

# Shell model in a quantum computer

Pérez-Obiol, Romero, Menéndez, Rios, García-Saez, Juliá-Díaz, [arxiv:2302.03641](#)



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Supercomputing  
Center  
Centro Nacional de Supercomputación



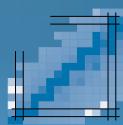
A Pérez-Obiol



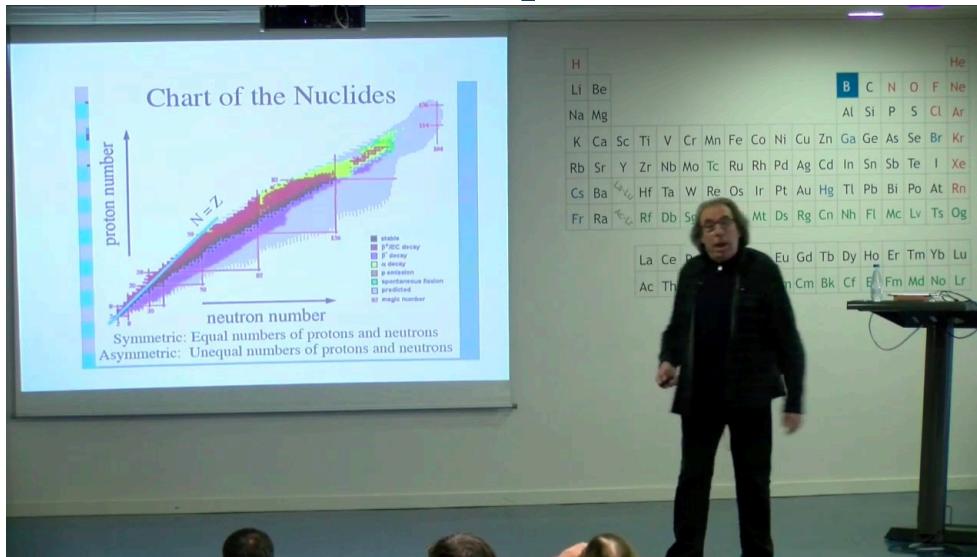
A García-Saez

**Arnaud Rios Huguet**  
Institute of Cosmos Sciences  
Universitat de Barcelona

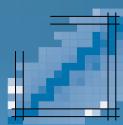
**Nuclear Tapas**  
Alfredo Poves' celebration  
April 2023



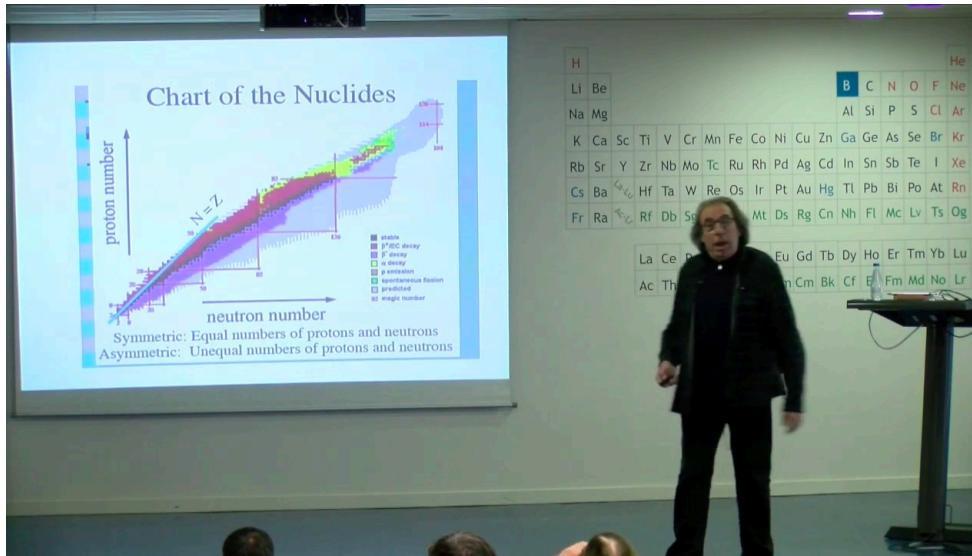
12 Dec 2020, Colloquium @ ICCUB



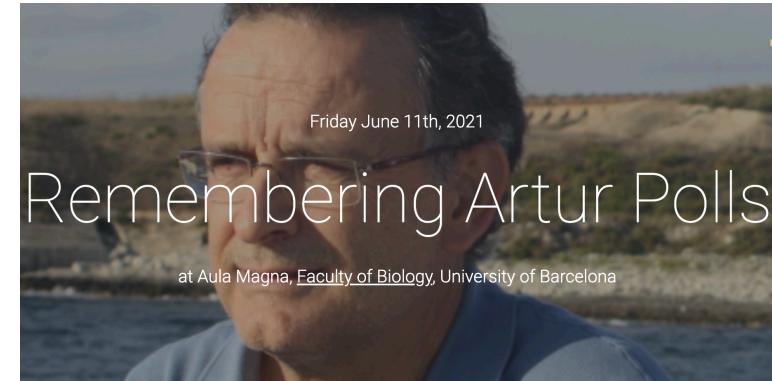
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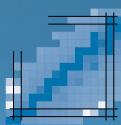


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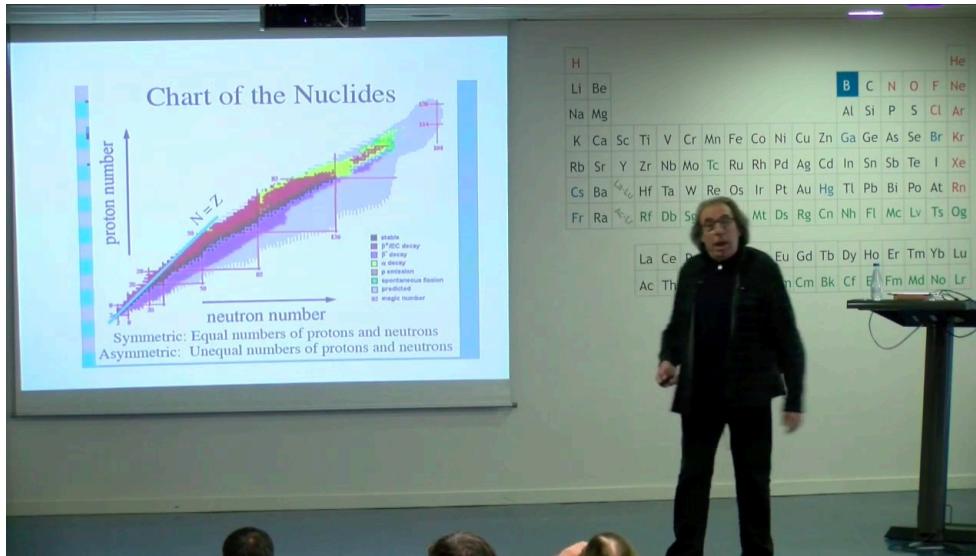
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# Alfredo

12 Dec 2020, Colloquium @ ICCUB



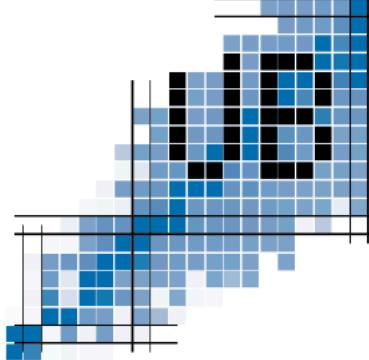
<https://www.youtube.com/watch?v=rOqp4xhKgCQ>



at Aula Magna, Faculty of Biology, University of Barcelona



- Me, as a young postdoc at MSU:
  - *I am from Barcelona!*
  - *Oh, so you work with Poves?*



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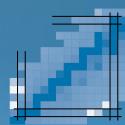
A Pérez-Obiol



A García-Saez

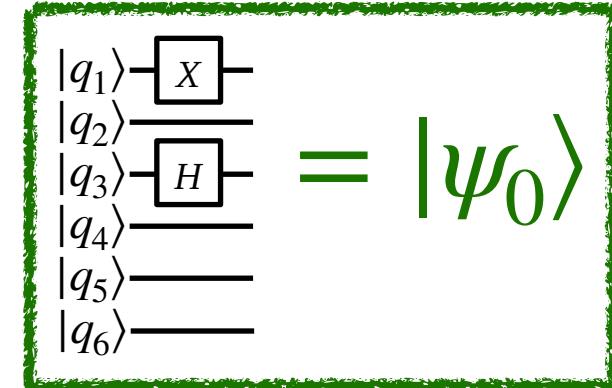
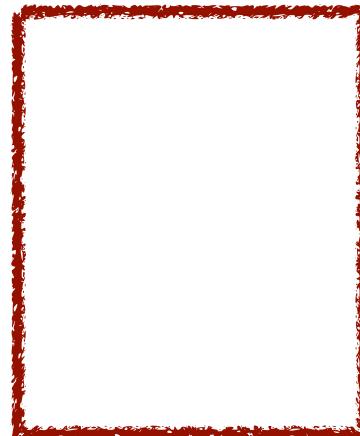
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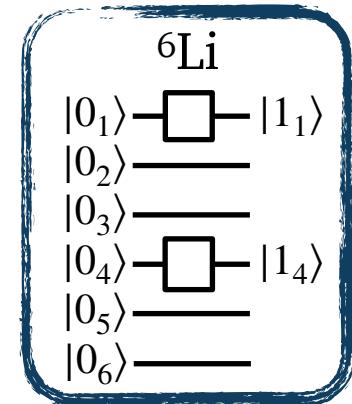
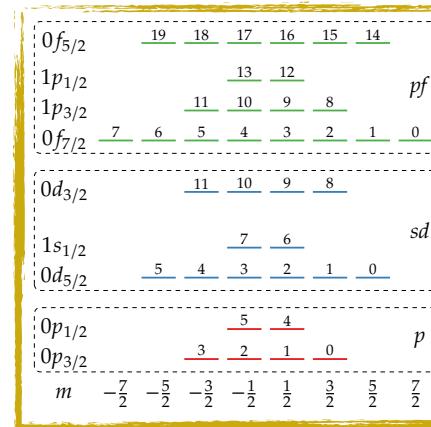


# Outline

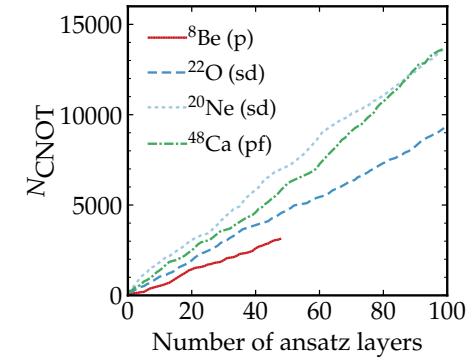
- Motivation

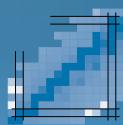


- How to?



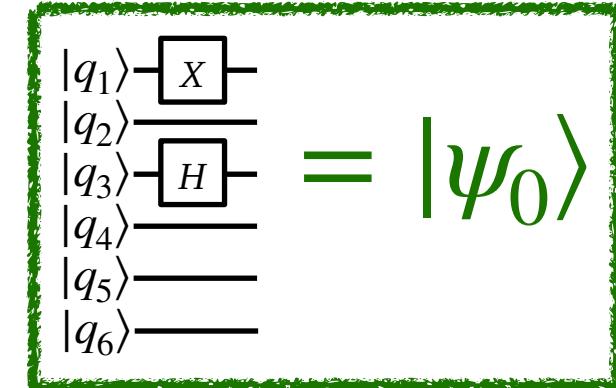
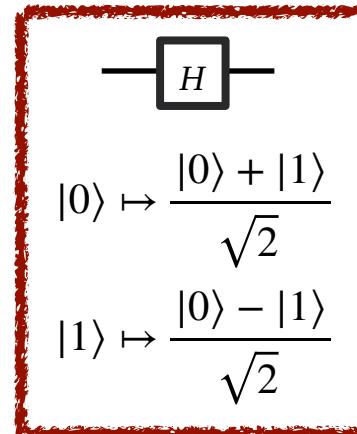
- Results & perspectives



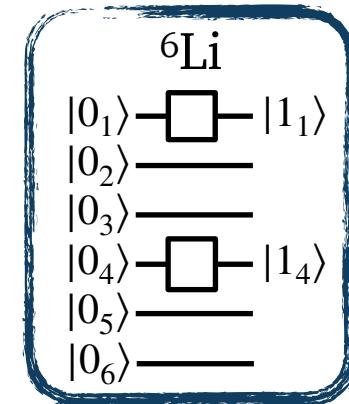
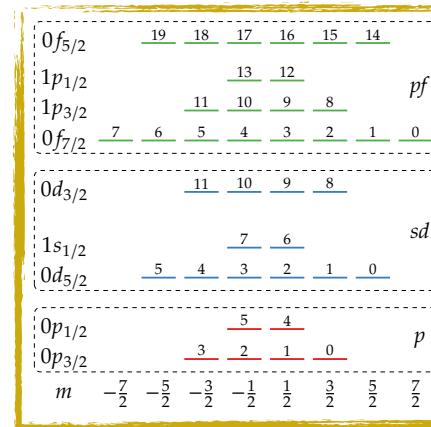


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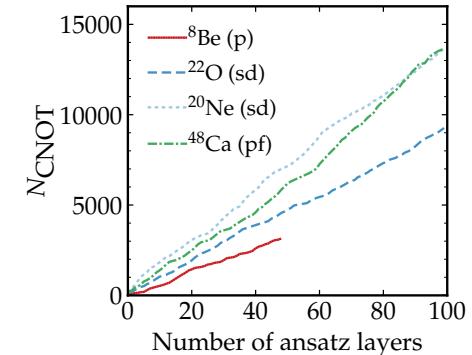
- Motivation



- How to?



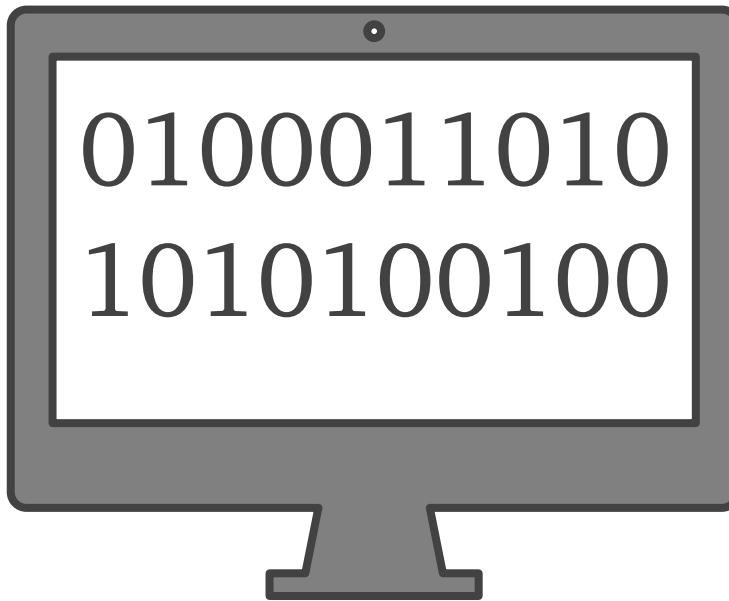
- Results & perspectives





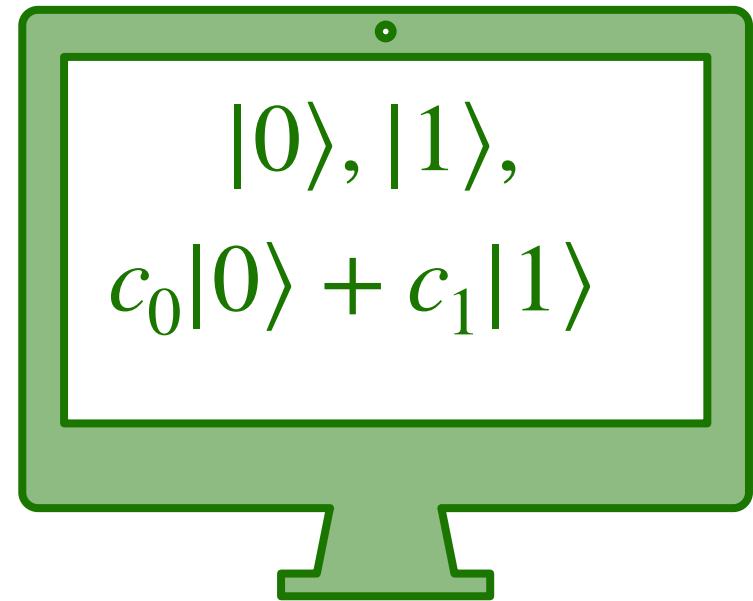
# What is quantum computing?

## Classical Computer

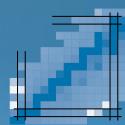


- Works with bits
- Bits are either 1 or 0

## Quantum Computer



- Works with **qubits**
- A **qubit** can be **superposition** of 1 or 0
- Many-qubits: **entanglement, interference**, etc



# Logic gates 1

*qubit*

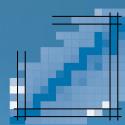
$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

*Logic gates*

$$|q_1\rangle \xrightarrow{\text{z}} |q_f\rangle$$

$$|q_1\rangle = |0\rangle \rightarrow |q_f\rangle = |0\rangle$$

$$|q_1\rangle = |1\rangle \rightarrow |q_f\rangle = -|1\rangle$$



# Logic gates 1

*qubit*

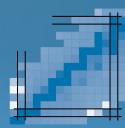
$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

*Logic gates*

$$|q_1\rangle \xrightarrow{\oplus} |q_f\rangle$$

$$|q_1\rangle = |0\rangle \rightarrow |q_f\rangle = |1\rangle$$

$$|q_1\rangle = |1\rangle \rightarrow |q_f\rangle = |0\rangle$$

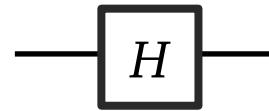


# Logic gates 1

*qubit*

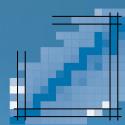
$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

*Logic gates*



$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

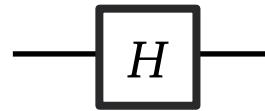


# Logic gates 1

*qubit*

$$|q_1\rangle \rightarrow \{|0\rangle, |1\rangle\}$$

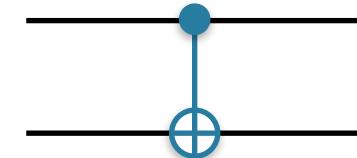
*Logic gates*



$$|0\rangle \mapsto \frac{|0\rangle + |1\rangle}{\sqrt{2}}$$

$$|1\rangle \mapsto \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

*2 qubit gates*

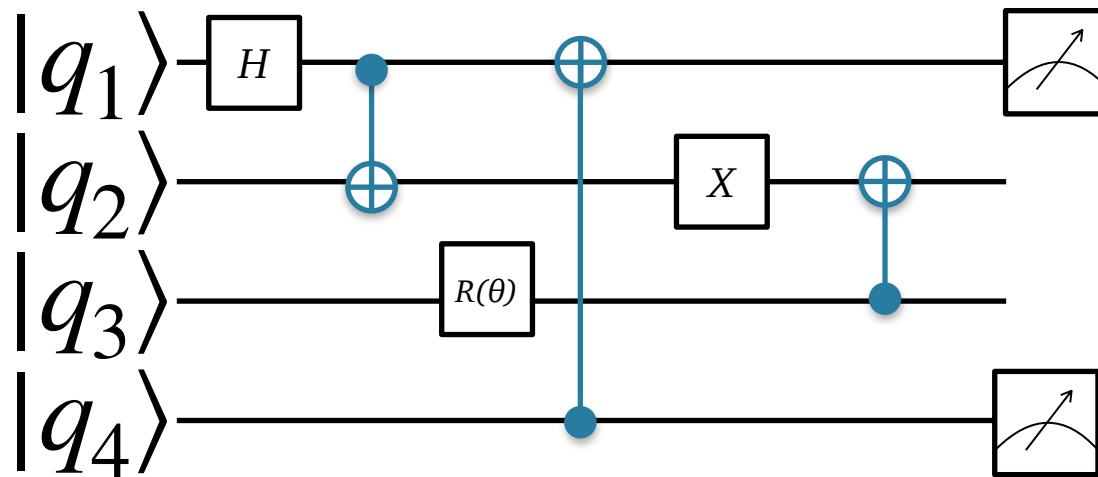
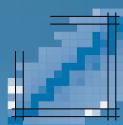


$$|00\rangle \mapsto |00\rangle$$

$$|01\rangle \mapsto |01\rangle$$

$$|10\rangle \mapsto |11\rangle$$

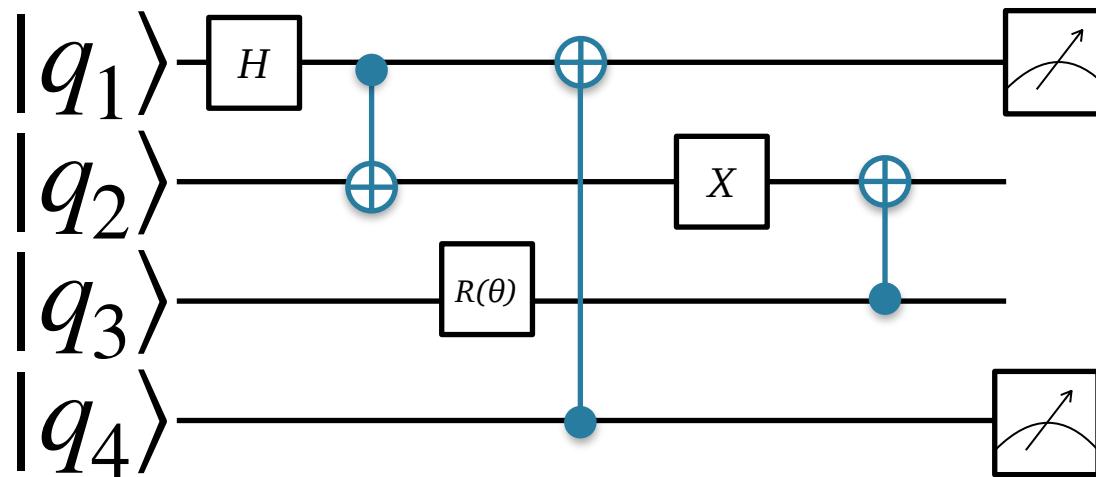
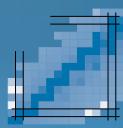
$$|11\rangle \mapsto |10\rangle$$



## Solovay-Kitaev theorem

A quantum circuit of  $m$  qubit gates can be approximated to  $\varepsilon$  error by a quantum circuit of  $O(m \log^c(m/\varepsilon))$  gates using a set of **finite universal gates**.

Kitaev, Russian Mathematical Surveys 52 (6) 1191 (1997)  
Nielsen & Chuang, Quantum Computation and Quantum Information



## Solovay-Kitaev theorem

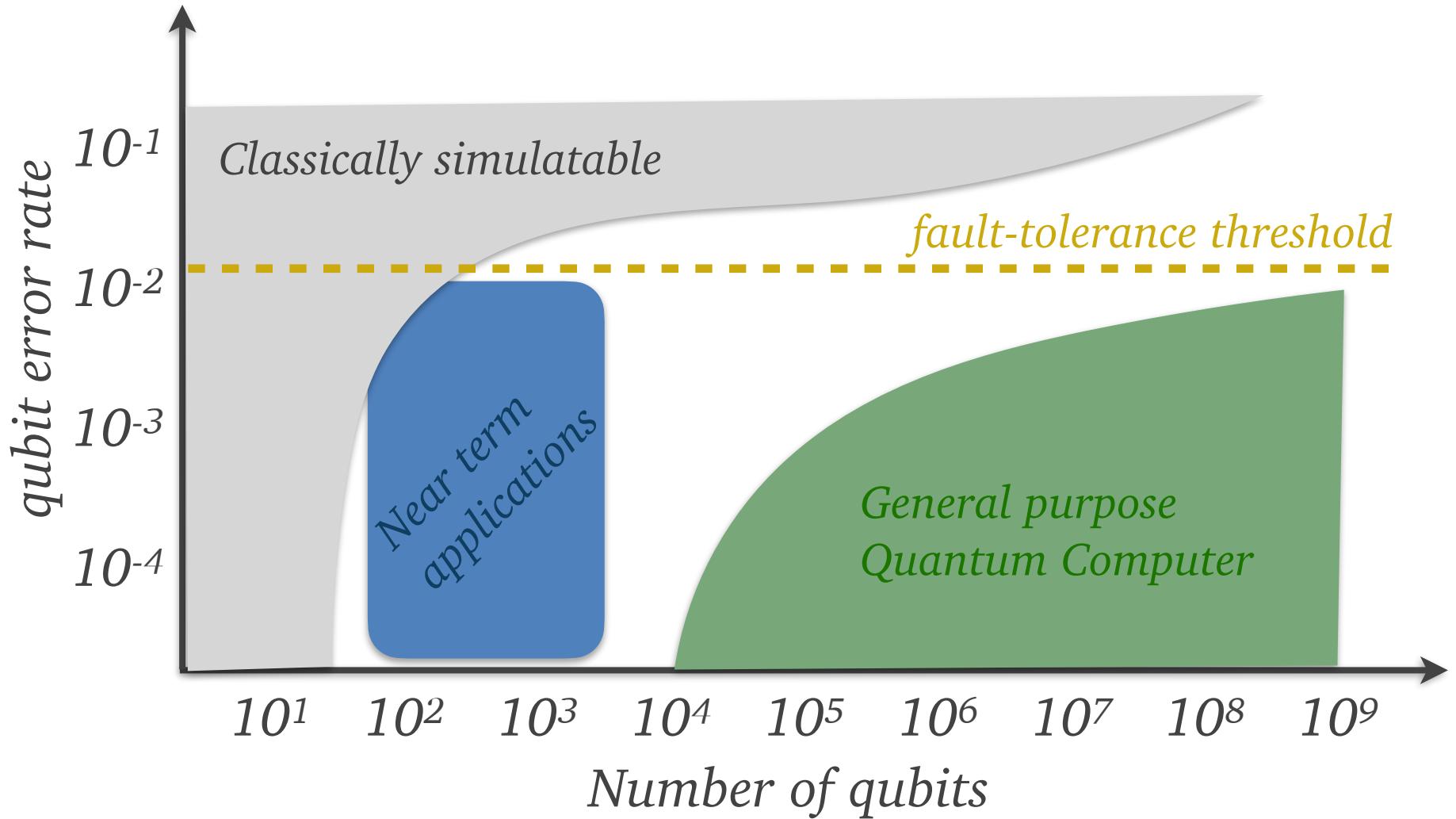
We can build a universal black box with only a finite number of buttons.

*(Alessandro Roggero)*

Kitaev, Russian Mathematical Surveys 52 (6) 1191 (1997)  
Nielsen & Chuang, *Quantum Computation and Quantum Information*

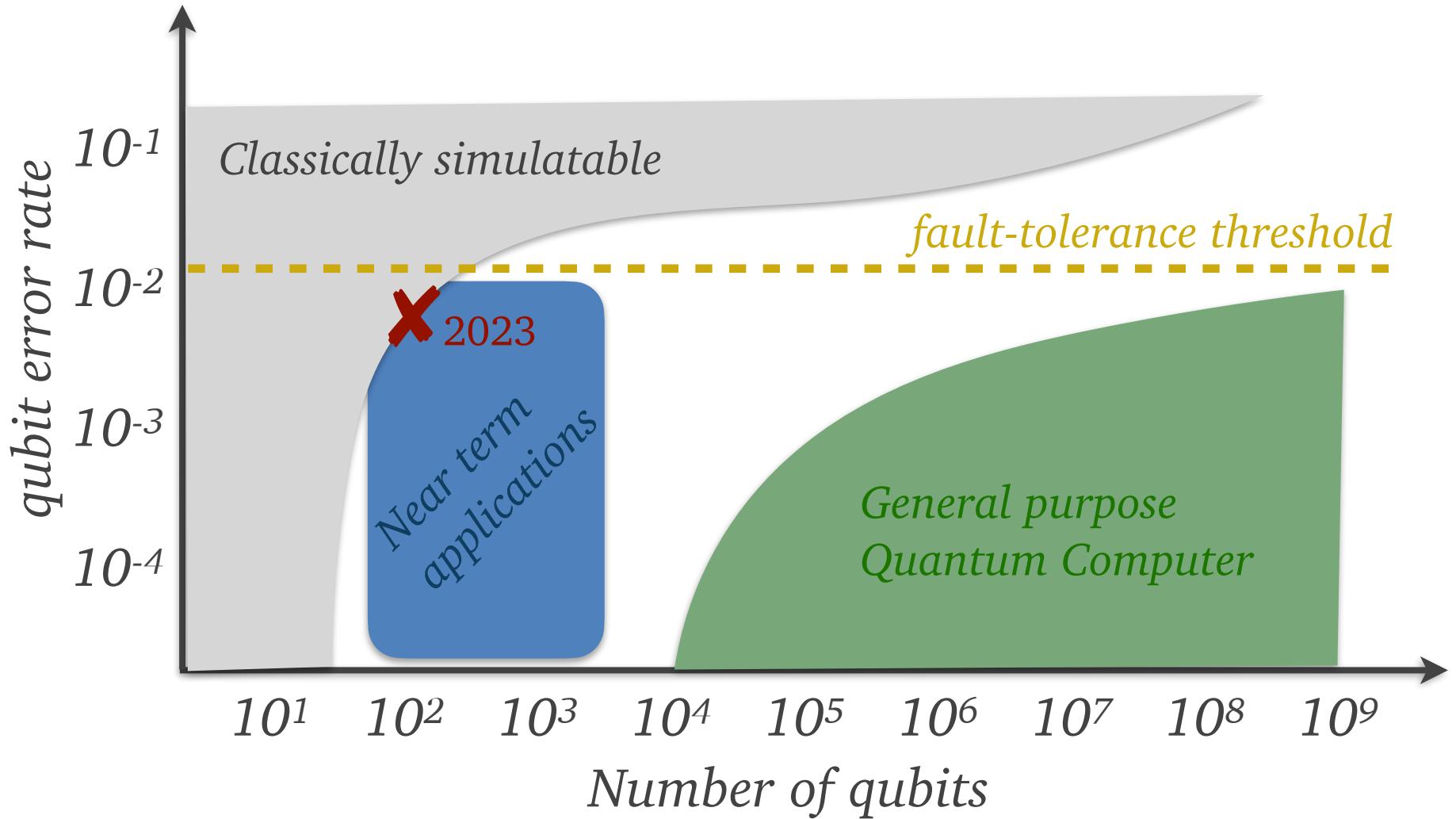


# Near-Intermediate Scale Quantum Tech



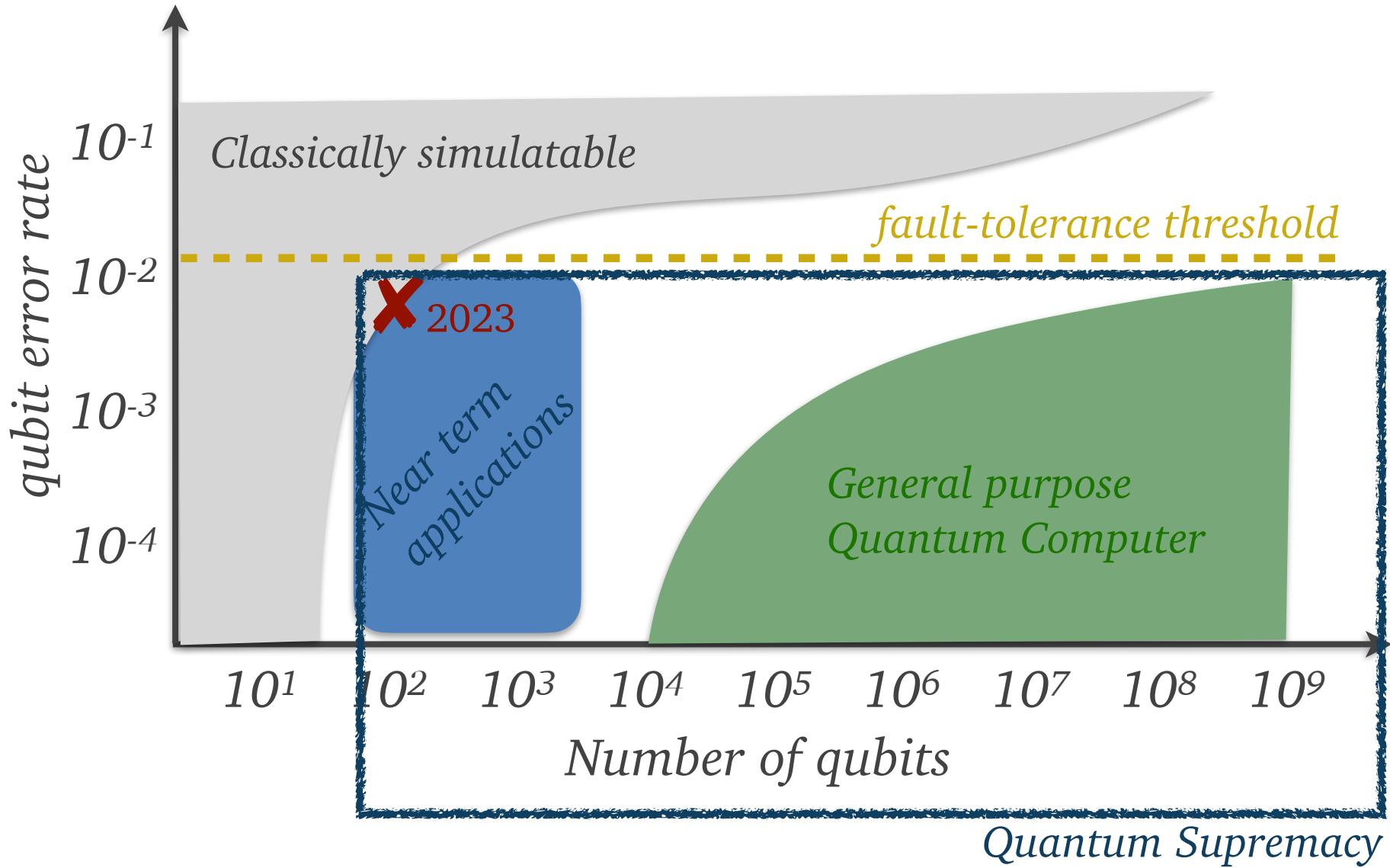


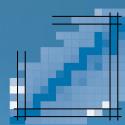
# Near-Intermediate Scale Quantum Tech





# Near-Intermediate Scale Quantum Tech



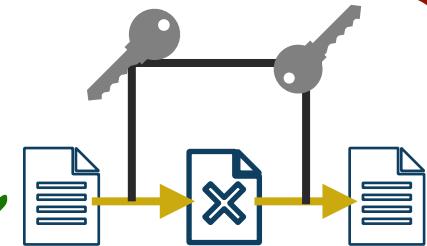


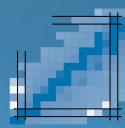
# Why quantum circuits?

## Shor's algorithm

“Find prime factors of an integer  $N$  with  $O(\log N)$  operations”

Classical ✗  
Quantum ✓



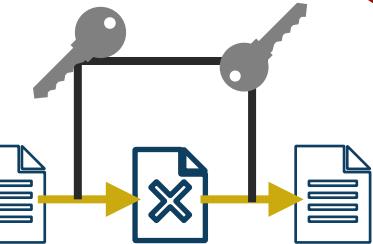


# Why quantum circuits?

## Shor's algorithm

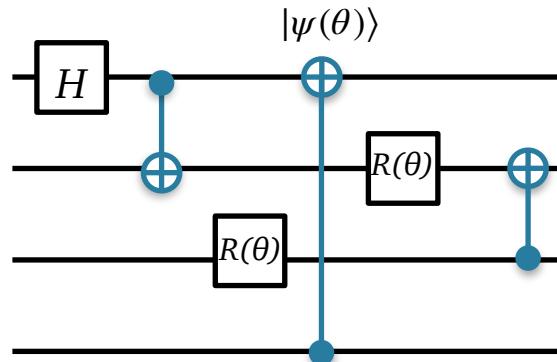
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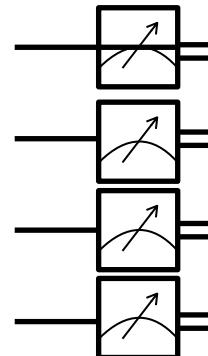


## Variational Quantum Eigensolver

### Quantum hardware

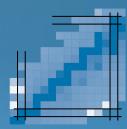


### Measurement

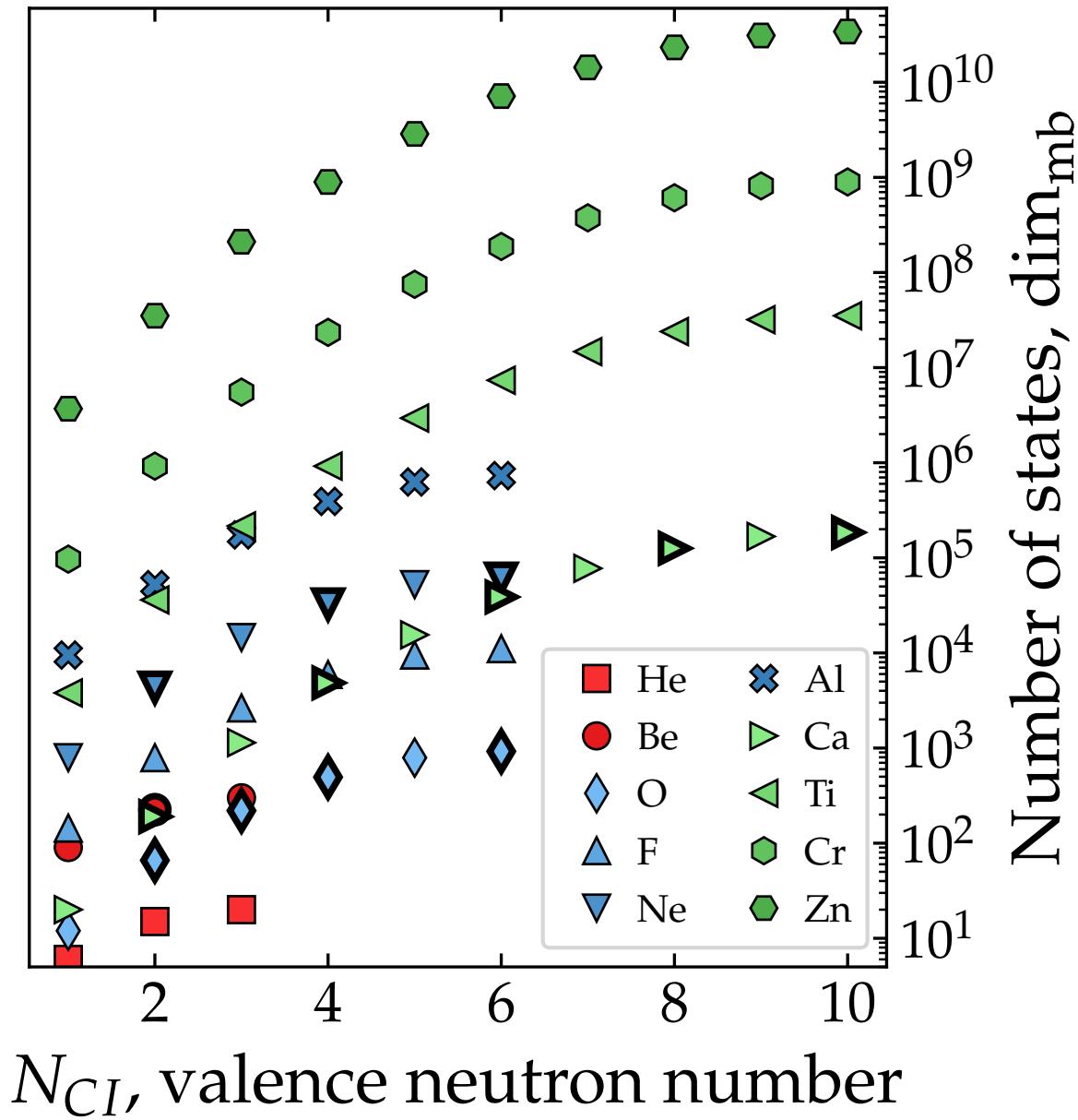


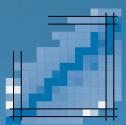
$$E(\theta) = \frac{\langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle}$$

Update parameters  $\theta$   
*Classical minimisation*



# Shell model complexity





# QC in nuclear structure

PHYSICAL REVIEW LETTERS 120, 210501 (2018)

S' Suggestion

Featured in Physics

## Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,<sup>1</sup> A. J. McCaskey,<sup>2</sup> G. Hagen,<sup>3,4</sup> G. R. Jansen,<sup>5,3</sup> T. D. Morris,<sup>4,3</sup> T. Papenbrock,<sup>4,3,\*</sup>  
R. C. Psoor,<sup>1,4</sup> D. J. Dean,<sup>3</sup> and P. Lougovski<sup>1,†</sup>

Phys. Rev. Lett. 120 210501 (2018)

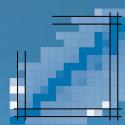
## • Previous work on nuclear structure

- Limited to **one minimisation strategy** (UCC)
- Only a handful of isotopes ( $^2\text{H}$ ,  $^6\text{Li}$ ,  $^8\text{Be}$ ,  $^{20-20}\text{O}$ ,  $^{20}\text{Ne}$ )

Lacroix *et al*, *Quantum computing with and for many-body physics*, arXiv:2303.04850  
Stetcu, Baroni, Carlson, Phys. Rev. C 105 064308 (2022)  
Kiss, Papenbrock *et al* Phys. Rev. C 106 034325 (2022)

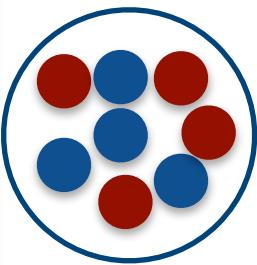
## • Our strategy

- Can we **beat exponential scaling**?
- Does it work **across shells**?
- “**Build**” circuits and **quantify** resources

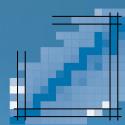


# Variational Quantum Eigensolver

## 1. Mapping

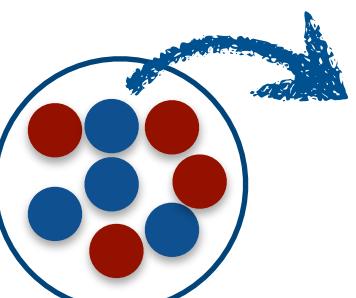


$|q_1\rangle$  —————  
 $|q_2\rangle$  —————  
 $|q_3\rangle$  —————  
 $|q_4\rangle$  —————  
 $|q_5\rangle$  —————  
 $|q_6\rangle$  —————

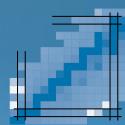


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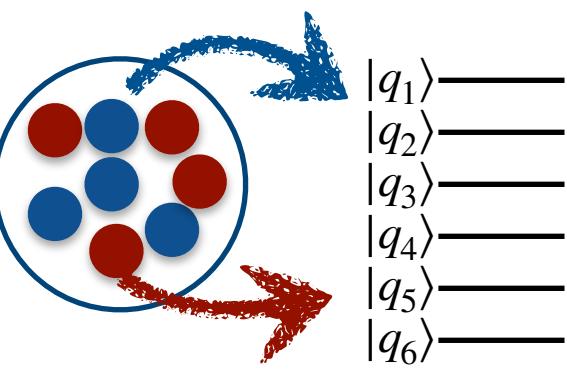


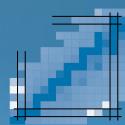
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# Variational Quantum Eigensolver

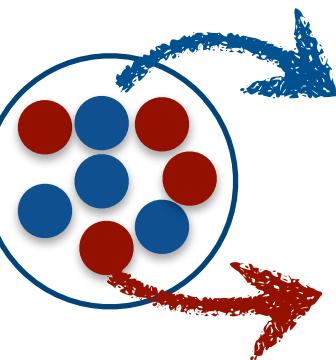
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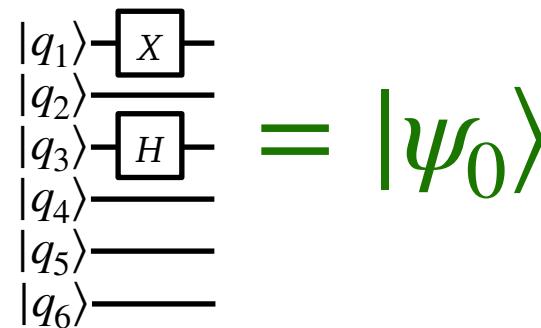


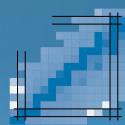
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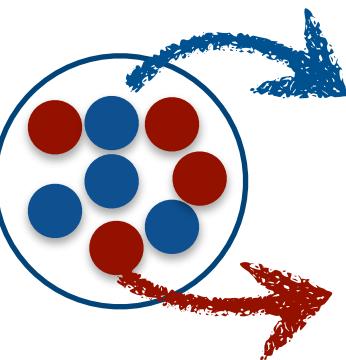
## 2.Reference state



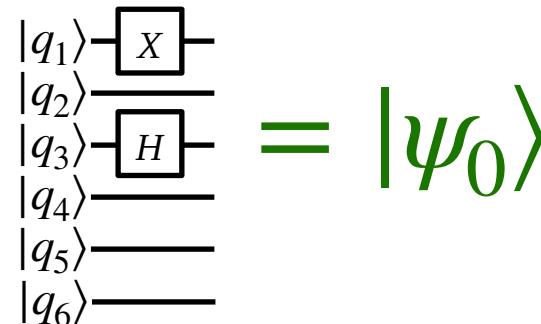


# Variational Quantum Eigensolver

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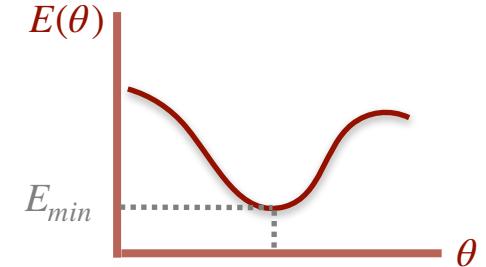


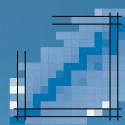
## 2. Reference state



## 3. Minimisation

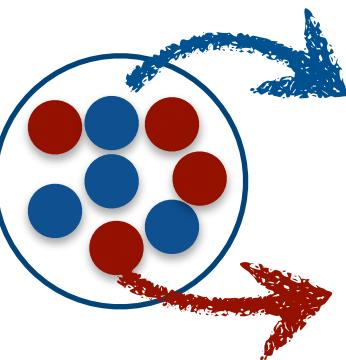
$$\min_{\theta} E(\theta) = \frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle}$$



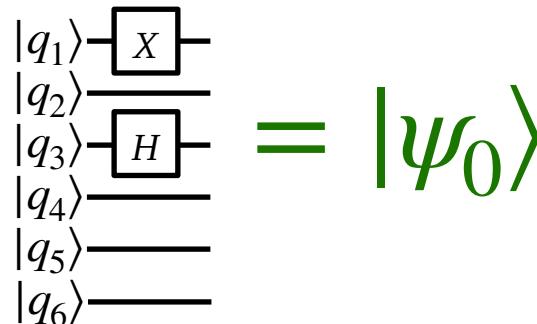


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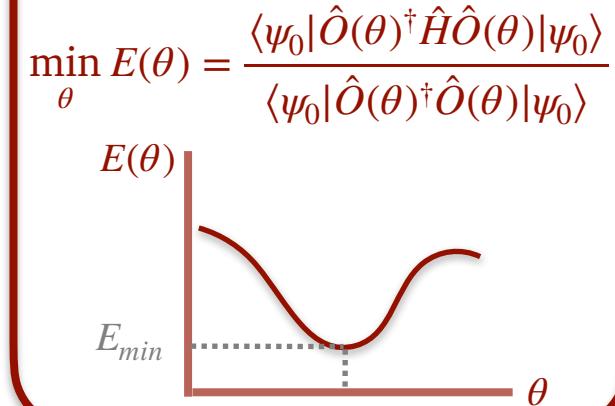
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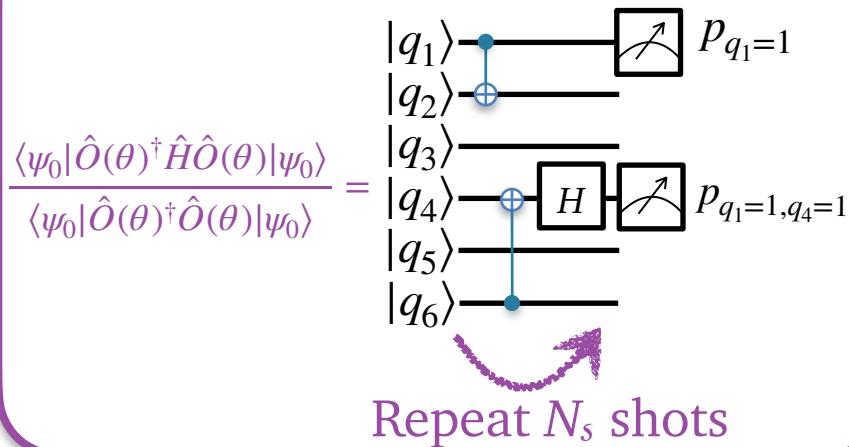
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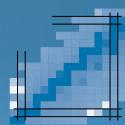


## 3. Minimisation



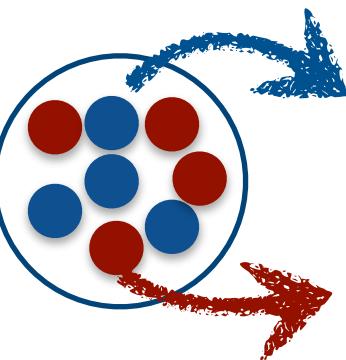
## 4. Measurement





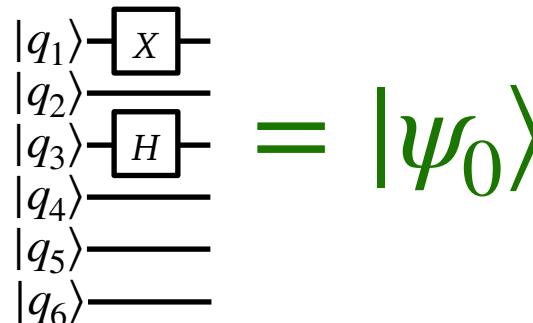
# Variational Quantum Eigensolver

## 1. Mapping

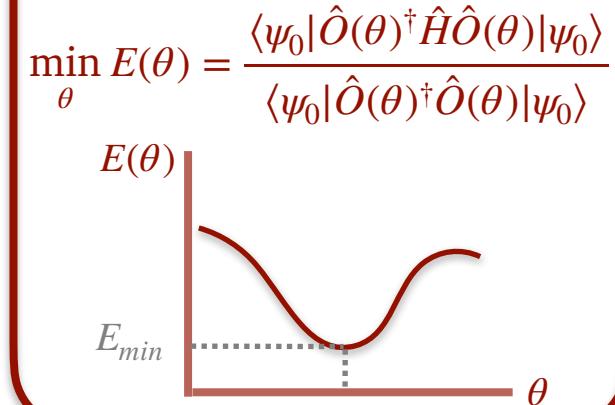


$|q_1\rangle$   
 $|q_2\rangle$   
 $|q_3\rangle$   
 $|q_4\rangle$   
 $|q_5\rangle$   
 $|q_6\rangle$

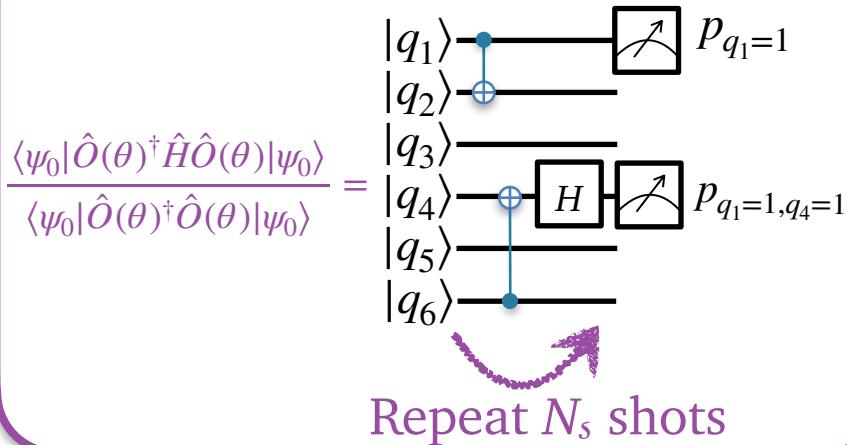
## 2. Reference state



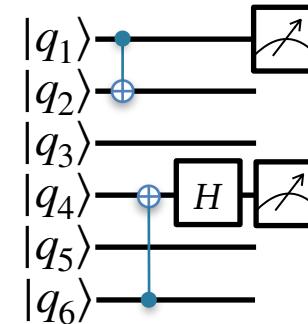
## 3. Minimisation

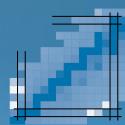


## 4. Measurement



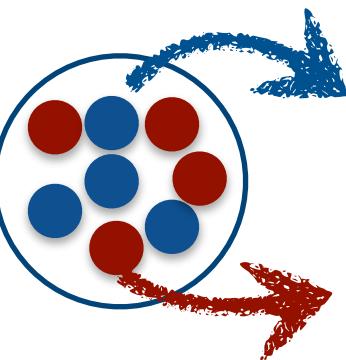
## 5. Error mitigation





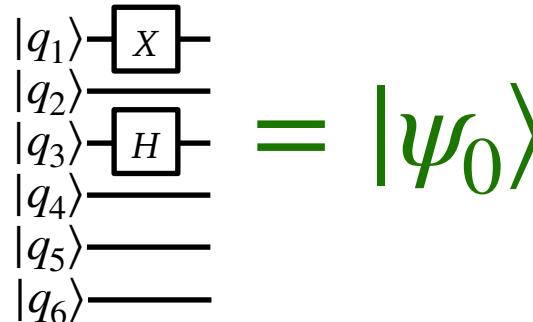
# Variational Quantum Eigensolver

## 1. Mapping



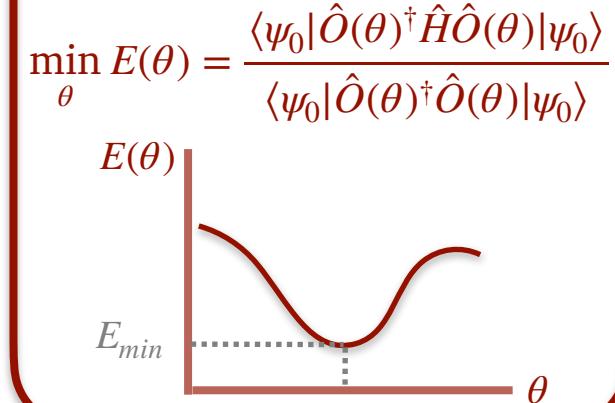
$|q_1\rangle$   
 $|q_2\rangle$   
 $|q_3\rangle$   
 $|q_4\rangle$   
 $|q_5\rangle$   
 $|q_6\rangle$

## 2. Reference state

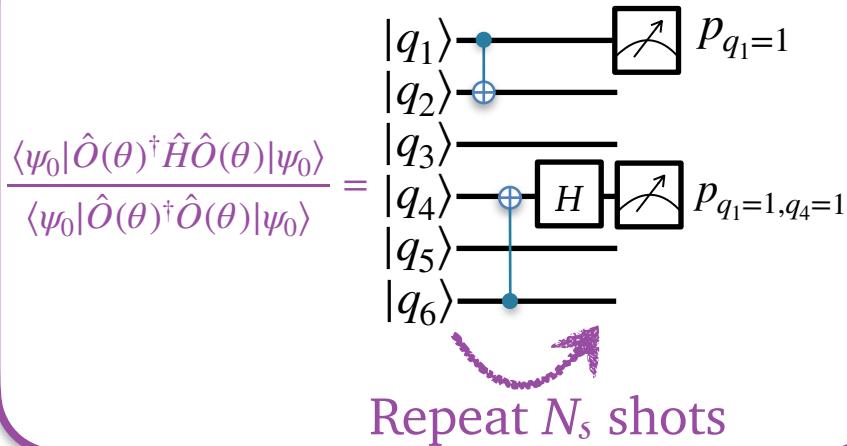


$|q_1\rangle$   $X$   
 $|q_2\rangle$   
 $|q_3\rangle$   $H$   
 $|q_4\rangle$   
 $|q_5\rangle$   
 $|q_6\rangle$

## 3. Minimisation



## 4. Measurement

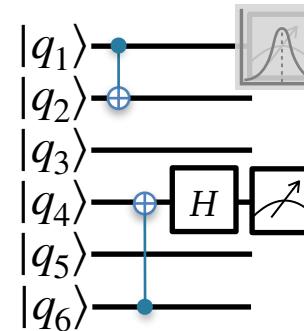


$|q_1\rangle$   $\text{CNOT}_{q1,q2}$   $p_{q_1=1}$   
 $|q_2\rangle$   
 $|q_3\rangle$   
 $|q_4\rangle$   $H$   $\text{CNOT}_{q4,q1}$   $p_{q_1=1, q_4=1}$   
 $|q_5\rangle$   
 $|q_6\rangle$

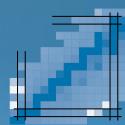
$\oplus$

Repeat  $N_s$  shots

## 5. Error mitigation

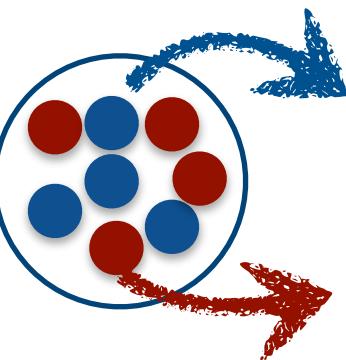


$|q_1\rangle$   $\text{CNOT}_{q1,q2}$   
 $|q_2\rangle$   
 $|q_3\rangle$   
 $|q_4\rangle$   $H$   $\text{CNOT}_{q4,q1}$



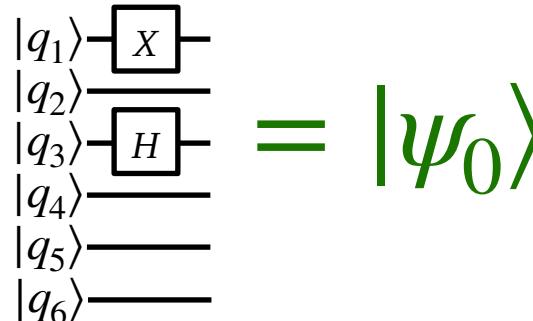
# Variational Quantum Eigensolver

## 1. Mapping



$|q_1\rangle$   
 $|q_2\rangle$   
 $|q_3\rangle$   
 $|q_4\rangle$   
 $|q_5\rangle$   
 $|q_6\rangle$

## 2. Reference state

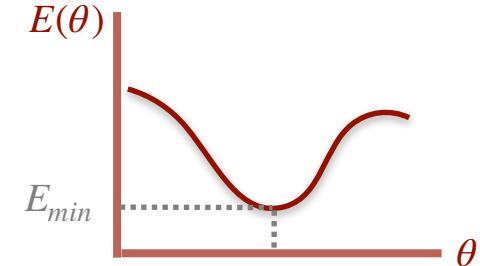


$|q_1\rangle$   $X$   
 $|q_2\rangle$   
 $|q_3\rangle$   $H$   
 $|q_4\rangle$   
 $|q_5\rangle$   
 $|q_6\rangle$

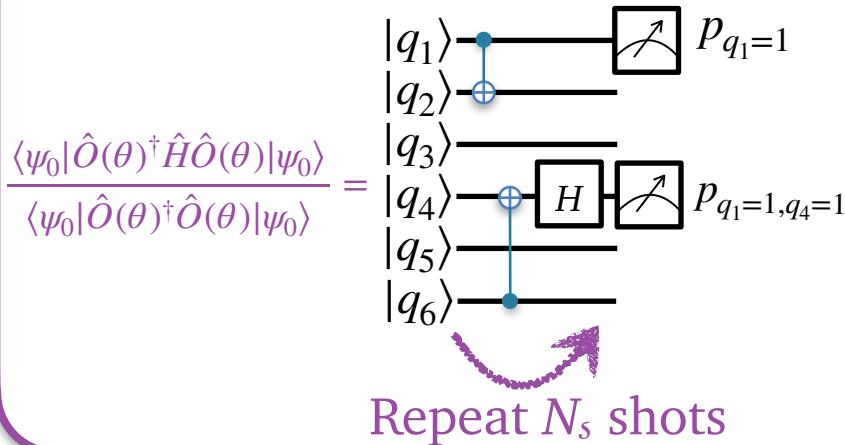
$$= |\psi_0\rangle$$

## 3. Minimisation

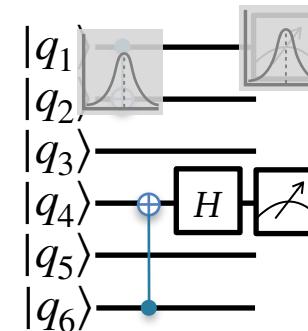
$$\min_{\theta} E(\theta) = \frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle}$$

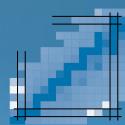


## 4. Measurement



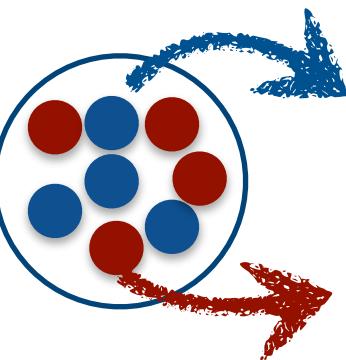
## 5. Error mitigation





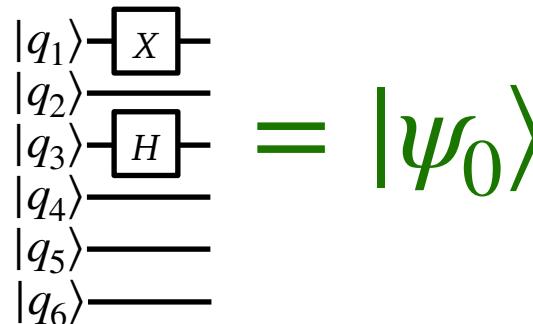
# Variational Quantum Eigensolver

## 1. Mapping

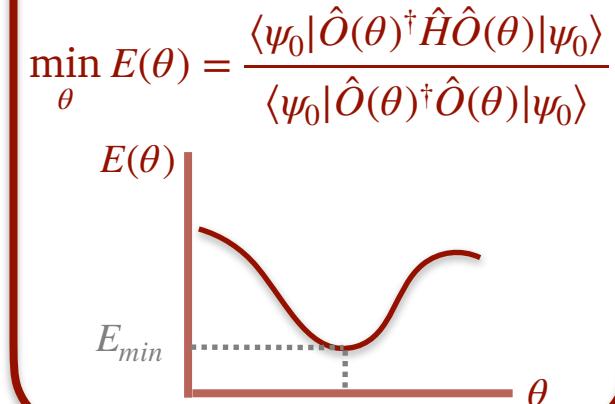


$|q_1\rangle$  —  
 $|q_2\rangle$  —  
 $|q_3\rangle$  —  
 $|q_4\rangle$  —  
 $|q_5\rangle$  —  
 $|q_6\rangle$  —

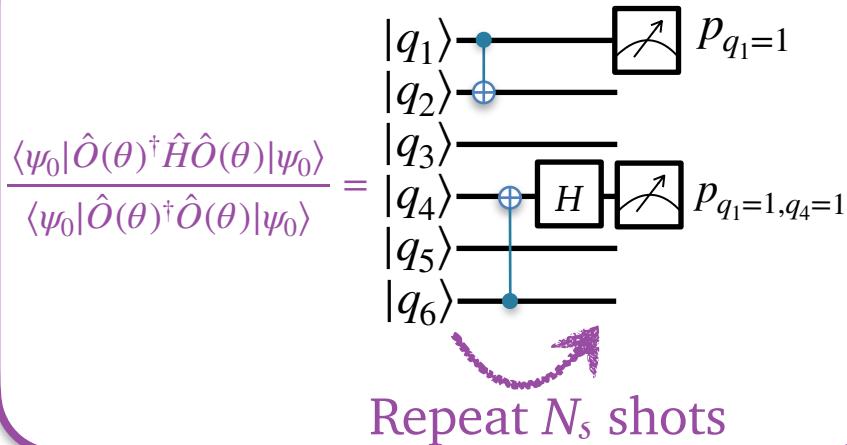
## 2. Reference state



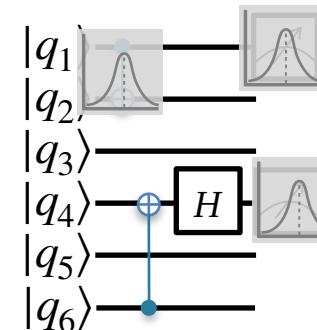
## 3. Minimisation

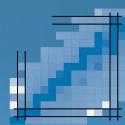


## 4. Measurement



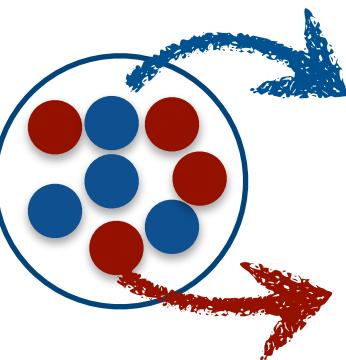
## 5. Error mitigation





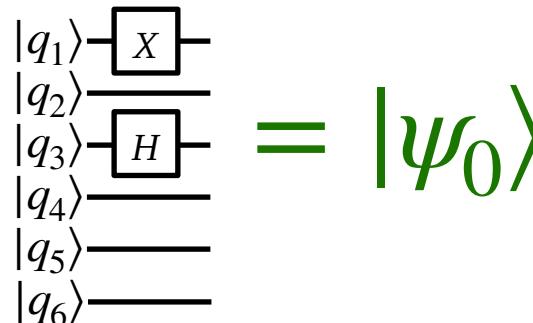
# Variational Quantum Eigensolver

## 1. Mapping



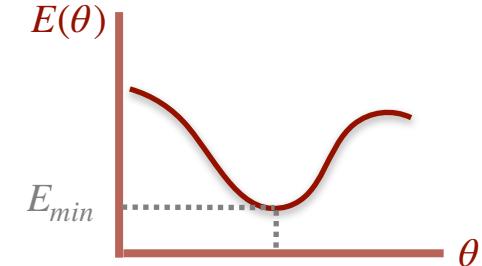
$|q_1\rangle$  —  
 $|q_2\rangle$  —  
 $|q_3\rangle$  —  
 $|q_4\rangle$  —  
 $|q_5\rangle$  —  
 $|q_6\rangle$  —

## 2. Reference state

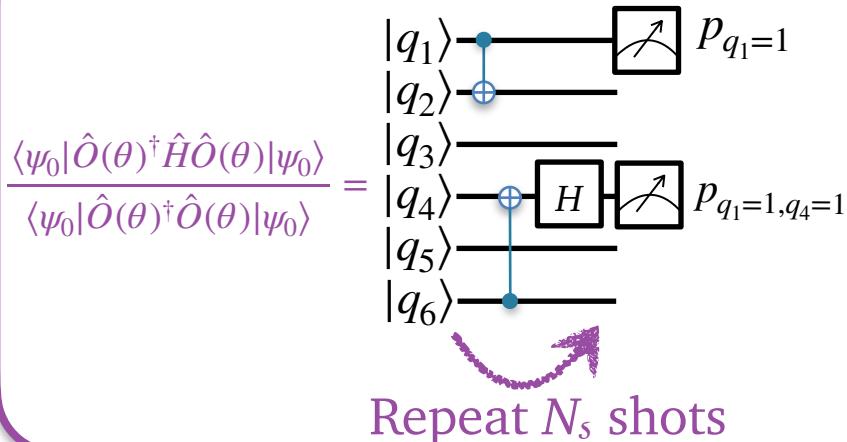


## 3. Minimisation

$$\min_{\theta} E(\theta) = \frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle}$$

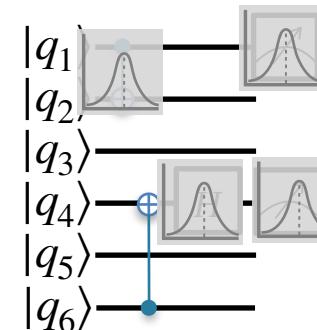


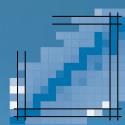
## 4. Measurement



$$\frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle} =$$

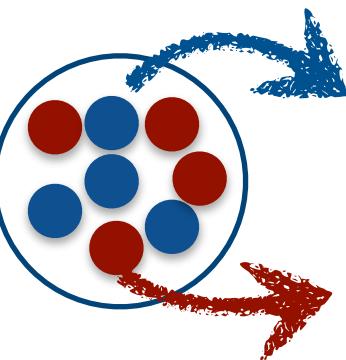
## 5. Error mitigation





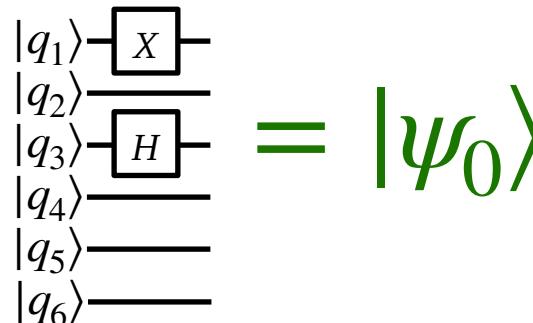
# Variational Quantum Eigensolver

## 1.Mapping



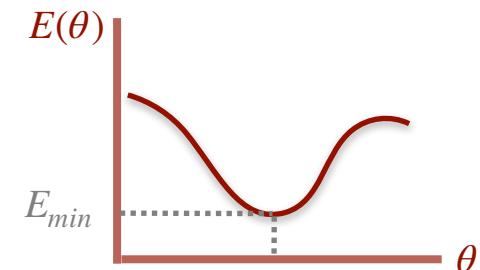
$|q_1\rangle$  —  
 $|q_2\rangle$  —  
 $|q_3\rangle$  —  
 $|q_4\rangle$  —  
 $|q_5\rangle$  —  
 $|q_6\rangle$  —

## 2.Reference state

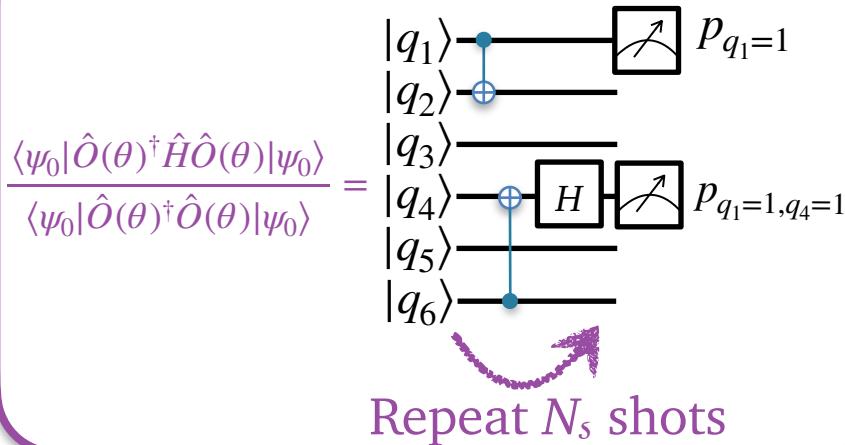


## 3.Minimisation

$$\min_{\theta} E(\theta) = \frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle}$$

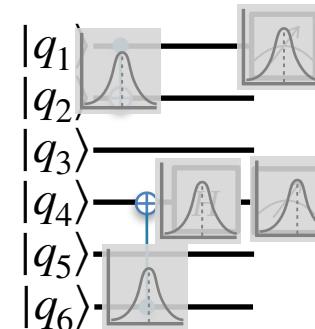


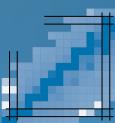
## 4.Measurement



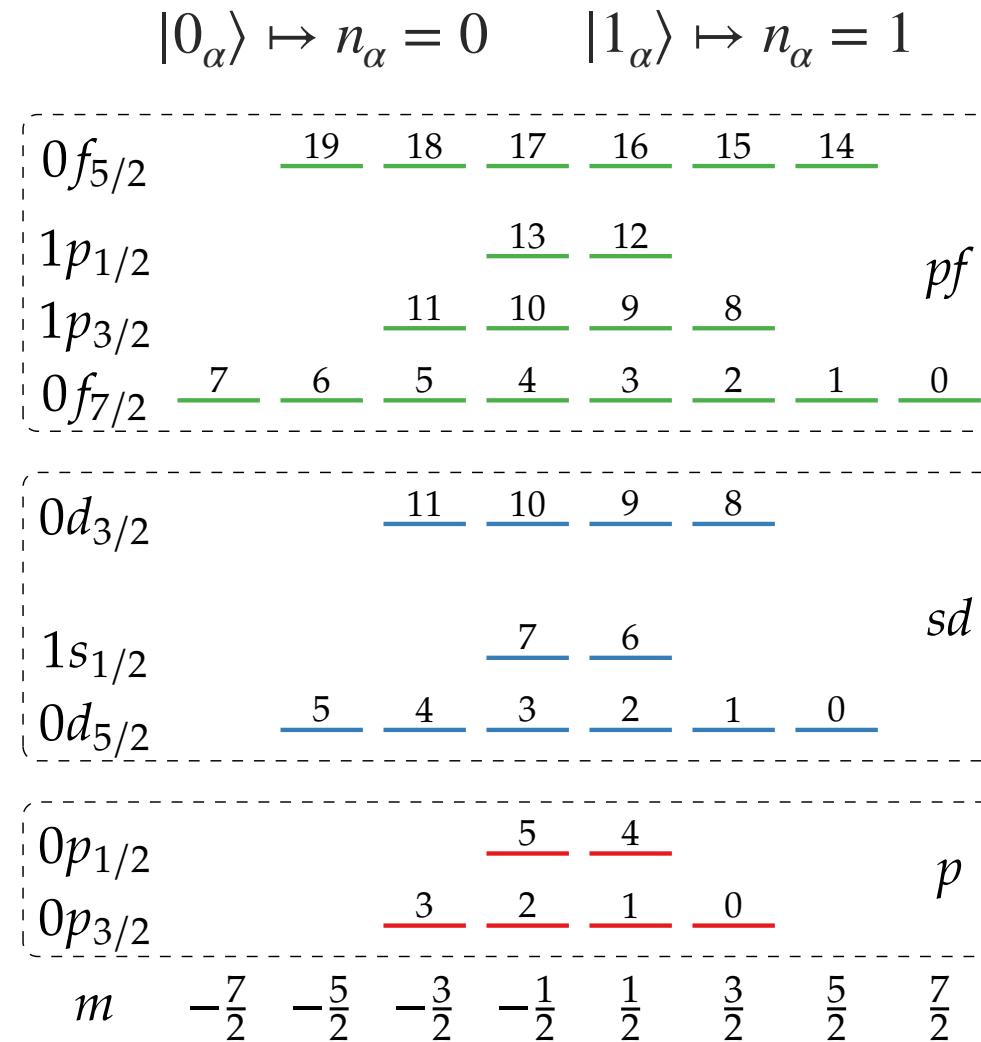
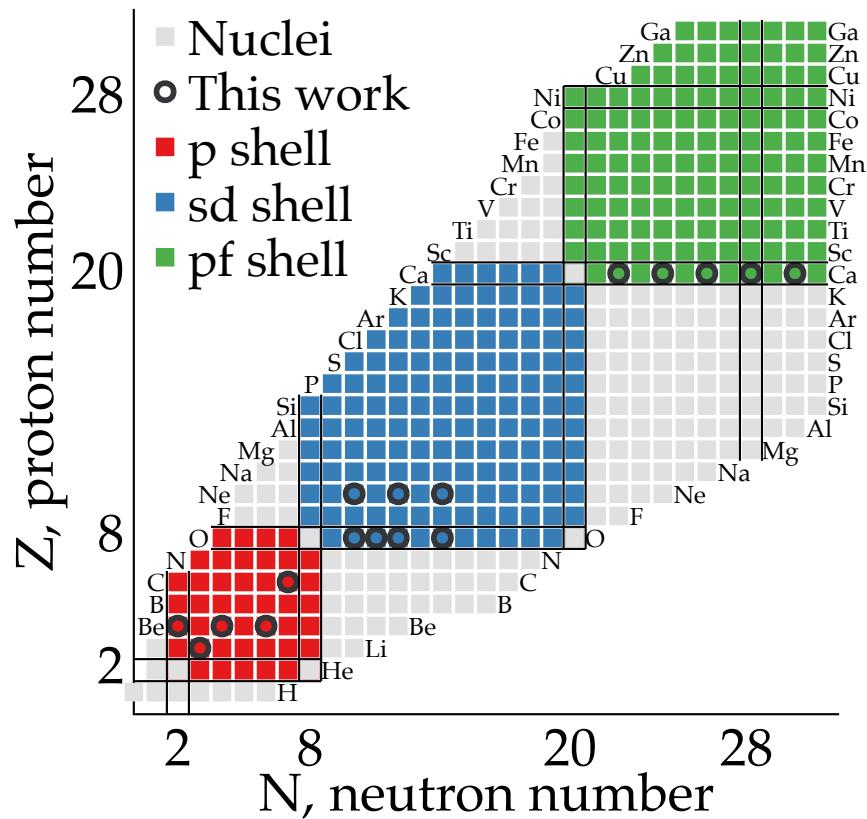
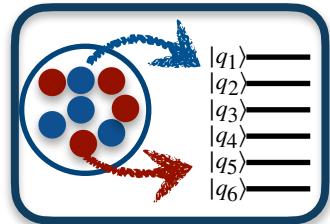
$$\frac{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{H} \hat{O}(\theta) | \psi_0 \rangle}{\langle \psi_0 | \hat{O}(\theta)^\dagger \hat{O}(\theta) | \psi_0 \rangle} =$$

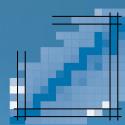
## 5.Error mitigation





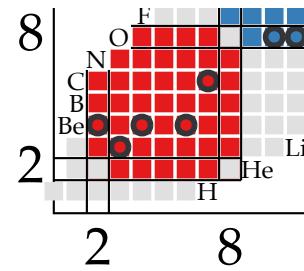
# Our work: mapping





# Our work: reference state

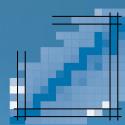
$$\begin{array}{c} |q_1\rangle \xrightarrow{X} \\ |q_2\rangle \\ |q_3\rangle \xrightarrow{H} \\ |q_4\rangle \\ |q_5\rangle \\ |q_6\rangle \end{array} = |\psi_0\rangle$$



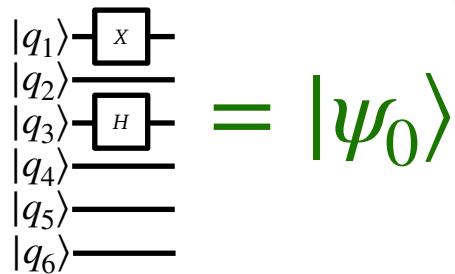
$$\begin{array}{c} {}^6\text{Be} \\ |0_1\rangle \xrightarrow{X} |1_1\rangle \\ |0_2\rangle \\ |0_3\rangle \\ |0_4\rangle \xrightarrow{X} |1_4\rangle \\ |0_5\rangle \\ |0_6\rangle \end{array}$$

$|100100\rangle$

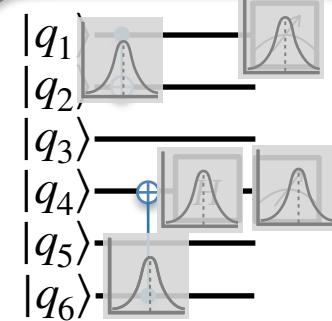
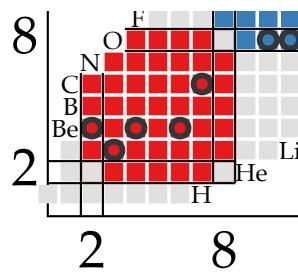
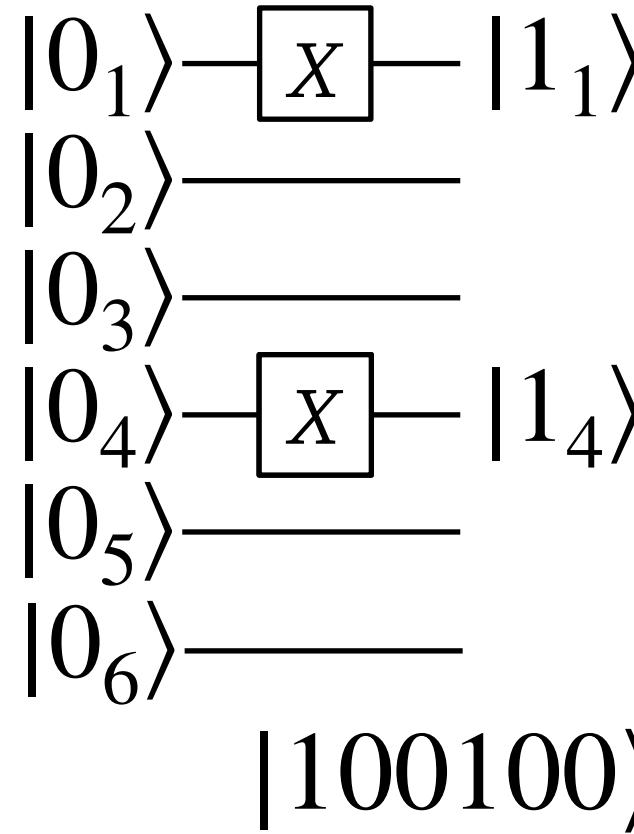
- Look for **minimum energy** Slater determinant



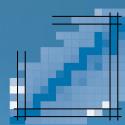
# Our work: reference state



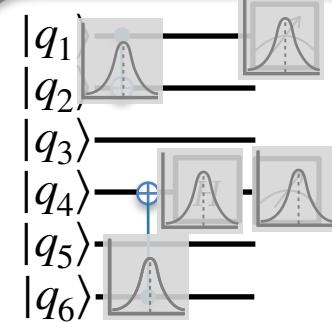
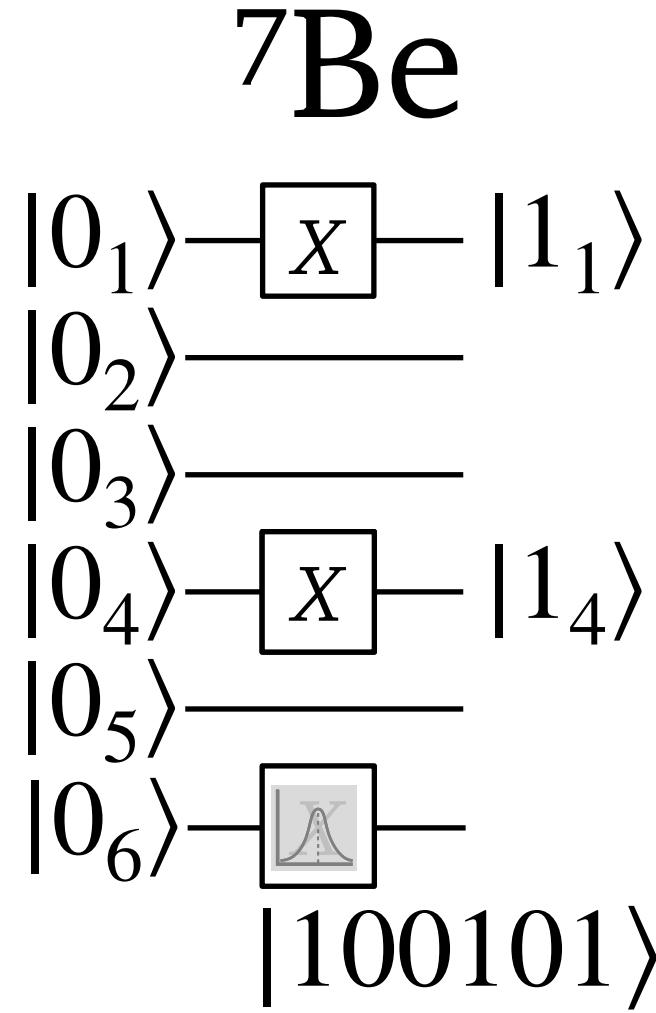
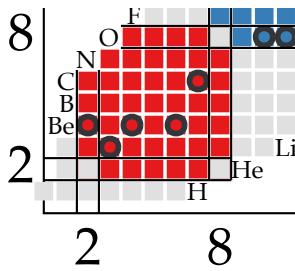
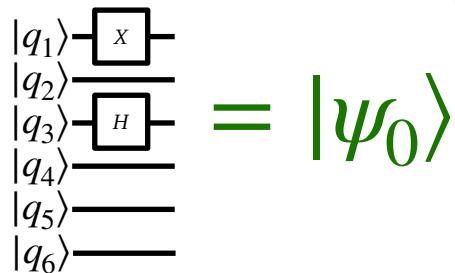
${}^6\text{Be}$



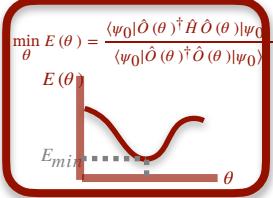
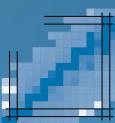
- Look for **minimum energy** Slater determinant



# Our work: reference state



- Look for **minimum energy** Slater determinant



## Layer 1

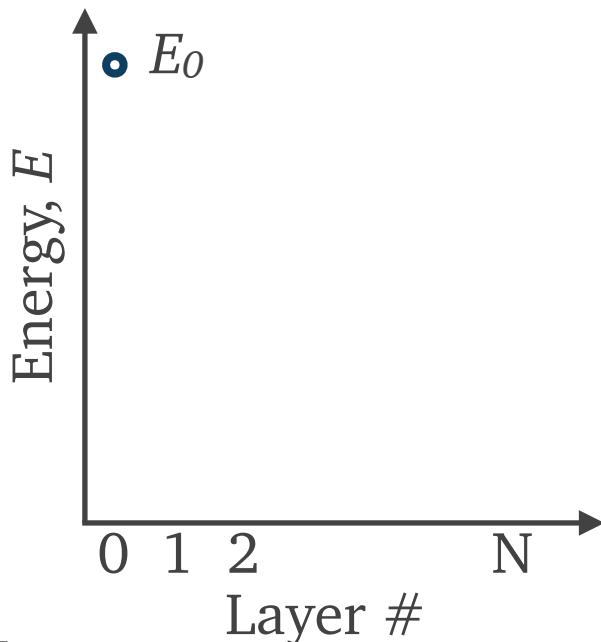
### 1. Ansatz

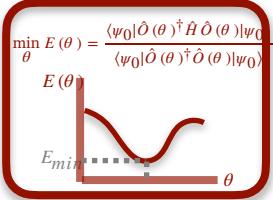
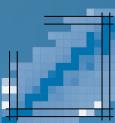
$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

## Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)





## Layer 1

### 1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

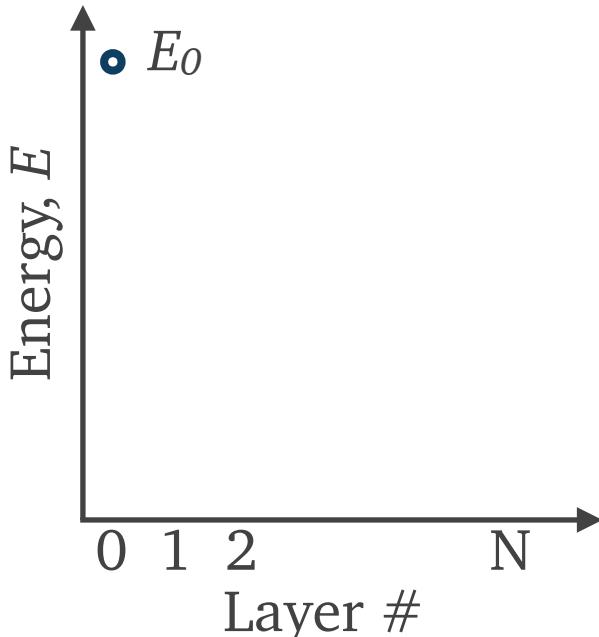
### 2. Compute gradients for k=1,M:

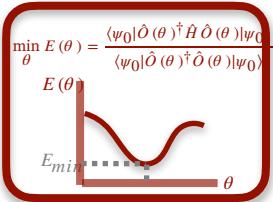
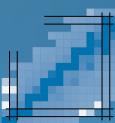
$$\frac{\partial E}{\partial \theta_k} \Big|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

## Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



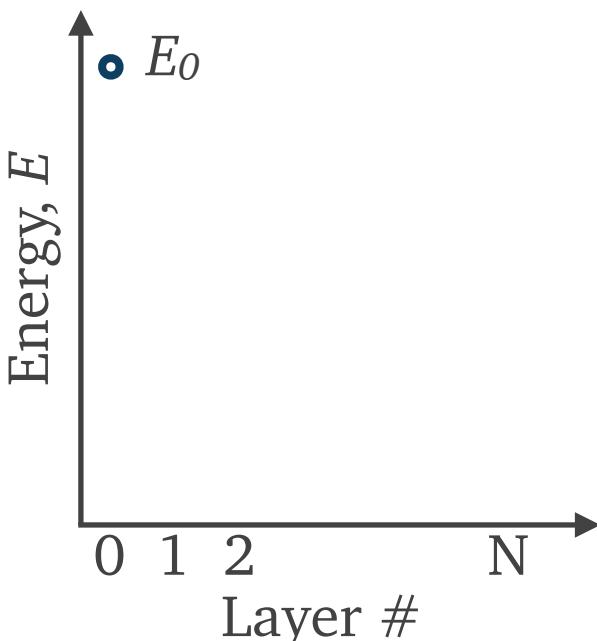


## Layer 1

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



#### 1. Ansatz

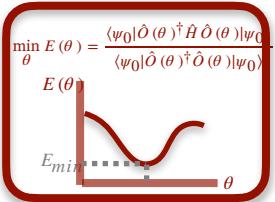
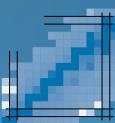
$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

#### 2. Compute gradients for k=1,M:

$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

#### 3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

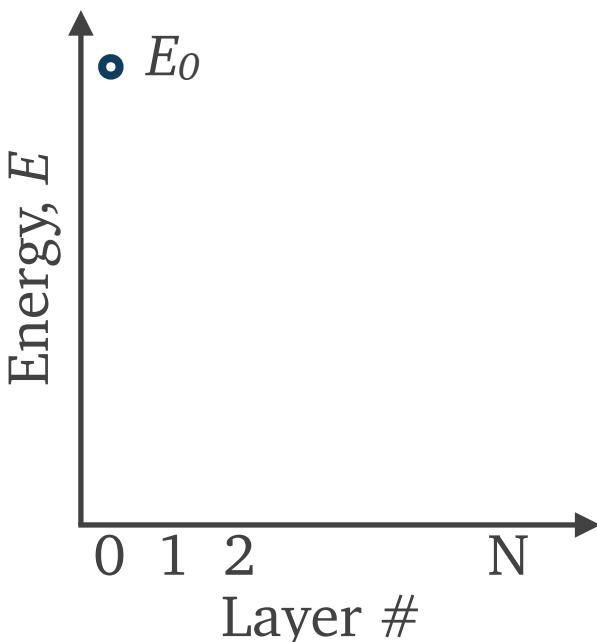


## Layer 1

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



### 1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

### 2. Compute gradients for k=1,M:

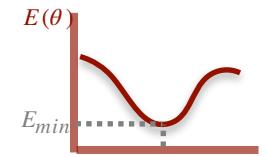
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

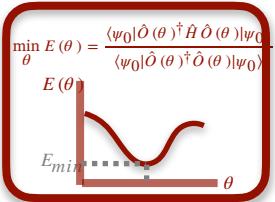
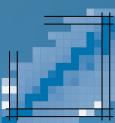
### 3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

### 4. Minimise the energy (classically)

$$\min_{\theta_1} E(\theta_1) = \langle \psi_0 | e^{-i\theta_1 \hat{A}_{k_1}} \hat{H} e^{i\theta_1 \hat{A}_{k_1}} | \psi_0 \rangle$$



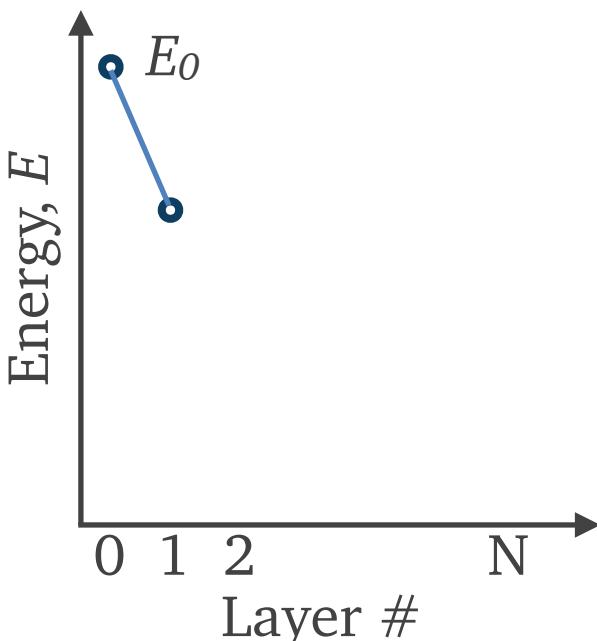


## Layer 1

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



### 1. Ansatz

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

### 2. Compute gradients for k=1,M:

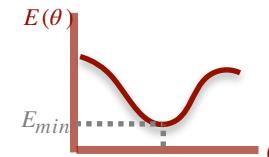
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

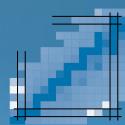
### 3. Keep the operator with largest gradient

$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

### 4. Minimise the energy (classically)

$$\min_{\theta_1} E(\theta_1) = \langle \psi_0 | e^{-i\theta_1 \hat{A}_{k_1}} \hat{H} e^{i\theta_1 \hat{A}_{k_1}} | \psi_0 \rangle$$



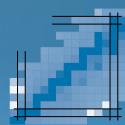


# Energy measurement strategy

$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$

One-body terms  $\langle \psi | \hat{H}_1 | \psi \rangle = \sum_p \epsilon_p \langle \psi | a_p^\dagger a_p | \psi \rangle$

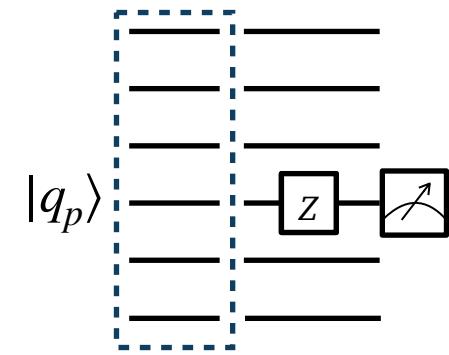
$$\langle \psi | a_p^\dagger a_p | \psi \rangle = \frac{1}{2} \langle \psi | 1 - Z_p | \psi \rangle = P_{p=1}$$



# Energy measurement strategy

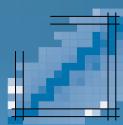
$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$

Measurement  
 $|\psi\rangle$



One-body terms  $\langle\psi|\hat{H}_1|\psi\rangle = \sum_p \epsilon_p \langle\psi|a_p^\dagger a_p|\psi\rangle$

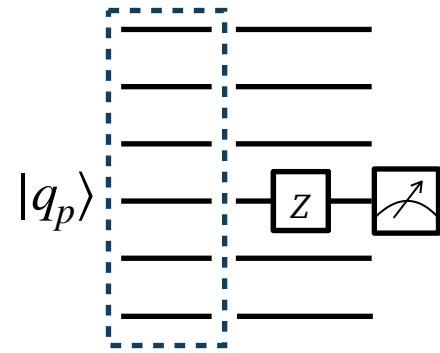
$$\langle\psi|a_p^\dagger a_p|\psi\rangle = \frac{1}{2} \langle\psi|1 - Z_p|\psi\rangle = P_{p=1}$$



# Energy measurement strategy

$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Measurement  
 $|\psi\rangle$



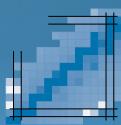
One-body terms  $\langle\psi|\hat{H}_1|\psi\rangle = \sum_p \epsilon_p \langle\psi|a_p^\dagger a_p|\psi\rangle$

$$\langle\psi|a_p^\dagger a_p|\psi\rangle = \frac{1}{2} \langle\psi|1 - Z_p|\psi\rangle = P_{p=1}$$

Two-body terms  $\langle\psi|\hat{H}_2|\psi\rangle = \sum_{pqrs} v_{pqrs} \langle\psi|a_p^\dagger a_q^\dagger a_r a_s|\psi\rangle$

$$\langle\psi|a_p^\dagger a_q^\dagger a_r a_s|\psi\rangle = \begin{cases} n_p n_q = P_{p=1} P_{q=1}, & p = r \text{ \& } q = s \\ P_{101}^{(pqrs)} - P_{110}^{(pqrs)}, & p = r \\ P_{1100}^{(pqrs)} - P_{0011}^{(pqrs)} & \end{cases}$$

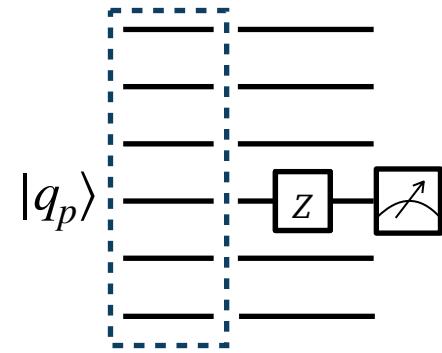
Non-contiguous case more difficult



# Energy measurement strategy

$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Measurement  
 $|\psi\rangle$



One-body terms  $\langle\psi|\hat{H}_1|\psi\rangle = \sum_p \epsilon_p \langle\psi|a_p^\dagger a_p|\psi\rangle$

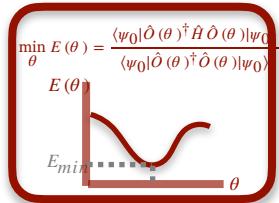
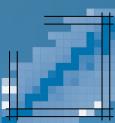
$$\langle\psi|a_p^\dagger a_p|\psi\rangle = \frac{1}{2} \langle\psi|1 - Z_p|\psi\rangle = P_{p=1}$$

Two-body terms  $\langle\psi|\hat{H}_2|\psi\rangle = \sum_{pqrs} v_{pqrs} \langle\psi|a_p^\dagger a_q^\dagger a_r a_s|\psi\rangle$

$$\langle\psi|a_p^\dagger a_q^\dagger a_r a_s|\psi\rangle = \begin{cases} n_p n_q = P_{p=1} P_{q=1}, & p = r \text{ & } q = s \\ P_{101}^{(pqrs)} - P_{110}^{(pqrs)}, & p = r \\ P_{1100}^{(pqrs)} - P_{0011}^{(pqrs)} & \end{cases}$$

Non-contiguous case more difficult

- Changes of basis for measurements
- Overhead of 0, 3 or 5 2-qubit gates for any nucleus!

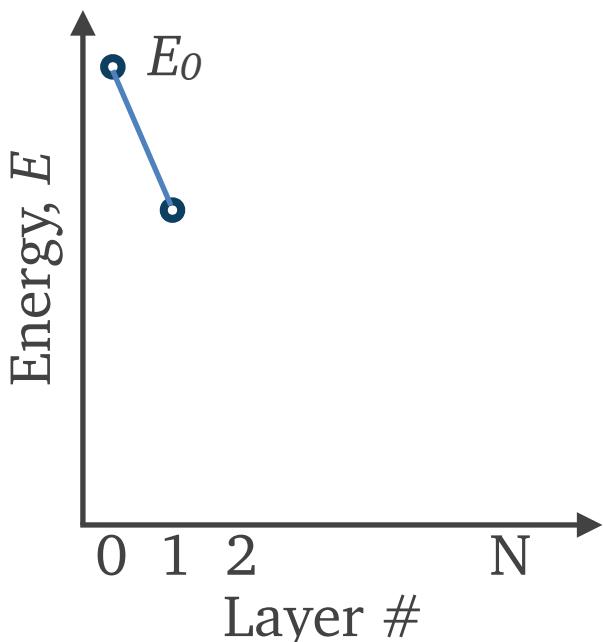


## Layer 2

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



#### 1. Ansatz

$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_k} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

#### 2. Compute gradients for $k=1, M$ :

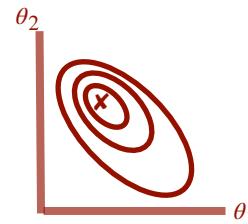
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

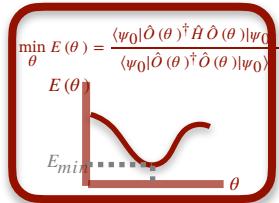
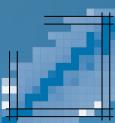
#### 3. Keep the operator with largest gradient

$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

#### 4. Minimise the energy (classically)

$$\min_{\theta_1, \theta_2} E(\theta_1, \theta_2) = \langle \psi_0 | e^{-i\theta_1 \hat{A}_{k_1}} e^{-i\theta_2 \hat{A}_{k_2}} \hat{H} e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} | \psi_0 \rangle$$



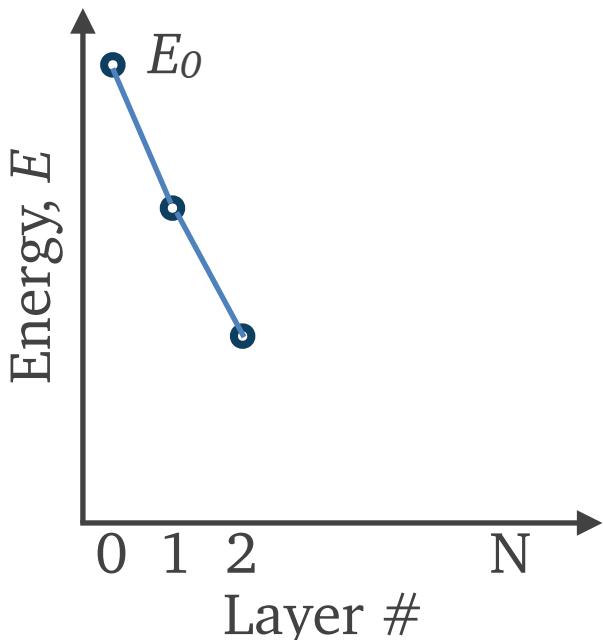


## Layer 2

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



#### 1. Ansatz

$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_k} e^{i\theta_1 \hat{A}_{k1}} |\psi_0\rangle$$

#### 2. Compute gradients for $k=1, M$ :

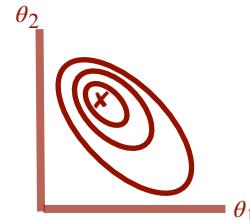
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

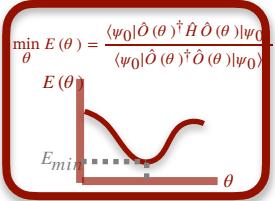
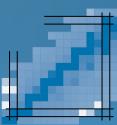
#### 3. Keep the operator with largest gradient

$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_{k2}} e^{i\theta_1 \hat{A}_{k1}} |\psi_0\rangle$$

#### 4. Minimise the energy (classically)

$$\min_{\theta_1, \theta_2} E(\theta_1, \theta_2) = \langle \psi_0 | e^{-i\theta_1 \hat{A}_{k1}} e^{-i\theta_2 \hat{A}_{k2}} \hat{H} e^{\theta_2 \hat{A}_{k2}} e^{\theta_1 \hat{A}_{k1}} | \psi_0 \rangle$$



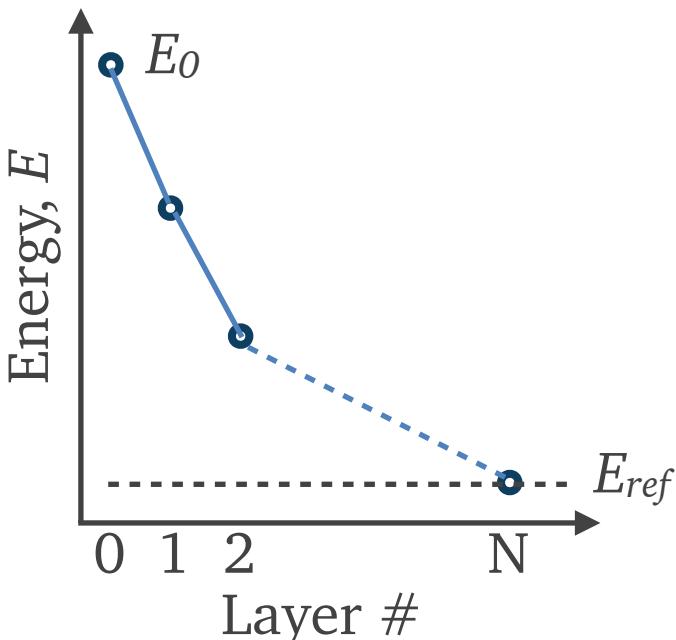


## Layer N

### Operator pool

$$\hat{A}_m : i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

M operators (consider symmetries!)



#### 1. Ansatz

$$|\psi_N(\vec{\theta})\rangle = \prod_{l=1}^N e^{i\theta_l \hat{A}_l} |\psi_0\rangle$$

#### 2. Compute gradients for k=1,M:

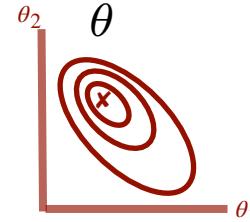
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

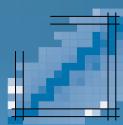
#### 3. Keep the operator with largest gradient

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

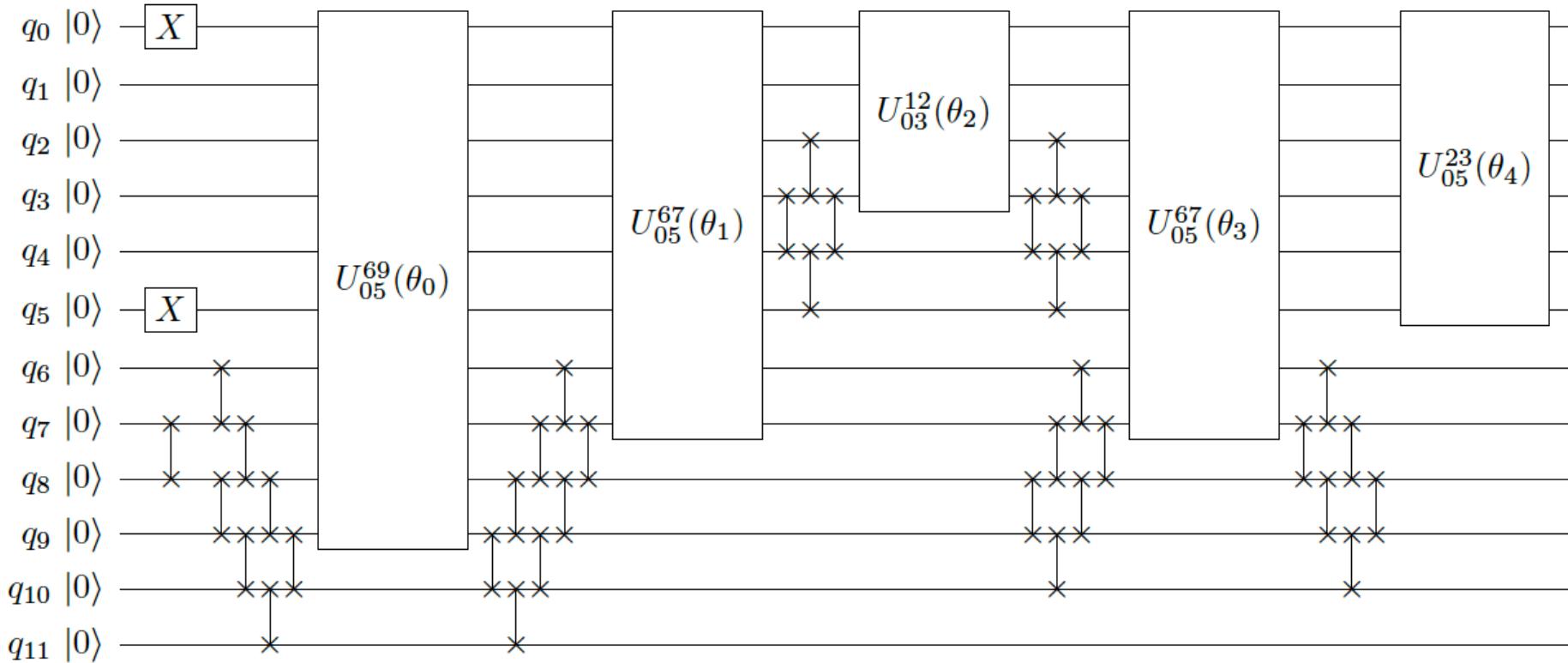
#### 4. Minimise the energy (classically)

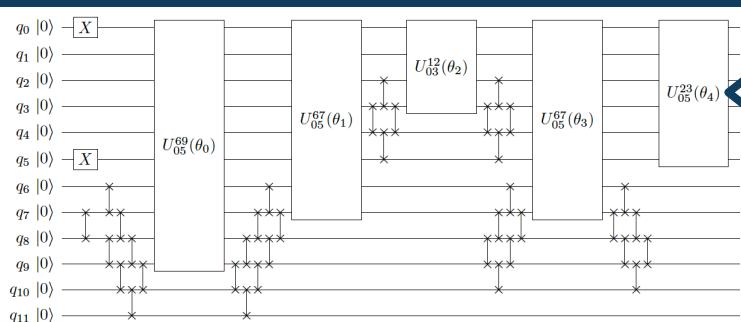
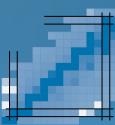
$$\min E(\vec{\theta})$$





## Circuit for the ground state of $^{18}\text{O}$



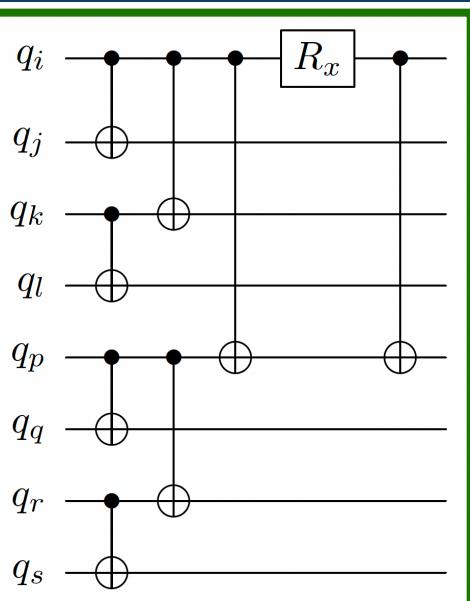


### 1. Ansatz

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_k} |\psi_{N-1}(\vec{\theta})\rangle$$

2. Compute gradients  
for  $k=1, M$ :

$$\frac{\partial E}{\partial \theta_k} \Big|_{\theta_k=0} = i\langle\psi(\theta)|[\hat{H}_{\text{eff}}, \hat{A}_k]|\psi(\theta)\rangle \Big|_{\theta_k=0}$$

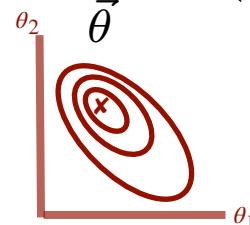


3. Keep the operator with largest gradient

$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

4. Minimise the energy (classically)

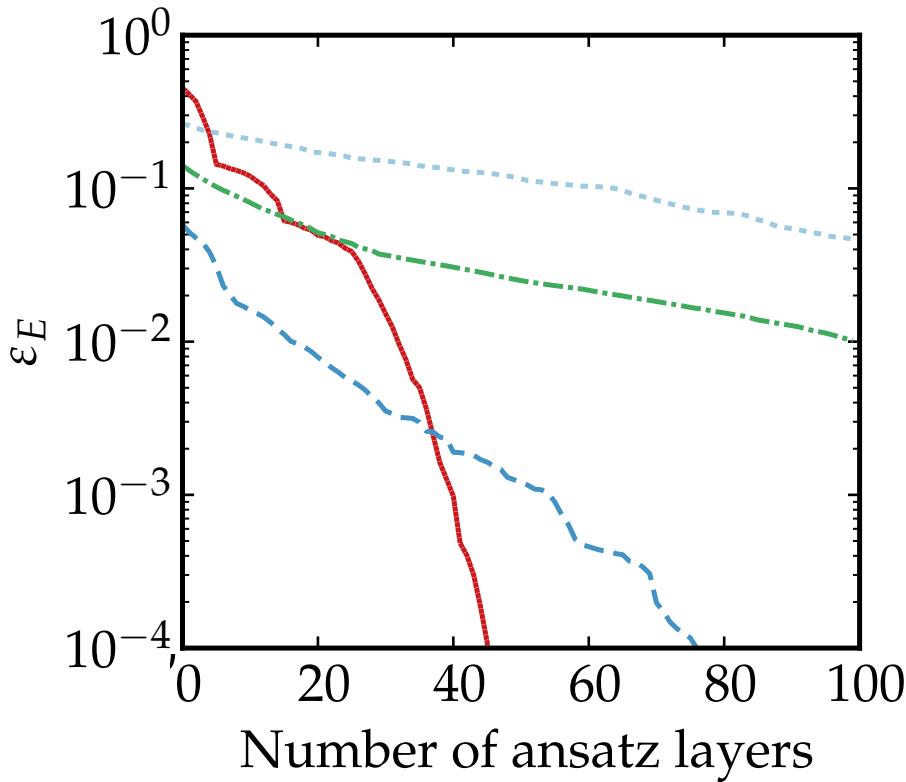
$$\min E(\vec{\theta})$$



`scipy.optimize.  
minimize`

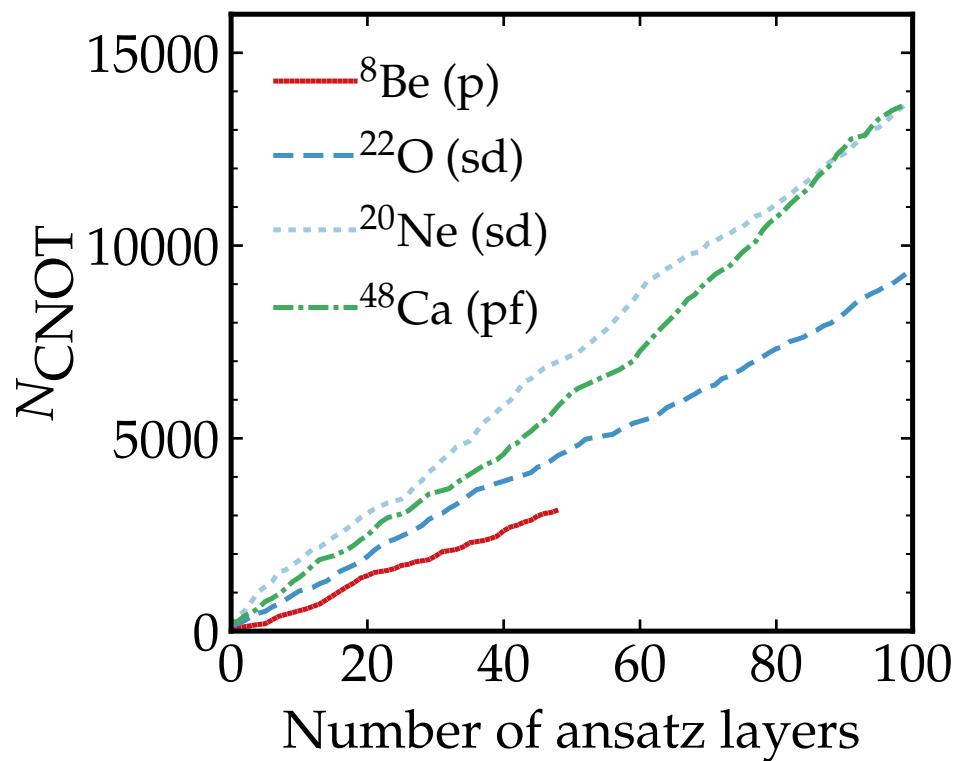


# Results



**Energy bound**

$$\epsilon_E = \frac{E_{ADAPT} - E_{SM}}{E_{SM}}$$



$N_{CNOT}$  is proxy for circuit depth

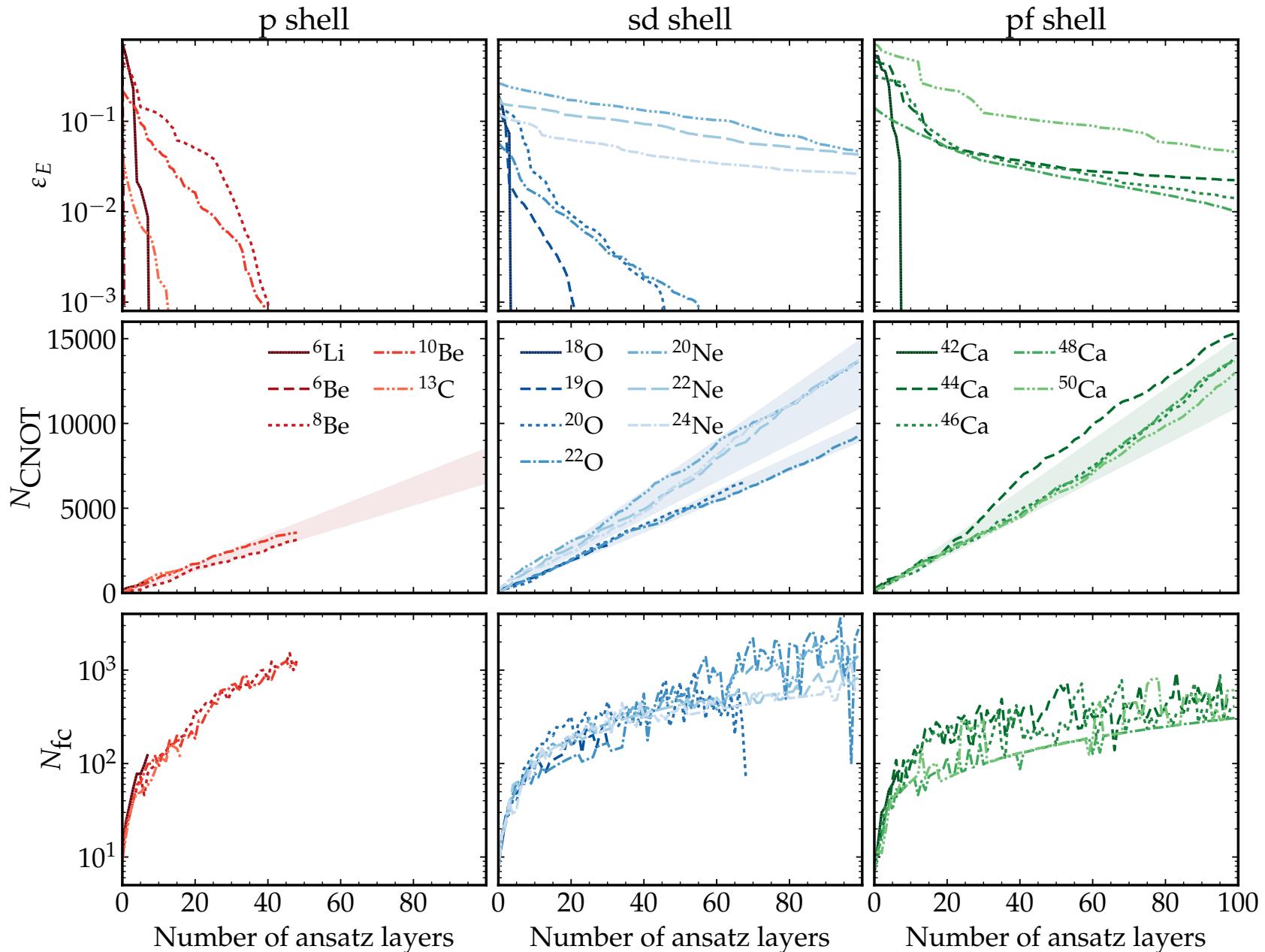


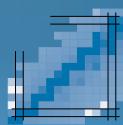
# Results

shell	$N_{qb}$	$N_{SD}$	nucleus	$N_{\text{layers}}$	$\varepsilon_E$ bound	$N_C$ (bound)
$p$	6	5	$^6\text{Be}$	2	$10^{-8}$	42 (80)
	12	10	$^6\text{Li}$	9	$10^{-7}$	92 (176)
		53	$^8\text{Be}$	48	$10^{-7}$	68 (176)
		51	$^{10}\text{Be}$	48	$10^{-7}$	62 (176)
		21	$^{13}\text{C}$	19	$10^{-7}$	77 (176)
$sd$	12	14	$^{18}\text{O}$	5	$10^{-6}$	99 (176)
		37	$^{19}\text{O}$	32	$10^{-6}$	85 (176)
		81	$^{20}\text{O}$	70	$10^{-6}$	98 (176)
		142	$^{22}\text{O}$	117	$10^{-6}$	93 (176)
	24	640	$^{20}\text{Ne}$	167	$2 \times 10^{-2}$	137 (368)
		4206	$^{22}\text{Ne}$	236	$2 \times 10^{-2}$	137 (368)
		7562	$^{24}\text{Ne}$	345	$2 \times 10^{-2}$	138 (368)
$pf$	20	30	$^{42}\text{Ca}$	9	$10^{-8}$	116 (304)
		565	$^{44}\text{Ca}$	132	$10^{-2}$	153 (304)
		3952	$^{46}\text{Ca}$	124	$10^{-2}$	139 (304)
		12022	$^{48}\text{Ca}$	101	$10^{-2}$	137 (304)
		17276	$^{50}\text{Ca}$	221	$10^{-2}$	130 (304)



# Results





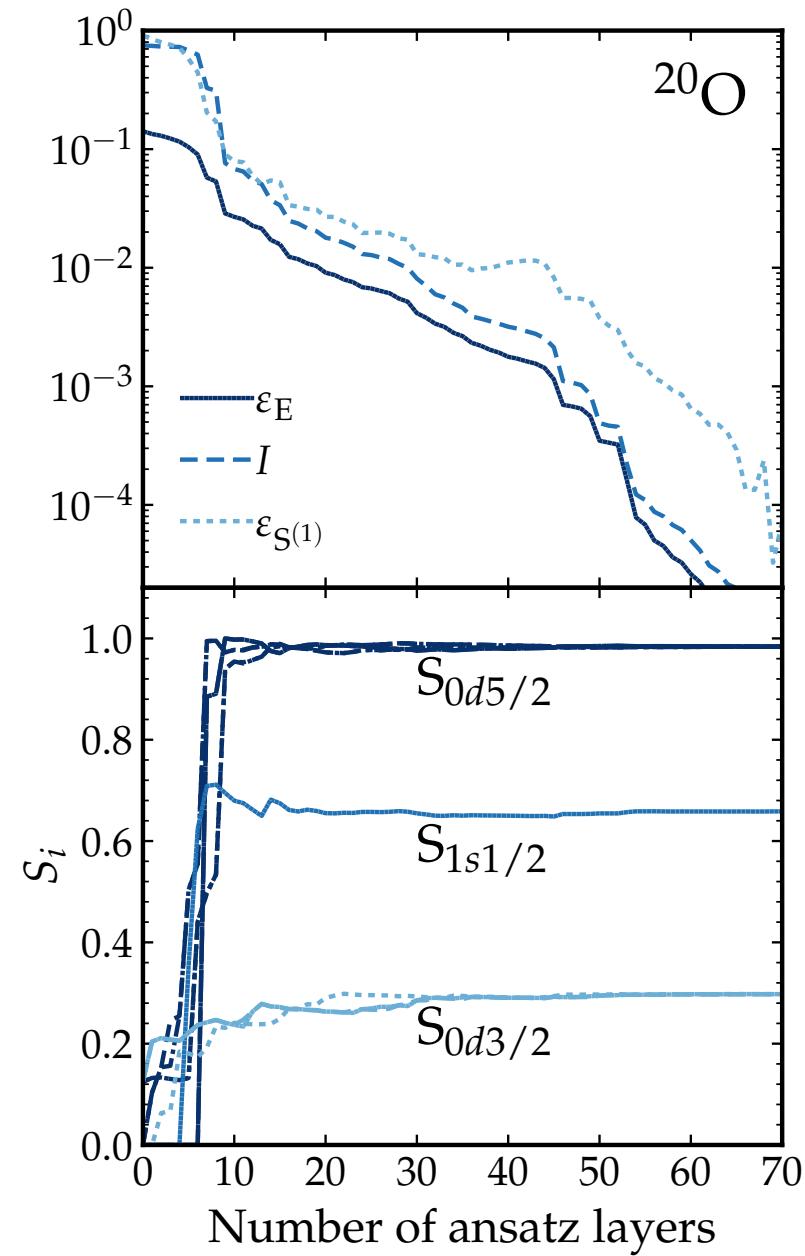
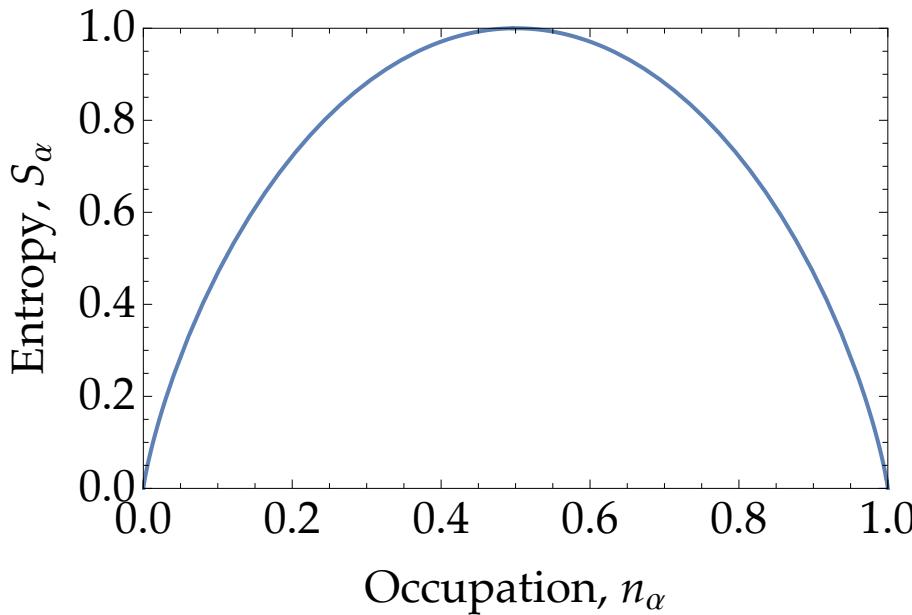
# Single-orbital entanglement

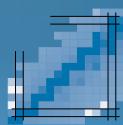
- A & B to be single-nucleon basis states

$$\hat{\rho}_A = \text{Tr}_B \hat{\rho}_{AB}$$

$$S(\hat{\rho}_A) = -\text{Tr} \hat{\rho}_A \log \hat{\rho}_A$$

$$S_\alpha = -n_\alpha \log_2 n_\alpha - (1 - n_\alpha) \log_2 (1 - n_\alpha)$$



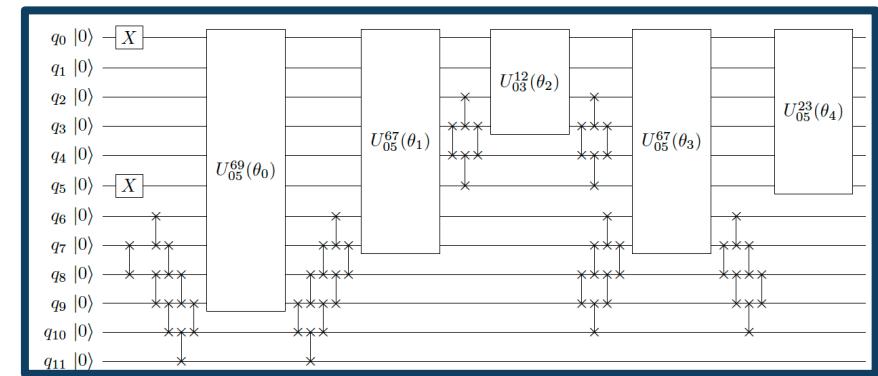


# Outlook & Perspectives

- VQEs can reproduce **shell model** wavefunctions
  - Number of qubits not an issue
  - Depth of circuit **is** an issue

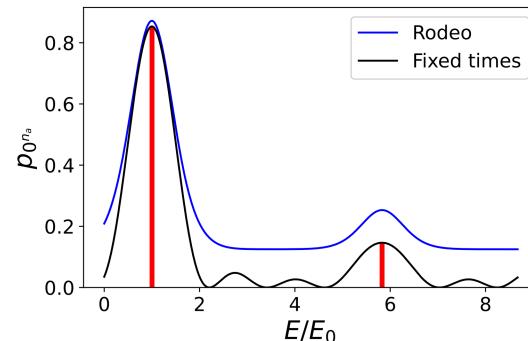
## To-Do List:

- Quantum computer
  - Simulations in “real” QCs
- Other methods
  - Unitary Coupled Cluster
- Entanglement
  - Quantification, exploitation
- Excited states
  - Rodeo algorithm



### ADAPT vs UCC

$$|\psi_N(\vec{\theta})\rangle = \prod_{l=1}^N e^{i\theta_l \hat{A}_l} |\psi_0\rangle \quad \text{vs} \quad |\psi_N(\vec{\theta})\rangle = e^{i \sum_l \theta_l \hat{A}_l} |\psi_0\rangle$$



# Thank you!

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