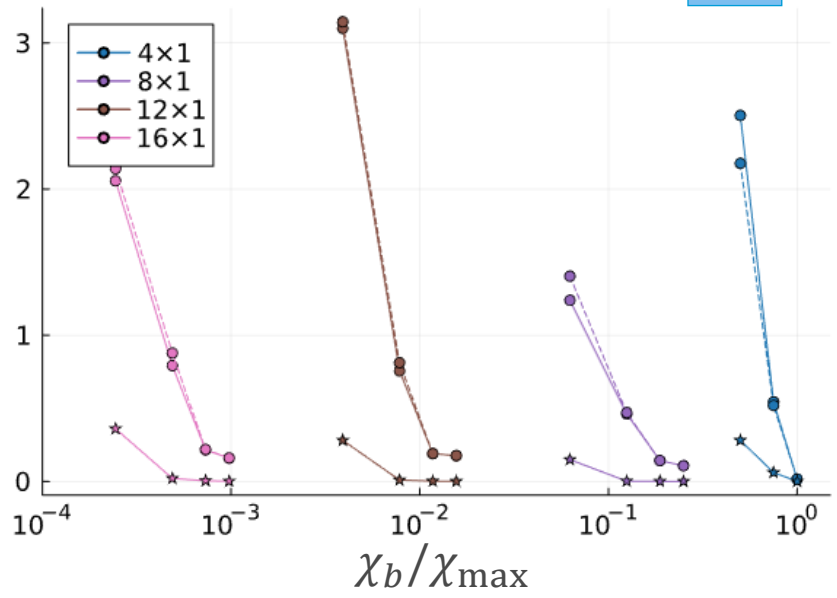


Computing Gradients

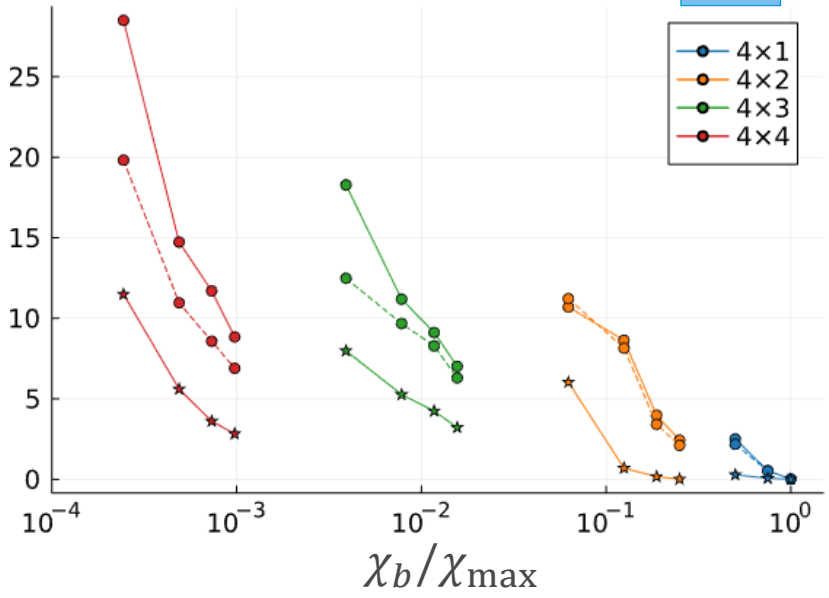


Results

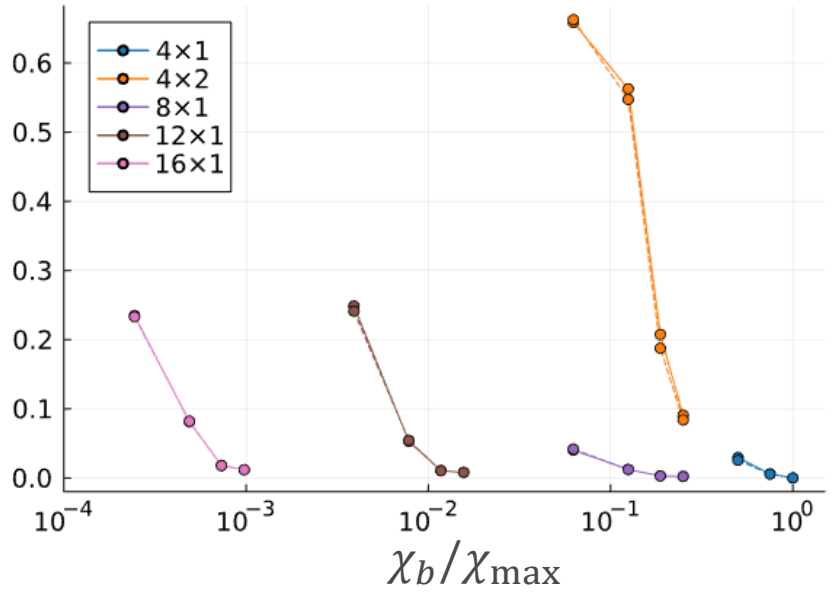
Relative Energy Error (%) 1D



Relative Energy Error (%) 2D



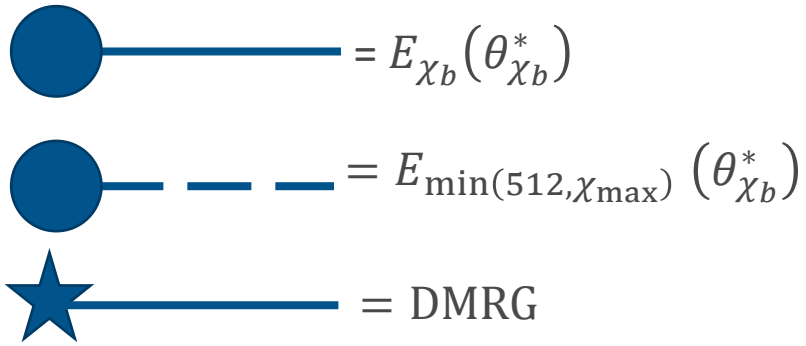
$1 - |\langle \psi(\theta^*_{\chi_b}) | \psi_{\text{exact}} \rangle|^2$



We perform VQE optimization with $\chi_b \in \{16, 32, 48, 64\}$

$$\theta^*_{\chi_b} = \underset{\theta}{\text{argmin}} \langle \psi_{\chi_b}(\theta) | H | \psi_{\chi_b}(\theta) \rangle$$

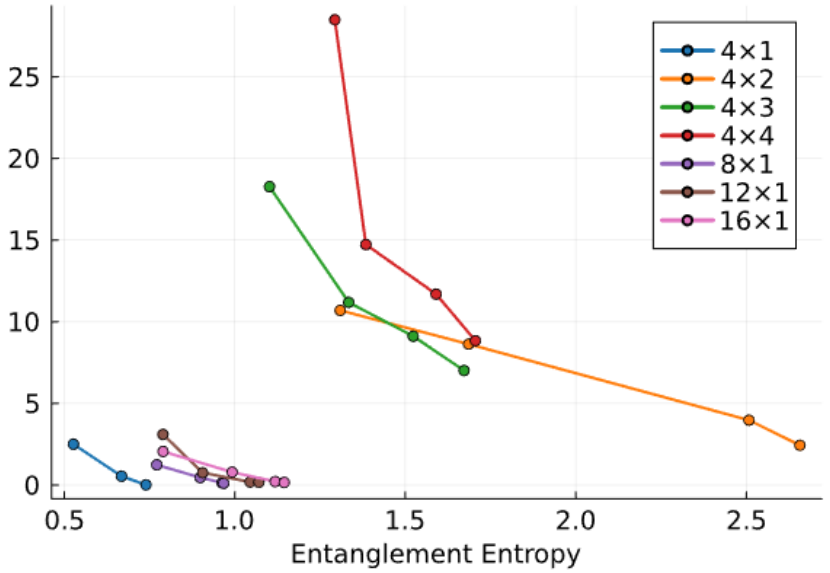
$$E_{\chi_a}(\theta^*_{\chi_b}) = \langle \psi_{\chi_a}(\theta^*_{\chi_b}) | H | \psi_{\chi_a}(\theta^*_{\chi_b}) \rangle$$



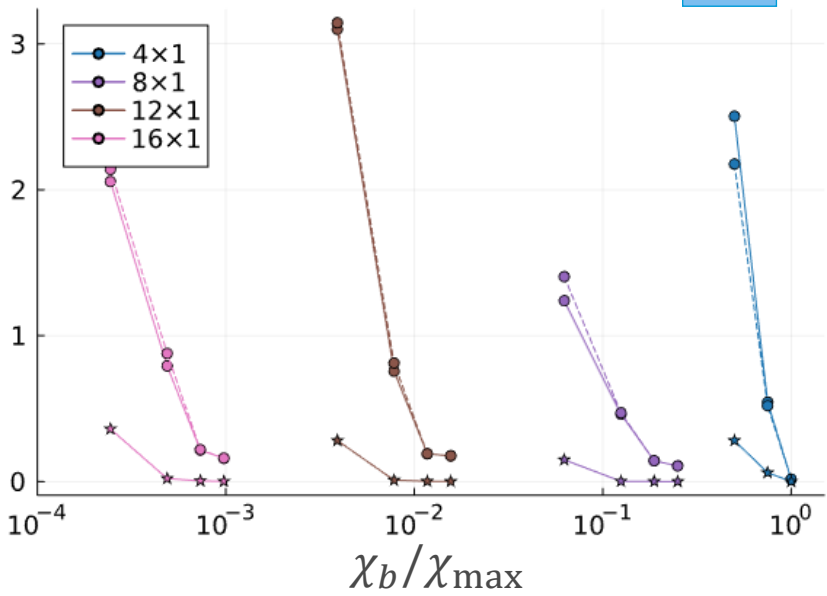
Takeaways

- Using the MPS bond dimension, we can trade computational resources with ground state accuracy
- The complexity of the circuit is bounded by its entanglement entropy, which is bounded by the MPS bond dimension
- Generally, when $\chi_1 < \chi_2$, $E_{\chi_2}(\theta^*_{\chi_1}) < E_{\chi_1}(\theta^*_{\chi_1})$
  - Optimizing at a low bond dimension yields circuits that yield more accurate target states when the circuit is evaluated exactly

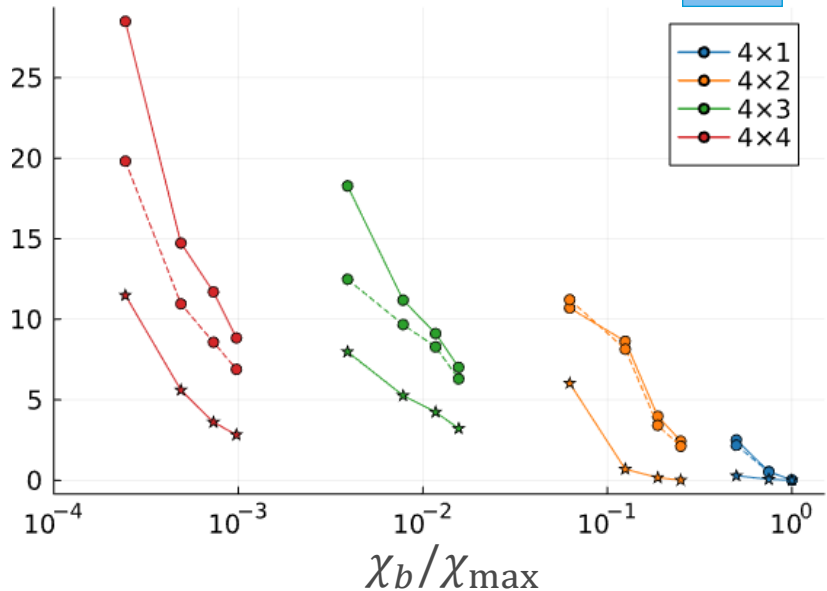
Relative Energy Error (%)



Relative Energy Error (%) 1D



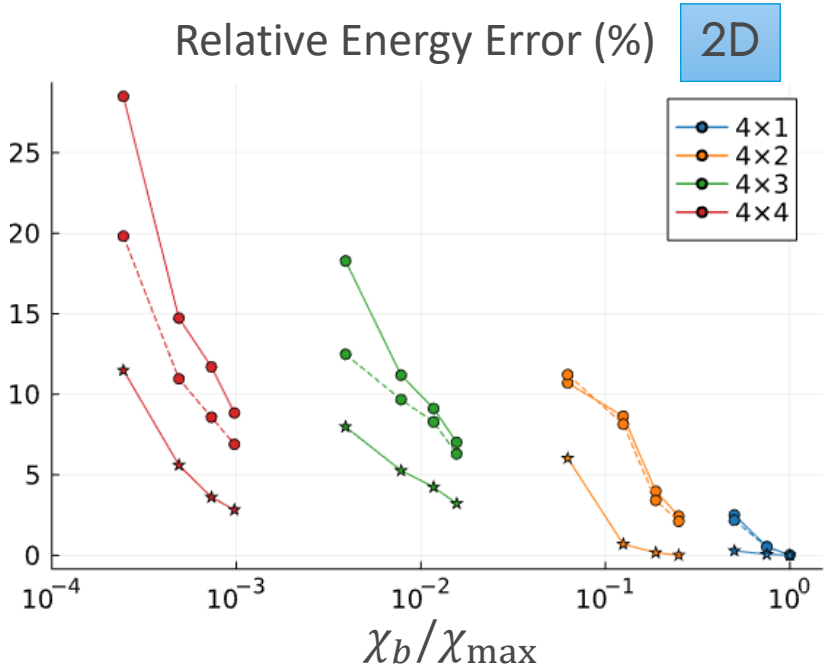
Relative Energy Error (%) 2D



Further Research

1. Instead of minimizing
   $E_\chi(\theta) = \langle\psi_\chi(\theta)|H|\psi_\chi(\theta)\rangle$,
   what if we minimized
   $1 - F(\theta) = 1 - \left|\langle\psi_\chi(\theta)|\psi_{\mathrm{DMRG}}\rangle\right|^2$

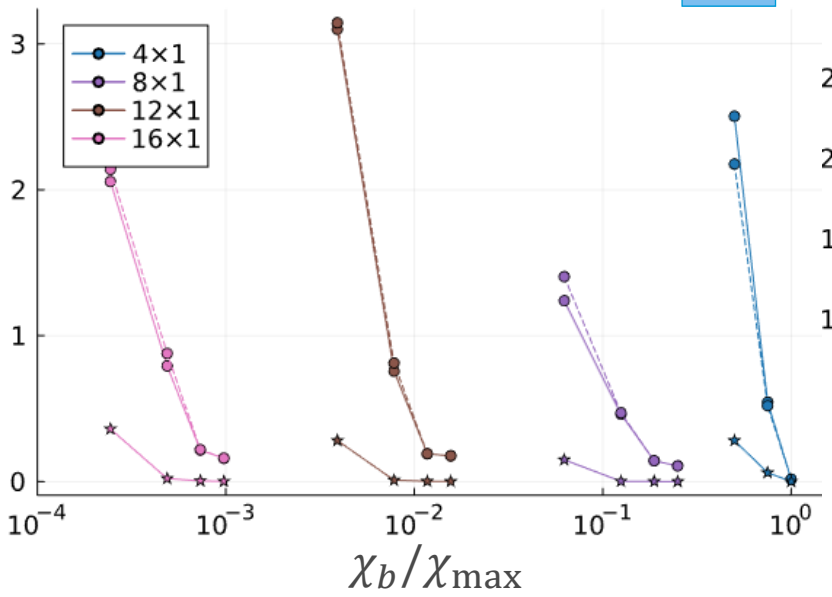
2. How well do these optimized parameters perform as initialization for true VQE?
   1. How many optimization steps
   2. Does this get us out of barren plateaus



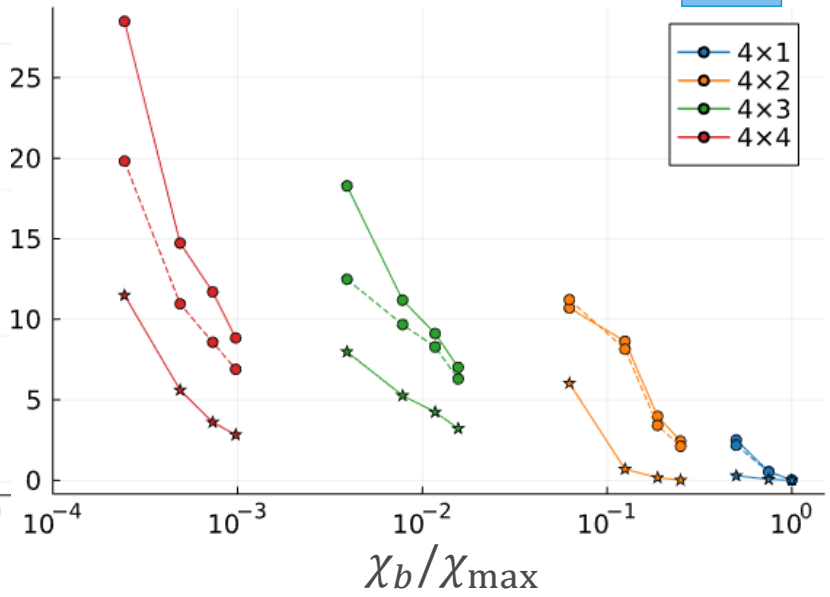
Conclusion

- Performed VQE simulations of up to 32 qubits
- MPS bond dimension tunes accuracy with resources
- Optimized parameters yield more accurate energies when circuits are evaluated exactly

Relative Energy Error (%) 1D



Relative Energy Error (%) 2D



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