

Studying $(2+1)$ -dimensional fermionic systems with adaptive variational quantum algorithms

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1. Overview
2. Setup
3. Variational quantum eigensolver
4. ADAPT-VQE
 - ▶ Naive ansatz
 - ▶ Best greedy ansatz
 - ▶ Symmetry-informed ansatz

Overview

Why $(2+1)$ -dimensional fermionic systems?

Why (adaptive) variational quantum algorithms?



From Google Gemini

Overview

Why (2+1)-dimensional fermionic systems?

- Higher dimensional testing ground

Why (adaptive) variational quantum algorithms?



From Google Gemini

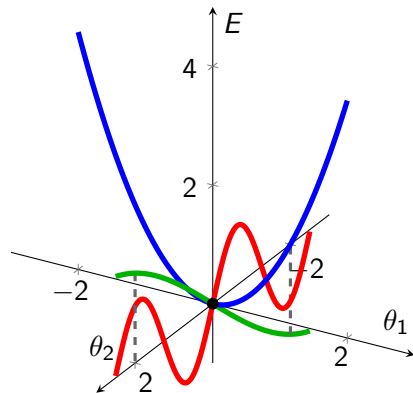
Overview

Why (2+1)-dimensional fermionic systems?

- Higher dimensional testing ground

Why (adaptive) variational quantum algorithms?

- (Ground-) state preparation



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Free Wilson fermions in 2+1D

Spatial discretization with Wilson term (PBC):

$$H = \sum_{n \in \Lambda} \left[-\frac{1}{2} \sum_j \left(\bar{\Psi}(n) (i\gamma^j + r) \Psi(n + \hat{j}) + \text{h.c.} \right) + \bar{\Psi}(n)(m + 2r)\Psi(n) \right]$$

- ▶ $N_x \times N_y$ physical lattice of spinors $\Psi(n)$
- ▶ $(2 \cdot N_x) \times N_y$ lattice of fermionic modes $\Phi(n)$

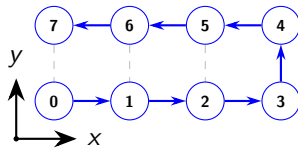
$$\Psi(n) = \Psi(n_x, n_y) =: \begin{pmatrix} \Phi(2n_x, n_y) \\ \Phi(2n_x + 1, n_y) \end{pmatrix}$$

Setup

- ▶ 2×2 physical lattice of spinors $\Psi(n)$
- ▶ 4×2 lattice of fermionic modes $\Phi(n)$
- ▶ Jordan Wigner transformation
- ▶ 0-charge sector:

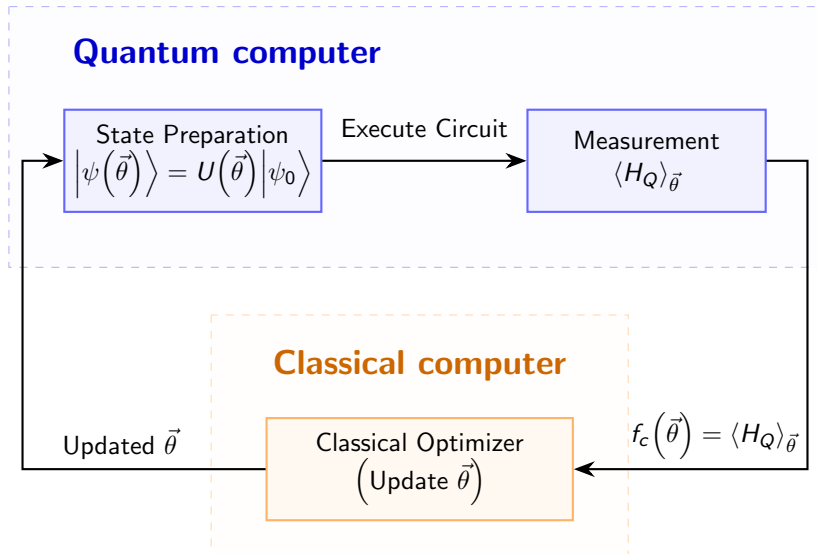
$$Q = \sum_{m_x=0}^3 \sum_{n_y=0}^1 \left(\Phi^\dagger(m_x, n_y) \Phi(m_x, n_y) - \frac{1}{2} \right)$$

$$H_Q = H + \lambda_Q Q^2 \quad \lambda_Q = 100$$

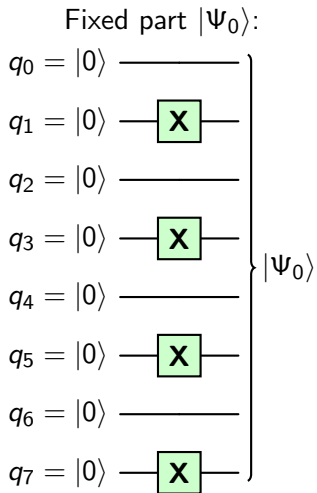


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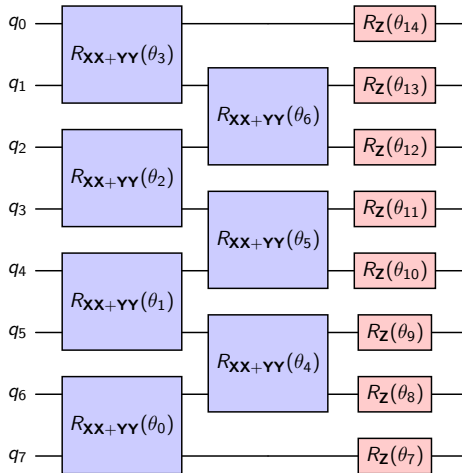
Variational quantum eigensolver (VQE)



VQE circuit



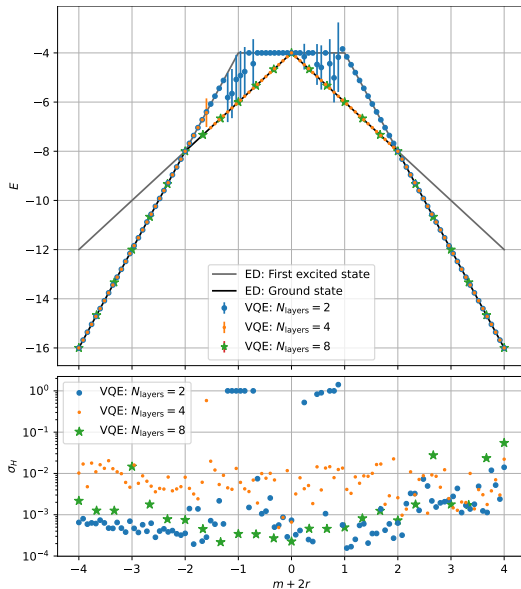
One layer (from Schuster et al. [Sch+24]):



VQE results for varying layer counts

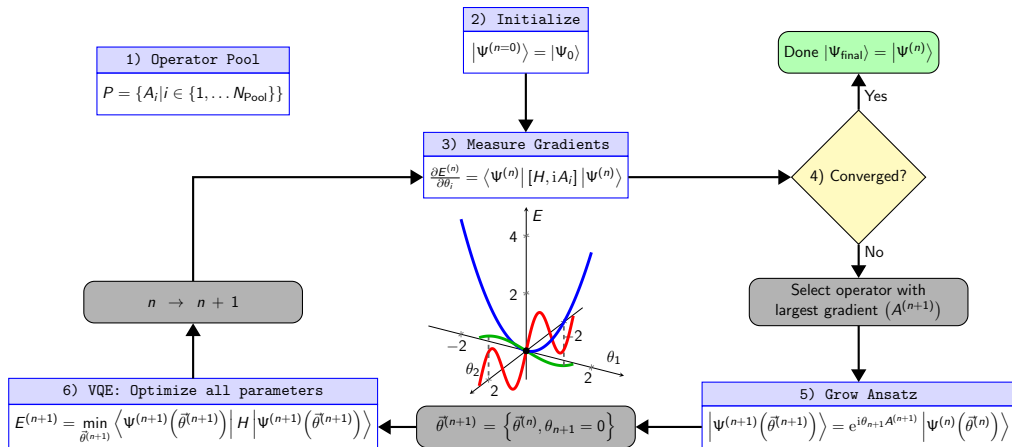
- ▶ $l_{\max} = 20000$
- ▶ $|\psi_0\rangle = |01010101\rangle$
- ▶ $\sigma_h = \sqrt{\text{Var}(H)}$

Four layers are sufficient
for ground state
reconstruction



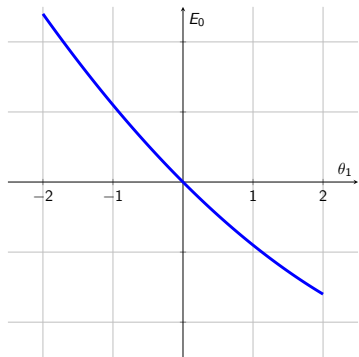
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Adaptive Derivative-Assembled Pseudo-Trotter ansatz VQE (ADAPT-VQE)

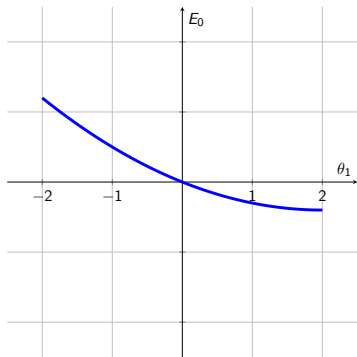


Adapted from Grimsley et al. [Gri+19]

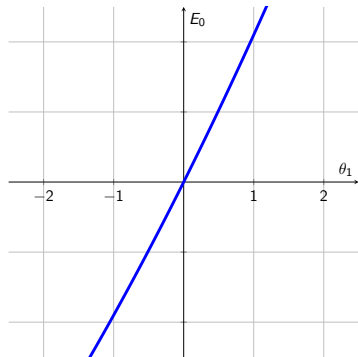
ADAPT-VQE: Pictorially - First iteration



A_1

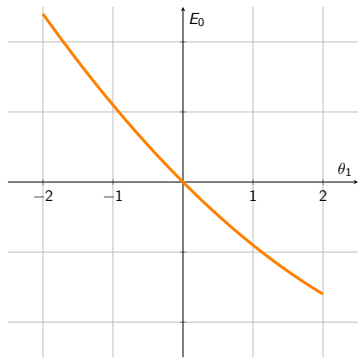


A_2

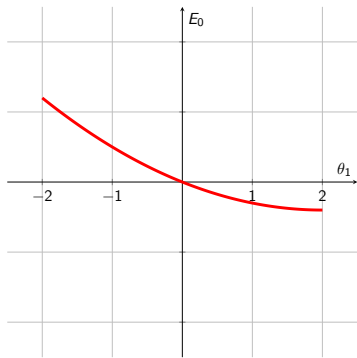


A_3

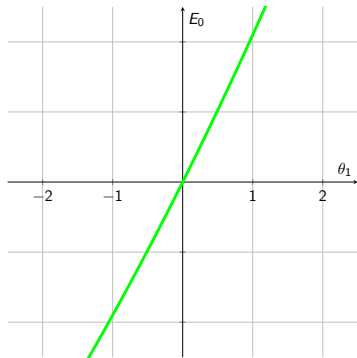
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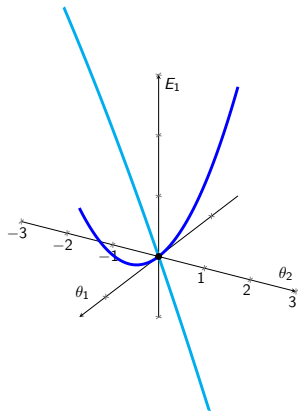


A_2

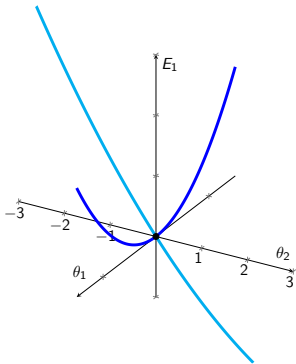


A_3

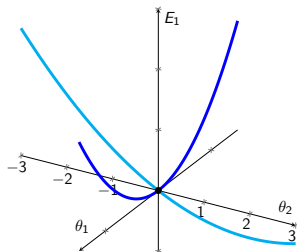
ADAPT-VQE: Pictorially - Second iteration



A_1

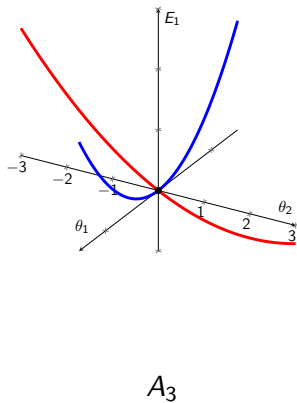
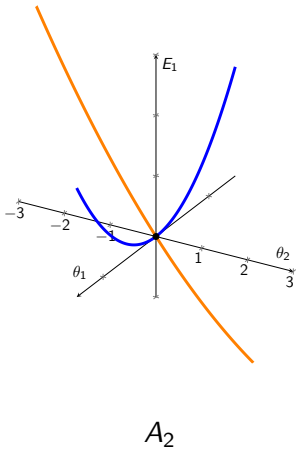
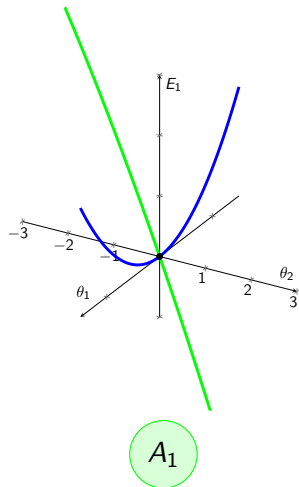


A_2



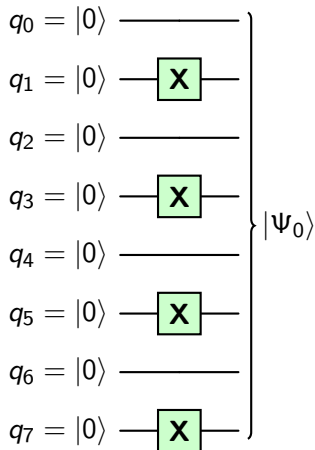
A_3

ADAPT-VQE: Pictorially - Second iteration



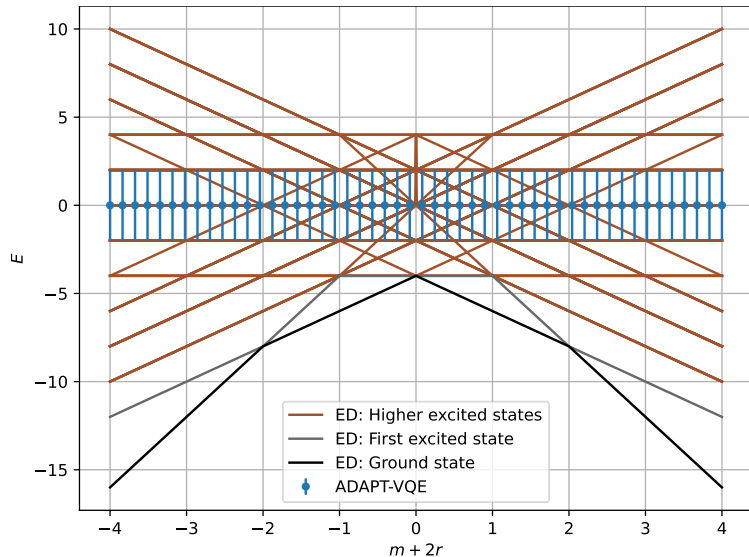
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ADAPT-VQE (naive greedy pool)



- ▶ Include penalty term in optimization, use H_Q
- ▶ Fixed part $|\Psi_0\rangle = |01010101\rangle$
- ▶ $P^{(0)} = \{(\mathbf{X}^{(i)}\mathbf{X}^{(i-1)} + \mathbf{Y}^{(i)}\mathbf{Y}^{(i-1)}), \mathbf{Z}^{(i)}\}$

ADAPT-VQE (naive greedy pool)

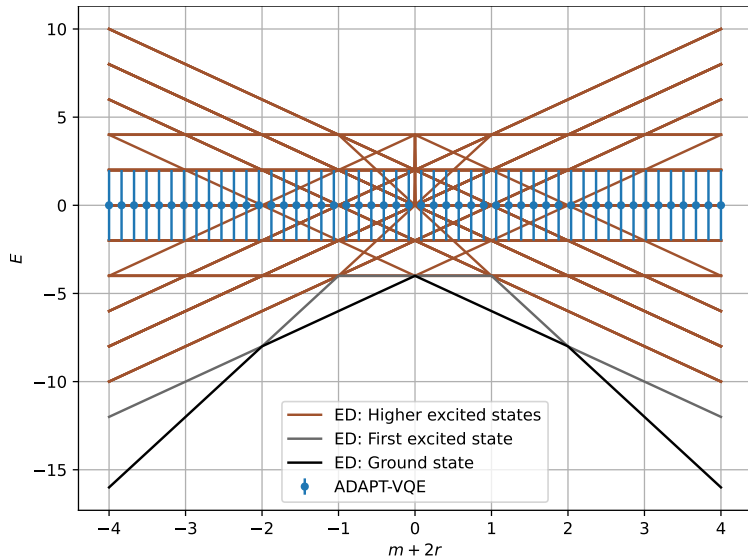


► $|\Psi_0\rangle = |01010101\rangle$

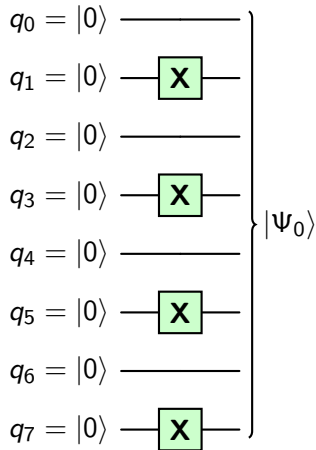
► Pool $P^{(0)}$

Optimization failed

ADAPT-VQE (naive greedy pool)



ADAPT-VQE exits in the first iteration



Limitations of ADAPT-VQE

- ▶ Write operator $A = X + iY$ where $X^\top = X, -Y^\top = Y \in \mathbb{R}$
- ▶ Real wave function: $\vec{C}_0 \in \mathbb{R}$
- ▶ Real mapped Hamiltonian: $H^\top = H \in \mathbb{R}$

Limitations of ADAPT-VQE

- ▶ Write operator $A = X + \mathrm{i}Y$ where $X^\mathrm{T} = X, -Y^\mathrm{T} = Y \in \mathbb{R}$
- ▶ Real wave function: $\vec{C}_0 \in \mathbb{R}$
- ▶ Real mapped Hamiltonian: $H^\mathrm{T} = H \in \mathbb{R}$

$$\Rightarrow \quad \frac{\partial E^{(n)}}{\partial \theta} = \left\langle \psi^{(n)} \left| [H, \mathrm{i}A] \right| \psi^{(n)} \right\rangle = \vec{C}_0^\mathrm{T} (-HY + YH) \vec{C}_0$$

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- ▶ Independent of X

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- ▶ Independent of X
- ▶ $\frac{\partial E^{(n)}}{\partial \theta_i} = 0$ for $Y = 0$

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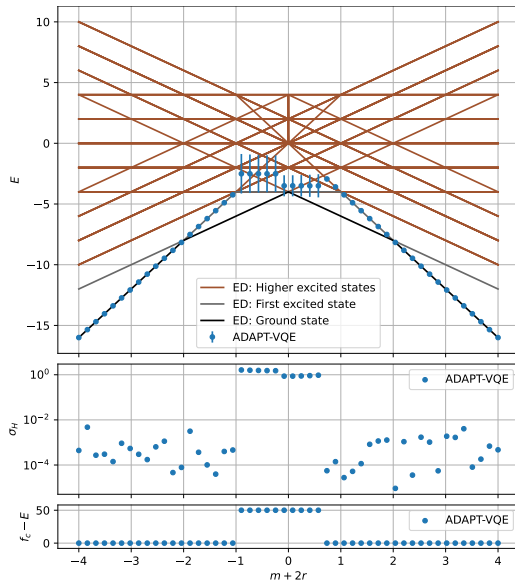
ADAPT-VQE (best greedy pool)

- ▶ Include penalty term in optimization, use H_Q
- ▶ Fixed part $|\Psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$
- ▶ $P^{(2)} = \{(\mathbf{X}^{(i)}\mathbf{X}^{(i-1)} + \mathbf{Y}^{(i)}\mathbf{Y}^{(i-1)}), (\mathbf{X}^{(i)}\mathbf{Y}^{(i-1)} - \mathbf{Y}^{(i)}\mathbf{X}^{(i-1)}), \mathbf{X}^{(i)}, \mathbf{Y}^{(i)}, \mathbf{Z}^{(i)}\}$

ADAPT-VQE (best greedy pool)

- ▶ $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$
- ▶ Pool $P^{(2)}$
- ▶ $l_{\max} = 20000$
- ▶ $\sigma_h = \sqrt{\text{Var}(H)}$
- ▶ $f_C - E = \lambda_Q \langle Q^2 \rangle$

Reliable reconstruction of
energy eigenstates for
 $m + 2r < -1$ and
 $1 < m + 2r$



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Using discrete symmetries for the operator pool construction

- ▶ P and T broken
- ▶ C unbroken: $[H, C] = 0$
- ▶ Pool $\{A_i | [A_i, C] = 0\}$
- ▶ Action of C:

$$\begin{aligned} C |\Psi(\theta_n, \dots, \theta_1)\rangle &= C e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} |\Psi_0\rangle \\ &= e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} C |\Psi_0\rangle \\ C |\Psi_0\rangle &= \alpha_0 |\Psi_0\rangle \quad \Rightarrow \quad C |\Psi(\theta_n, \dots, \theta_1)\rangle = \alpha_0 |\Psi(\theta_n, \dots, \theta_1)\rangle \end{aligned}$$

Going beyond a greedy ansatz: "C invariant" ansatz

$$[A_i, C] \stackrel{!}{=} 0$$

Use parts of H like Farrell et al. [Far+24] in 1+1D:

$$O_1(n) = \bar{\Psi}(n)\Psi(n) = O_1^\dagger(n) \xrightarrow{C} O_1(n)$$

$$O_2(n, j) = \bar{\Psi}(n) i \gamma^j \Psi(n + \hat{j}) \xrightarrow{C} O_2^\dagger(n, j)$$

$$O_4(n, j) = \bar{\Psi}(n) \Psi(n + \hat{j}) \xrightarrow{C} O_4^\dagger(n, j)$$

Combine O_i to C invariant and complex operators:

$$A_1(n) = O_2(n, 1) + O_2^\dagger(n, 1)$$

$$A_2(n) = i \left[O_1(n), O_2(n, 2) + O_2^\dagger(n, 2) \right]$$

$$A_3(n) = i \left[O_1(n), O_4(n, 1) + O_4^\dagger(n, 1) \right]$$

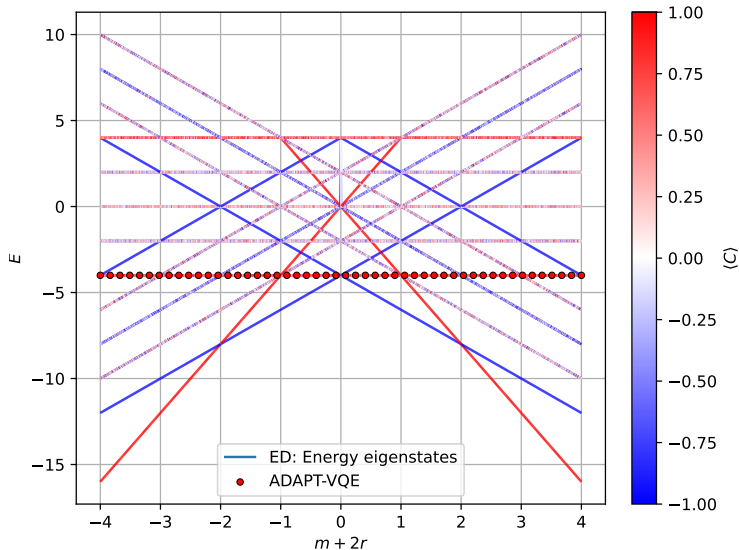
$$A_4(n) = i \left[O_1(n), O_4(n, 2) + O_4^\dagger(n, 2) \right]$$

$$C |\Psi_0\rangle \stackrel{!}{=} \alpha_{C, \Omega} |\Psi_0\rangle \text{ and } P^{(3)} = \{A_i(n)\}$$

ADAPT-VQE (C invariant ansatz 1)

- ▶ Initial state:
 $C|\Psi_0\rangle = +1|\Psi_0\rangle$
- ▶ $|\Psi_0\rangle = |01010101\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$

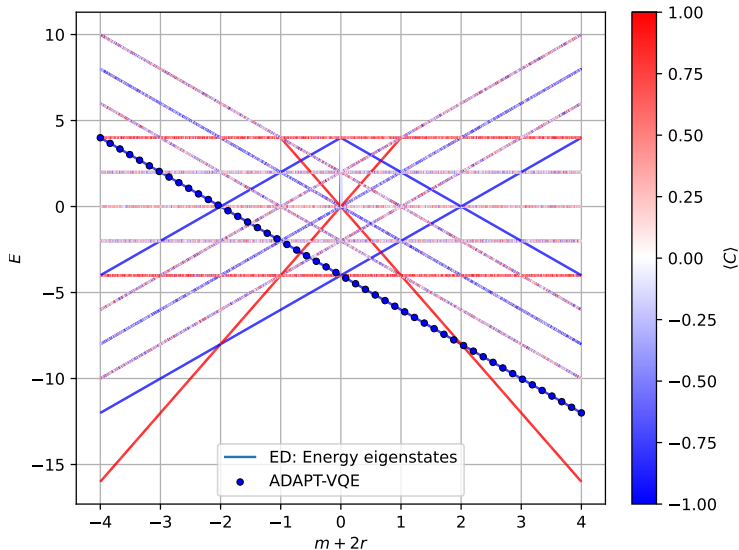
Correct reconstruction of
first excited state for
 $-1 < m + 2r < 1$



ADAPT-VQE (C invariant ansatz 2)

- ▶ Initial state:
 $C|\Psi_0\rangle = -1|\Psi_0\rangle$
- ▶ $|\Psi_0\rangle = |01010110\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$

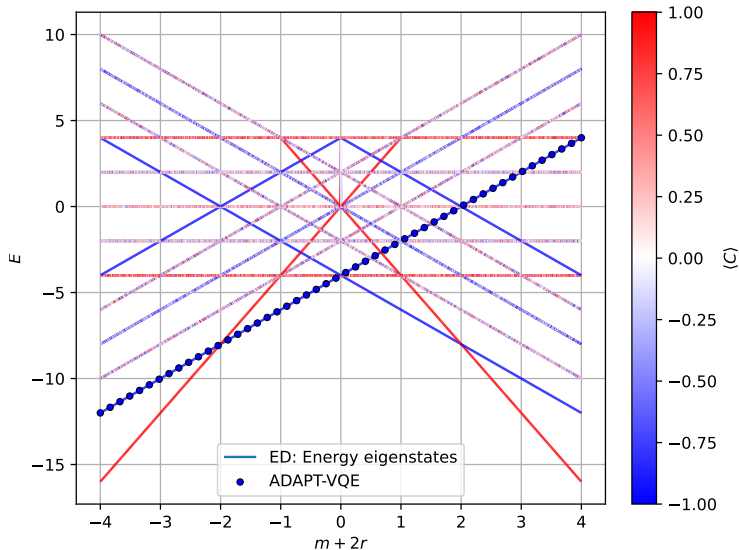
Correct reconstruction of
ground state for
 $0 < m + 2r < 2$



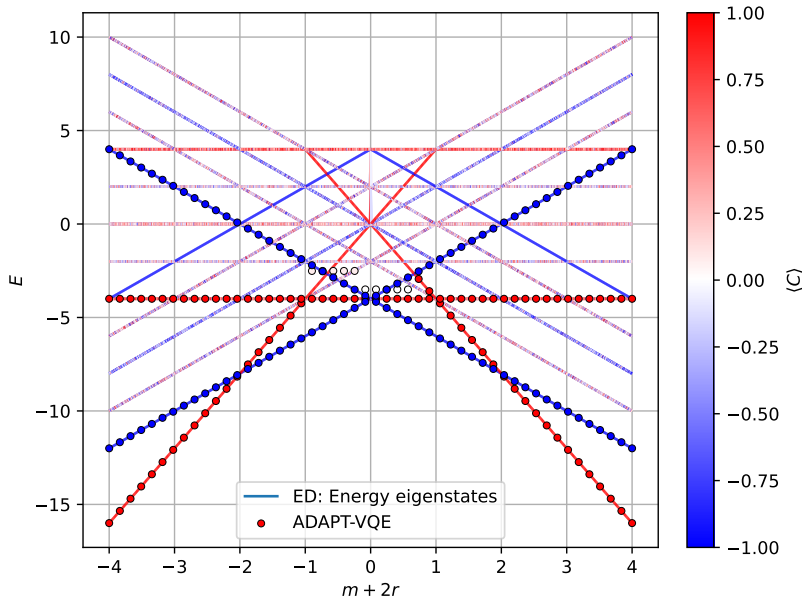
ADAPT-VQE (C invariant ansatz 3)

- ▶ Initial state:
 $C|\Psi_0\rangle = -1|\Psi_0\rangle$
- ▶ $|\Psi_0\rangle = |10010101\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$

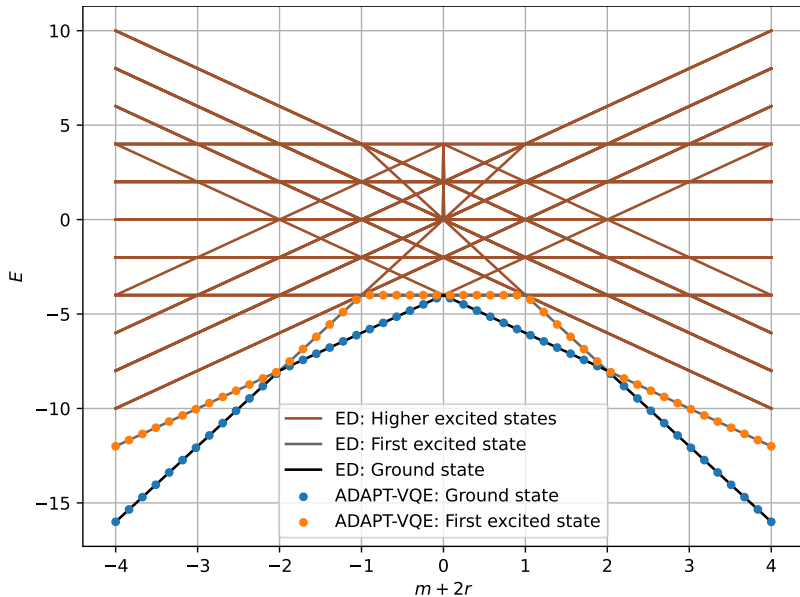
Correct reconstruction of
ground state for
 $-2 < m + 2r < 0$



ADAPT-VQE combined results



ADAPT-VQE combined results



Summary and Outlook

Summary:

- ▶ ADAPT-VQE is not universal
- ▶ Symmetries can mitigate problem of excited states
- ▶ Reconstruction of ground and first excited state

Outlook:

- ▶ Add gauge fields
- ▶ Incorporate more symmetries
- ▶ Larger lattices
- ▶ Scalable ADAPT-VQE

References I

- [Alg+24] Manuel G. Algaba et al. “Low-depth simulations of fermionic systems on square-grid quantum hardware”. In: *Quantum* 8 (Apr. 2024), p. 1327. ISSN: 2521-327X. DOI: 10.22331/q-2024-04-30-1327. URL: <https://doi.org/10.22331/q-2024-04-30-1327>.
- [CCB10] M. Cardoso, N. Cardoso, and P. Bicudo. “Lattice QCD computation of the color fields for the static hybrid quark-gluon-antiquark system, and microscopic study of the Casimir scaling”. In: *Phys. Rev. D* 81 (3 Feb. 2010), p. 034504. DOI: 10.1103/PhysRevD.81.034504. URL: <https://link.aps.org/doi/10.1103/PhysRevD.81.034504>.
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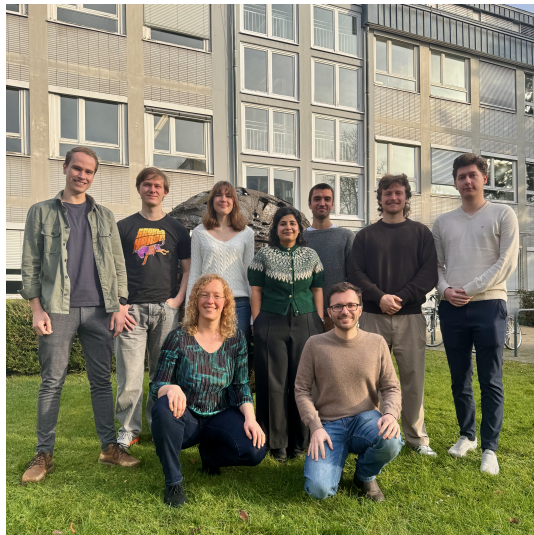
References II

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- [Sch+24] Stephan Schuster et al. “Studying the phase diagram of the three-flavor Schwinger model in the presence of a chemical potential with measurement- and gate-based quantum computing”. In: *Phys. Rev. D* 109 (11 June 2024), p. 114508. DOI: [10.1103/PhysRevD.109.114508](https://doi.org/10.1103/PhysRevD.109.114508). URL: <https://link.aps.org/doi/10.1103/PhysRevD.109.114508>.

References III

- [VC05] F Verstraete and J I Cirac. “Mapping local Hamiltonians of fermions to local Hamiltonians of spins”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2005.09 (Sept. 2005), P09012. DOI: 10.1088/1742-5468/2005/09/P09012.

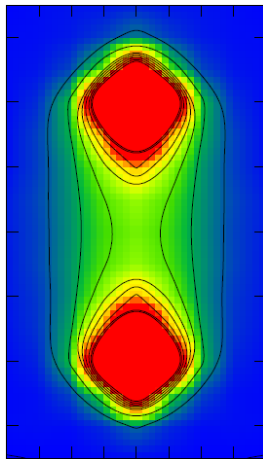
Questions?



Overview: Why $(2+1)$ -dimensional fermionic systems?

Particle physics

- Confinement in QCD in $3+1D$

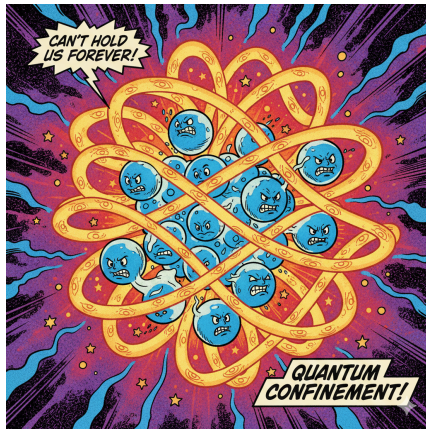


Flux tube from Cardoso et al. [CCB10]

Overview: Why $(2+1)$ -dimensional fermionic systems?

Particle physics

- ▶ Confinement in QCD in $3+1D$
- ▶ Confinement in QED in $2+1D$



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Particle physics

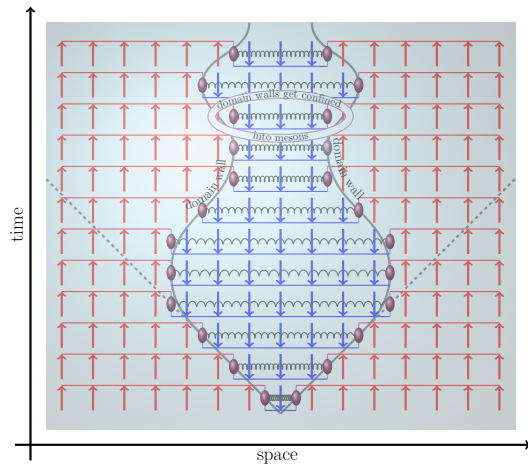
- ▶ Confinement in QCD in $3+1D$
- ▶ Confinement in QED in $2+1D$
- ▶ Free fermions in $2+1D$



From Google Gemini

Overview: Why variational quantum algorithms?

- Non equilibrium / real time dynamics



Confinement sketch from Kormos et al. [Kor+16]

Overview: Why variational quantum algorithms?

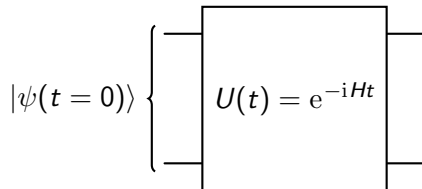
- ▶ Non equilibrium / real time dynamics
 - ▶ Monte Carlo methods suffer from sign problem



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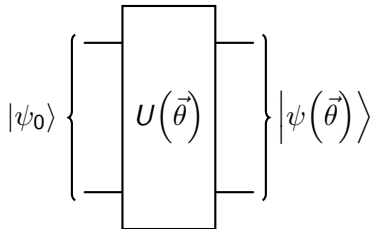
Overview: Why variational quantum algorithms?

- ▶ Non equilibrium / real time dynamics
 - ▶ Monte Carlo methods suffer from sign problem
 - ▶ Quantum computing



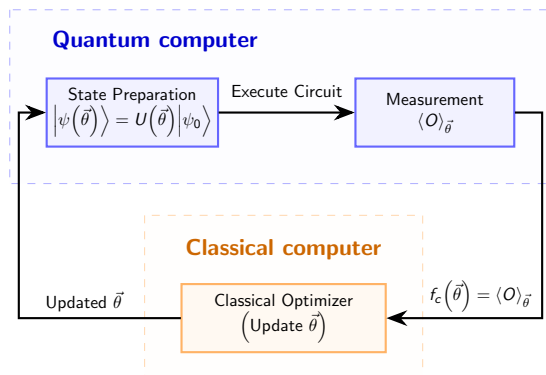
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 - ▶ Monte Carlo methods suffer from sign problem
 - ▶ Quantum computing
- ▶ (Ground-) state preparation:



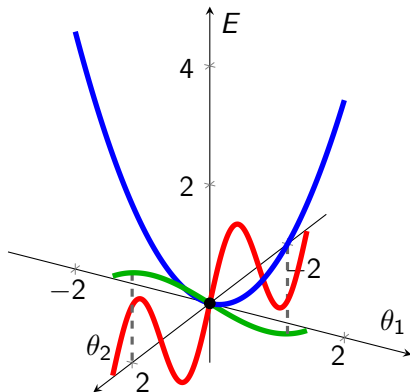
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 - ▶ Quantum computing
- ▶ (Ground-) state preparation:
 - ▶ Variational quantum eigensolver



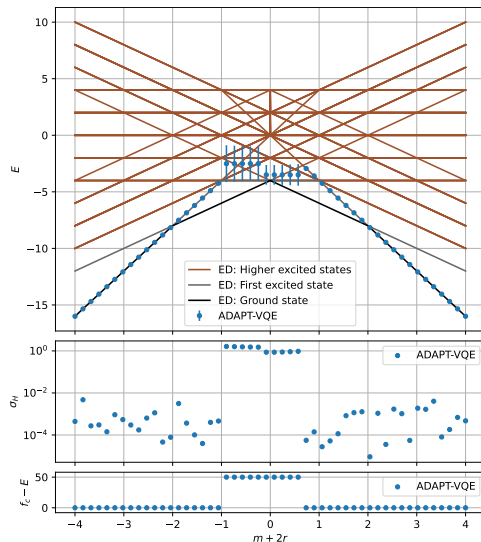
Overview: Why variational quantum algorithms?

- ▶ Non equilibrium / real time dynamics
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- ▶ (Ground-) state preparation:
 - ▶ Variational quantum eigensolver
 - ▶ ADAPT-VQE



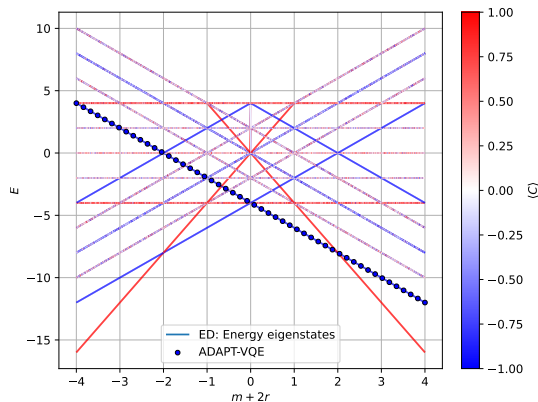
Overview: This work

- First application of ADAPT-VQE to 2+1D
Case study: Free Wilson fermions



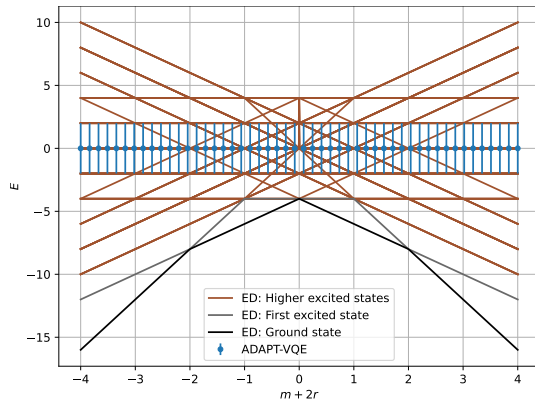
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- ▶ First application of ADAPT-VQE to 2+1D
Case study: Free Wilson fermions
- ▶ Exploiting discrete symmetries



Overview: This work

- ▶ First application of ADAPT-VQE to 2+1D
Case study: Free Wilson fermions
- ▶ Exploiting discrete symmetries
- ▶ Limitations of ADAPT-VQE

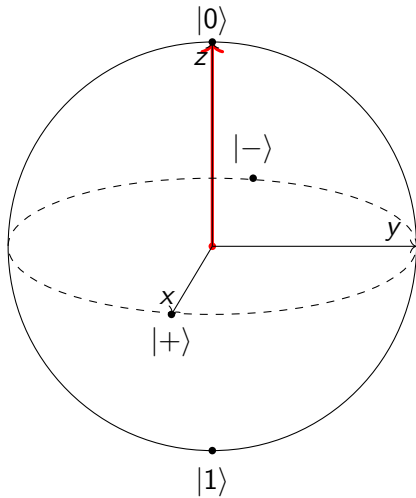


Quantum computing (Gate based)

Classical computing

- Bits either 0

Quantum computing

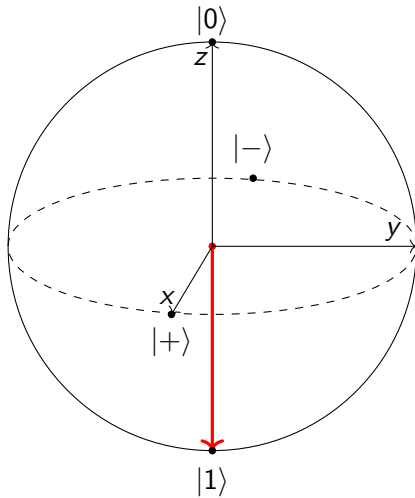


Quantum computing (Gate based)

Classical computing

- Bits either 0 or 1

Quantum computing



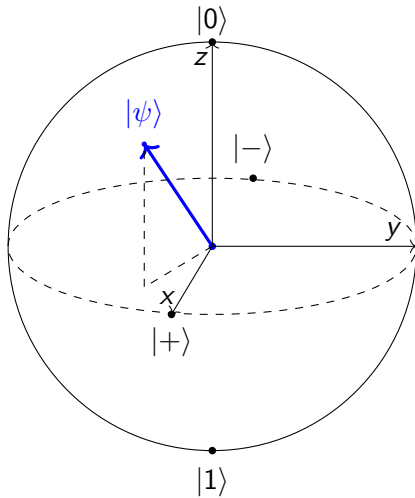
Quantum computing (Gate based)

Classical computing

- Bits either 0 or 1

Quantum computing

- Qubits $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$



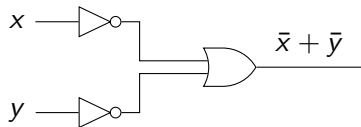
Quantum computing (Gate based)

Classical computing

- ▶ Bits either 0 or 1
- ▶ Circuits of logic gates

Quantum computing

- ▶ Qubits $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$



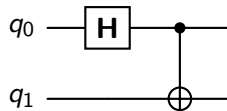
Quantum computing (Gate based)

Classical computing

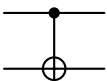
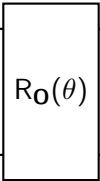
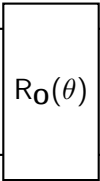
- ▶ Bits either 0 or 1
- ▶ Circuits of logic gates

Quantum computing

- ▶ Qubits $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$
- ▶ Quantum circuits of quantum gates



Unitary gates

Name	Circuit representation	Matrix representation
X	q_i —  —	$\mathbf{X}^{(i)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{(i)}$
Hadamard	q_i —  —	$\mathbf{H}^{(i)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}^{(i)}$
CNOT	q_i —  — q_j —  —	$\text{CNOT}^{(i,j)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}^{(i,j)}$
O -rotation	q_i —  — $\vdots$ q_{i+l} —  —	$\mathbf{R}_{\mathbf{O}}^{(i,\dots,i+l)}(\theta) = \exp\left(-i\frac{\theta}{2}\mathbf{O}^{(i,\dots,i+l)}\right)$

Free fermions in 2+1D

Continuum:

$$\mathcal{L}_{\text{Free}}(\Psi, \bar{\Psi}, \partial_\mu \Psi, x^\mu) = [\bar{\Psi} (i\gamma^\mu \partial_\mu - m) \Psi]_x$$

$$H_{\text{free}} = \int \mathcal{H}_{\text{free}} d^2x = \int \{-i\bar{\Psi}\gamma^j \partial_j \Psi + m\bar{\Psi}\Psi\} d^2x$$

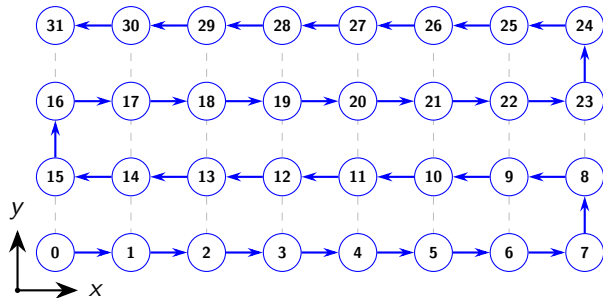
Mapping fermionic modes to qubits

► Jordan Wigner transformation

$$\Phi(m_x, n_y) =: \Phi(j(m_x, n_y))$$

$$= \Phi_j = \left(\prod_{n=0}^{j-1} \mathbf{z}^{(n)} \right) (\sigma^+)^{(j)}$$

$$\sigma^\pm = \frac{1}{2}(\mathbf{X} \pm i\mathbf{Y})$$



Mapping fermionic modes to qubits

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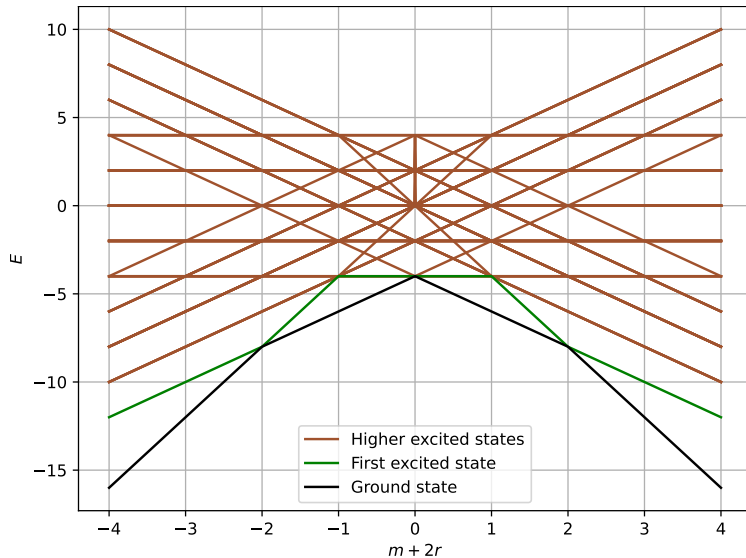
$$\sigma^\pm = \frac{1}{2}(\mathbf{X} \pm i\mathbf{Y})$$

$$|\psi\rangle = \sum_{i_0, \dots, i_{N-1}=0}^1 C_{i_0, \dots, i_{N-1}} \underbrace{\left(\Phi_0^\dagger\right)^{i_0} \dots \left(\Phi_{N-1}^\dagger\right)^{i_{N-1}}}_{=: |i_0, \dots, i_{N-1}\rangle} |\omega\rangle$$

$$= \sum_{i_0, \dots, i_{N-1}=0}^1 C_{i_0, \dots, i_{N-1}} |i_0, \dots, i_{N-1}\rangle$$

$$\forall j \in \{0, \dots, N-1\} : \Phi_j |\omega\rangle = 0,$$

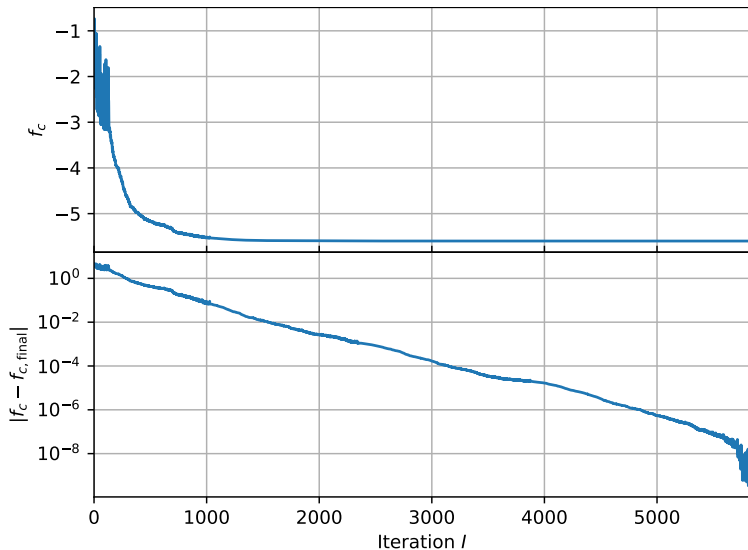
Exact diagonalization



VQE minimization

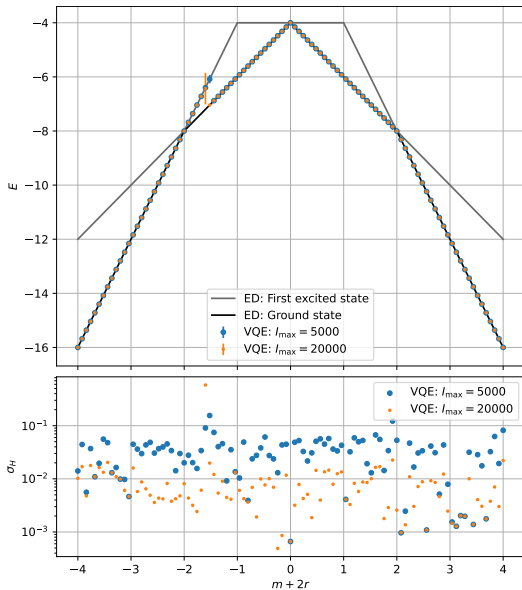
- ▶ $m = -2.8$
- ▶ $N_{\text{layers}} = 4$
- ▶ $I_{\text{max}} = 20000$
- ▶ $|\psi_0\rangle = |01010101\rangle$
- ▶ $f_c = \langle H_Q \rangle$

Exponential convergence



VQE varying $l_{\max}$

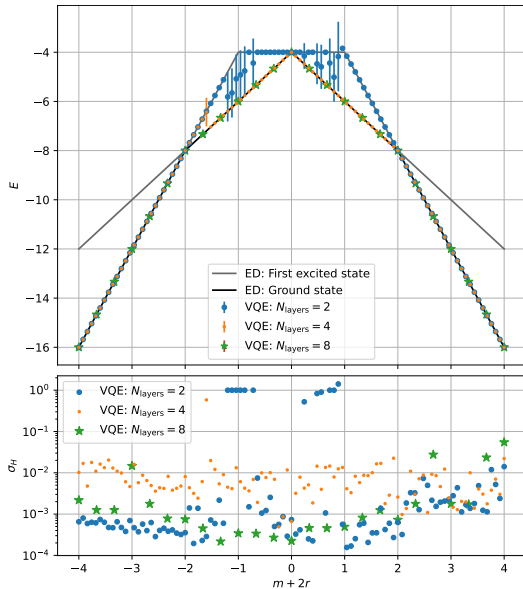
- ▶ $N_{\text{layers}} = 4$
- ▶ $|\psi_0\rangle = |01010101\rangle$



VQE varying N_{layers}

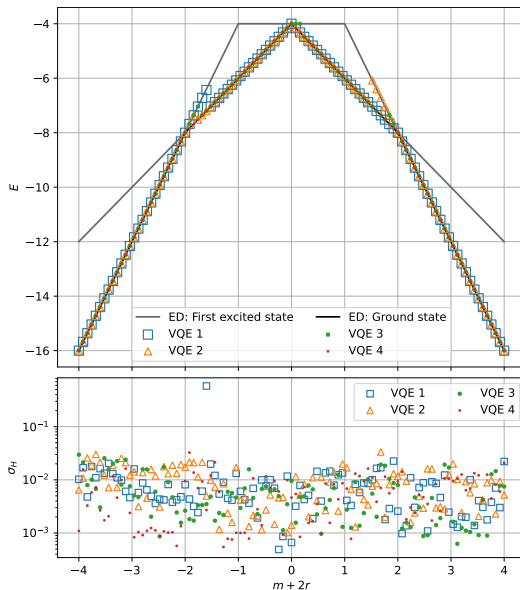
► $l_{\text{max}} = 20000$

► $|\psi_0\rangle = |01010101\rangle$



VQE varying seeds

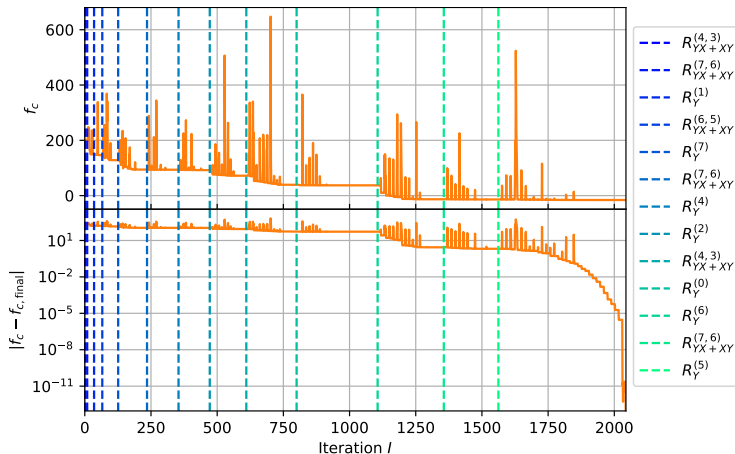
- ▶ $N_{\text{layers}} = 4$
- ▶ $I_{\text{max}} = 20000$
- ▶ $|\psi_0\rangle = |01010101\rangle$



ADAPT-VQE (not so naive greedy pool) minimization

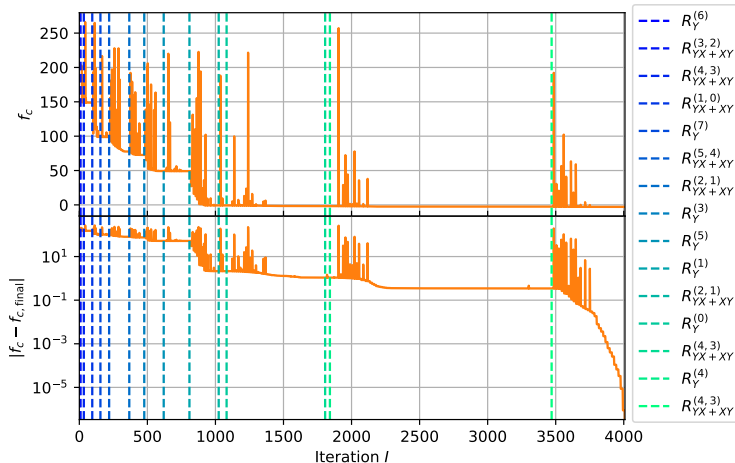
- ▶ $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$
- ▶ Pool $P^{(1)}$
- ▶ $l_{\max} = 20000$
- ▶ $m = -6$
- ▶ $f_c = \langle H_Q \rangle$

Added operators have
varying impacts on the
minimization

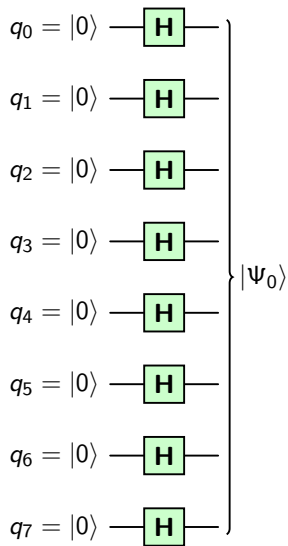


ADAPT-VQE (not so naive greedy pool) minimization

- ▶ $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$
- ▶ Pool $P^{(1)}$
- ▶ $l_{\max} = 20000$
- ▶ $m = -2.735$



ADAPT-VQE (not so naive greedy pool)



- ▶ Include penalty term in optimization, use H_Q
- ▶ Fixed part $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$
- ▶ $P^{(1)} = \{(\mathbf{X}^{(i)}\mathbf{Y}^{(i-1)} + \mathbf{Y}^{(i)}\mathbf{X}^{(i-1)}), \mathbf{X}^{(i)}, \mathbf{Y}^{(i)}, \mathbf{Z}^{(i)}\}$

ADAPT-VQE (not so naive greedy pool)

► $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$

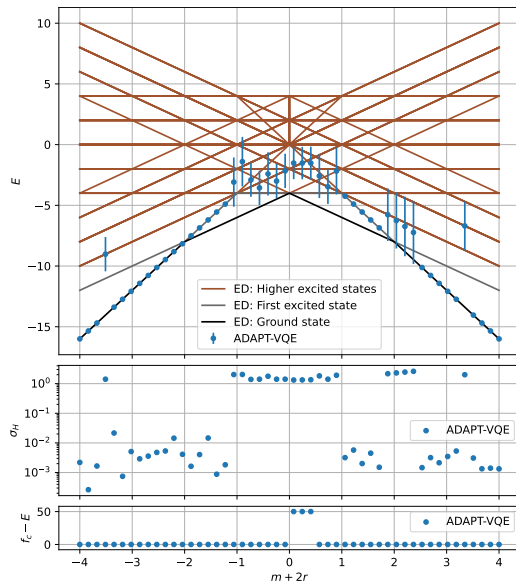
► Pool $P^{(1)}$

► $l_{\max} = 20000$

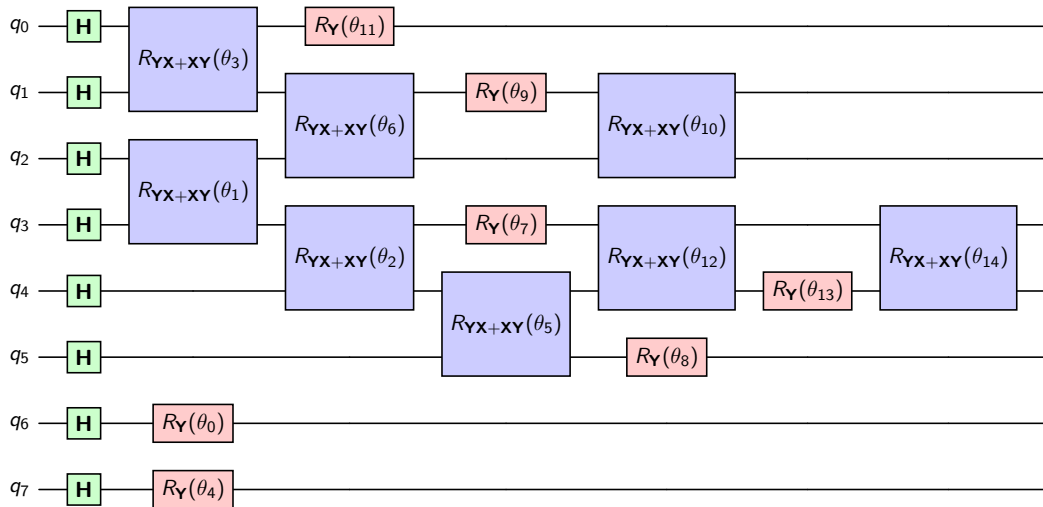
► $\sigma_h = \sqrt{\text{Var}(H)}$

► $f_C - E = \lambda_Q \langle Q^2 \rangle$

Energy level reconstruction
with suboptimal reliability



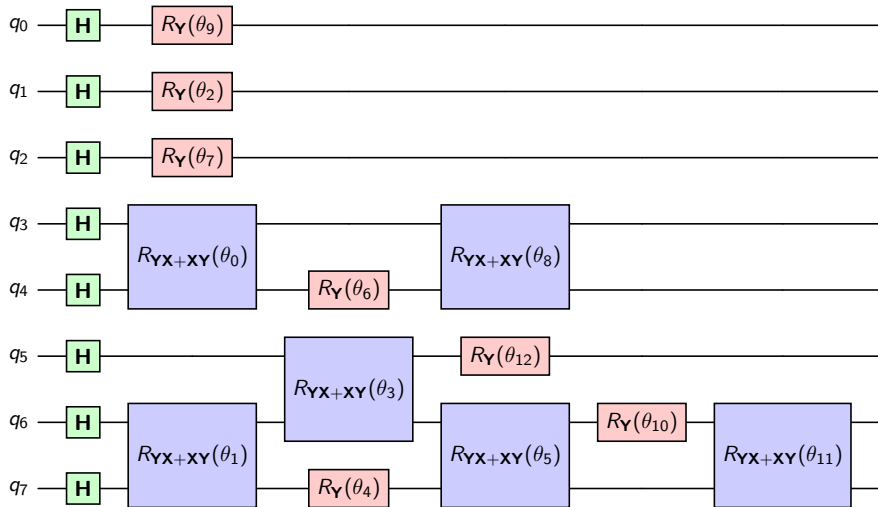
ADAPT-VQE (not so naive greedy pool) circuit ($m = -2.735$)



ADAPT-VQE (not so naive greedy pool) circuit ($m = -6$)

Optimal gates
on qubits 0-2

Non-optimal
gates on
qubits 3-7

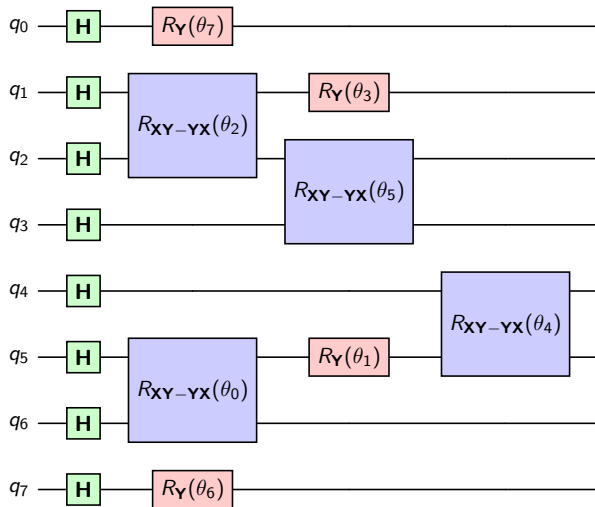


ADAPT-VQE (best greedy pool) circuit ($m = -2.735$)

► $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$

► Pool $P^{(2)}$

► $I_{\max} = 20000$

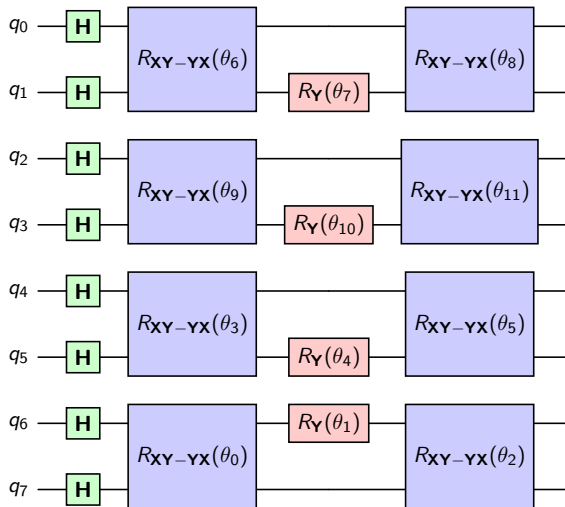


ADAPT-VQE (best greedy pool) circuit ($m = 2$)

► $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$

► Pool $P^{(2)}$

► $I_{\max} = 20000$



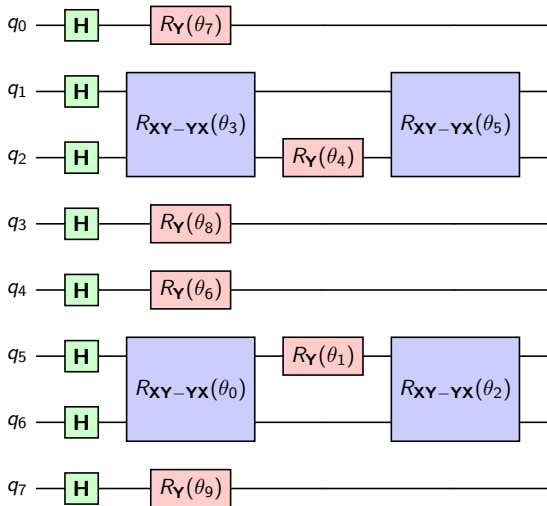
ADAPT-VQE (best greedy pool) circuit ($m = -6$)

► $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$

► Pool $P^{(2)}$

► $I_{\max} = 20000$

Circuit symmetries follow
physical symmetries



Using discrete symmetries for the operator pool construction

- ▶ P and T broken
- ▶ C unbroken: $[H, C] = 0$
- ▶ Pool $\{A_i | [A_i, C] = 0\}$
- ▶ Action of C:

$$\begin{aligned} C |\Psi(\theta_n, \dots, \theta_1)\rangle &= C e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} |\Psi_0\rangle \\ &= e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} C |\Psi_0\rangle \end{aligned}$$

$$C |\Psi_0\rangle = \alpha_0 |\Psi_0\rangle \quad \Rightarrow \quad C |\Psi(\theta_n, \dots, \theta_1)\rangle = \alpha_0 |\Psi(\theta_n, \dots, \theta_1)\rangle$$

- ▶ Convention: $C |\Omega\rangle = \alpha_{C,\Omega} |\Omega\rangle$

$$|00\rangle \xrightarrow{C} |11\rangle \quad |01\rangle \xrightarrow{C} |01\rangle \quad |10\rangle \xrightarrow{C} -|10\rangle \quad |11\rangle \xrightarrow{C} |00\rangle$$

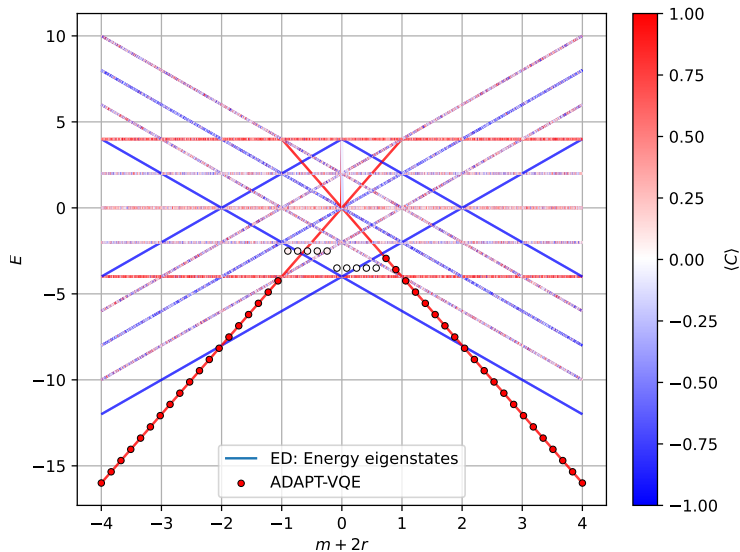
ADAPT-VQE (best greedy pool)

► $|\psi_0\rangle = \frac{1}{\sqrt{2^8}} \sum_{k=0}^{2^8-1} |k\rangle$

► Pool $P^{(2)}$

► $l_{\max} = 20000$

Correct reproduction
of $\langle C \rangle$ for $m + 2r < -1$
and $1 < m + 2r$



C invariant state construction

- ▶ Use $\{A_i\}$ as operator pool ($[A_i, C] = 0$)

- ▶ Final state:

$$|\Psi(\theta_n, \dots, \theta_1)\rangle = e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} |\Psi_0\rangle$$

- ▶ Action of C:

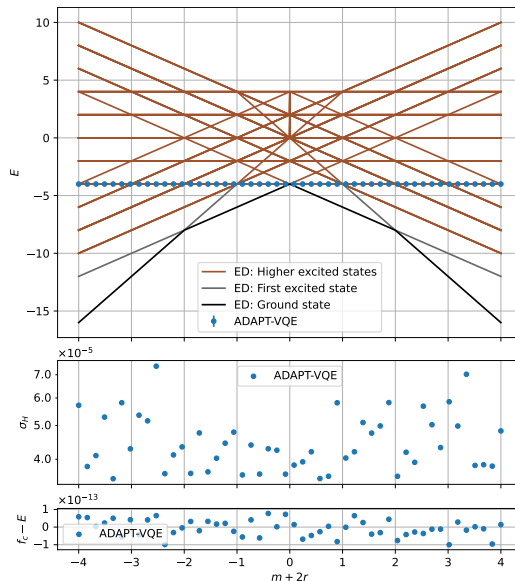
$$\begin{aligned} C |\Psi(\theta_n, \dots, \theta_1)\rangle &= C e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} |\Psi_0\rangle \\ &= e^{i\theta_n A_{i_n}} \dots e^{i\theta_1 A_{i_1}} C |\Psi_0\rangle \end{aligned}$$

- ▶ If $C |\Psi_0\rangle = \alpha_0 |\Psi_0\rangle$ then $C |\Psi(\theta_n, \dots, \theta_1)\rangle = \alpha_0 |\Psi(\theta_n, \dots, \theta_1)\rangle$

ADAPT-VQE (C invariant ansatz 1)

- ▶ Initial state:
 $C|\Psi_0\rangle = +1|\Psi_0\rangle$
- ▶ $|\Psi_0\rangle = |01010101\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$
- ▶ $\sigma_h = \sqrt{\text{Var}(H)}$
- ▶ $f_C - E = \lambda_Q \langle Q^2 \rangle$

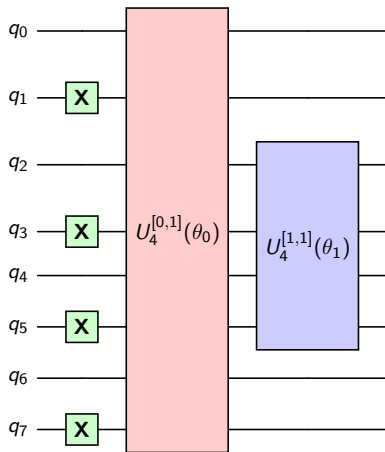
Improvements in
reconstruction fidelity



ADAPT-VQE (C invariant ansatz 1) circuit

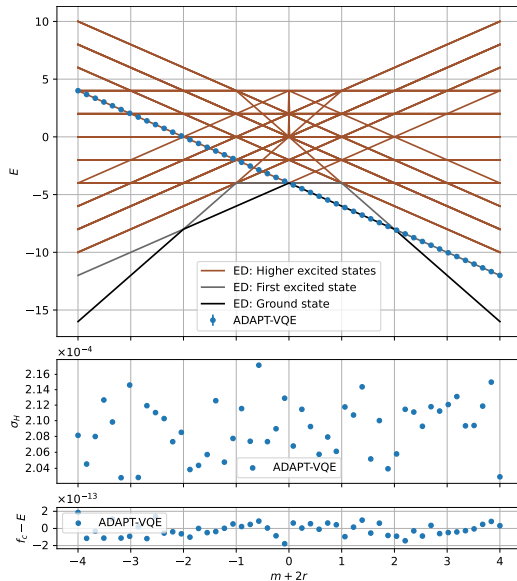
- ▶ Initial state:
 $C|\Psi_0\rangle = +1|\Psi_0\rangle$
- ▶ $|\Psi_0\rangle = |01010101\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$
- ▶ $U_i^{[n]}(\theta) := e^{i\theta A_i(n)}$

Two gates sufficient for all
parameter values



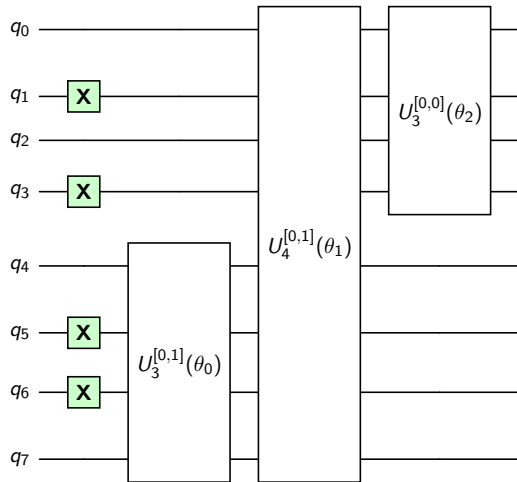
ADAPT-VQE (C invariant ansatz 2)

- ▶ $|\psi_0\rangle = |01010110\rangle$
- ▶ $C|\psi_0\rangle = -1|\psi_0\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$



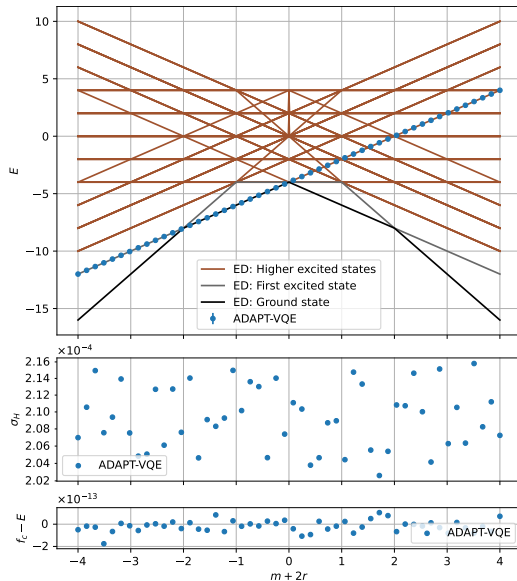
ADAPT-VQE (C invariant ansatz 2) circuit

- ▶ $|\Psi_0\rangle = |01010110\rangle$
- ▶ $C|\Psi_0\rangle = -1|\Psi_0\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$
- ▶ $U_i^{[n]}(\theta) := e^{i\theta A_i(n)}$



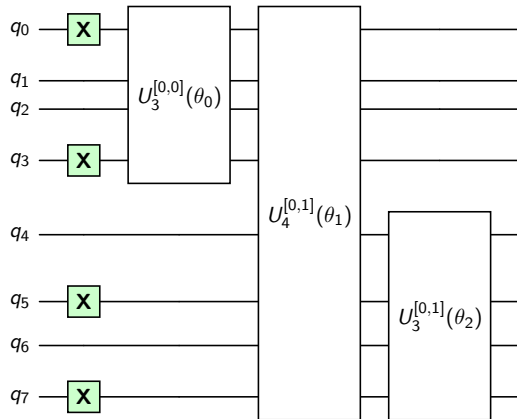
ADAPT-VQE (C invariant ansatz 3)

- ▶ $|\Psi_0\rangle = |10010101\rangle$
- ▶ $C|\Psi_0\rangle = -1|\Psi_0\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$



ADAPT-VQE (C invariant ansatz 3) circuit

- ▶ $|\Psi_0\rangle = |10010101\rangle$
- ▶ $C|\Psi_0\rangle = -1|\Psi_0\rangle$
- ▶ Pool $P^{(3)}$
- ▶ $l_{\max} = 20000$
- ▶ $U_i^{[n]}(\theta) := e^{i\theta A_i(n)}$



The cost (CNOT depth/count after transpilation for ibm_marrakesh)

► VQE:

- $N_{\text{layers}} = 4$ is baseline

► ADAPT-VQE:

1. Not so naive greedy
2. Best greedy
3. C invariant $\alpha_0 = +1$
4. C invariant $\alpha_0 = -1$
5. C invariant $\alpha_0 = -1$

