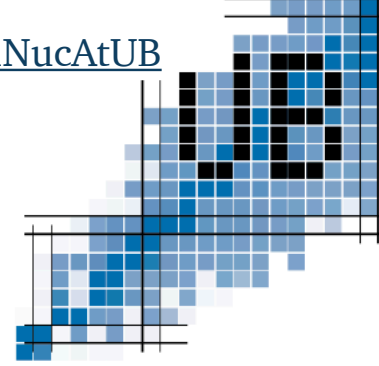




Quantum algorithms for the nuclear shell model



UNIVERSITAT DE
BARCELONA



Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

UAB
Universitat Autònoma
de Barcelona



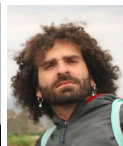
UNIVERSITAT POLITÈCNICA
DE CATALUNYA
BARCELONATECH



B Julià-Díaz



J Menéndez



E Costa



K Gallego



J Ainaud



A Morón



AM Romero



A García-Saez



S Masot-Llima



A Pérez-Obiol



M Carrasco-Codina

Digital: [Scientific Reports 13, 12291 \(2023\)](#) + [EPJA 59, 240 \(2023\)](#) + [arXiv:2409.04510](#) + [arXiv:2507.13819](#)

Adiabatic (Ema's talk): [SciPost Physics 19 062 \(2025\)](#) + [arXiv:2411.06954](#)

Arnau Rios Huguet

Associate Professor
Institute of Cosmos Sciences
Universitat de Barcelona
arnau.rios@fqa.ub.edu

**AQAM 2025
Montpellier**
20 November 2025

Nuclear Physics in Barcelona

Open Postdoc & PhD opportunities

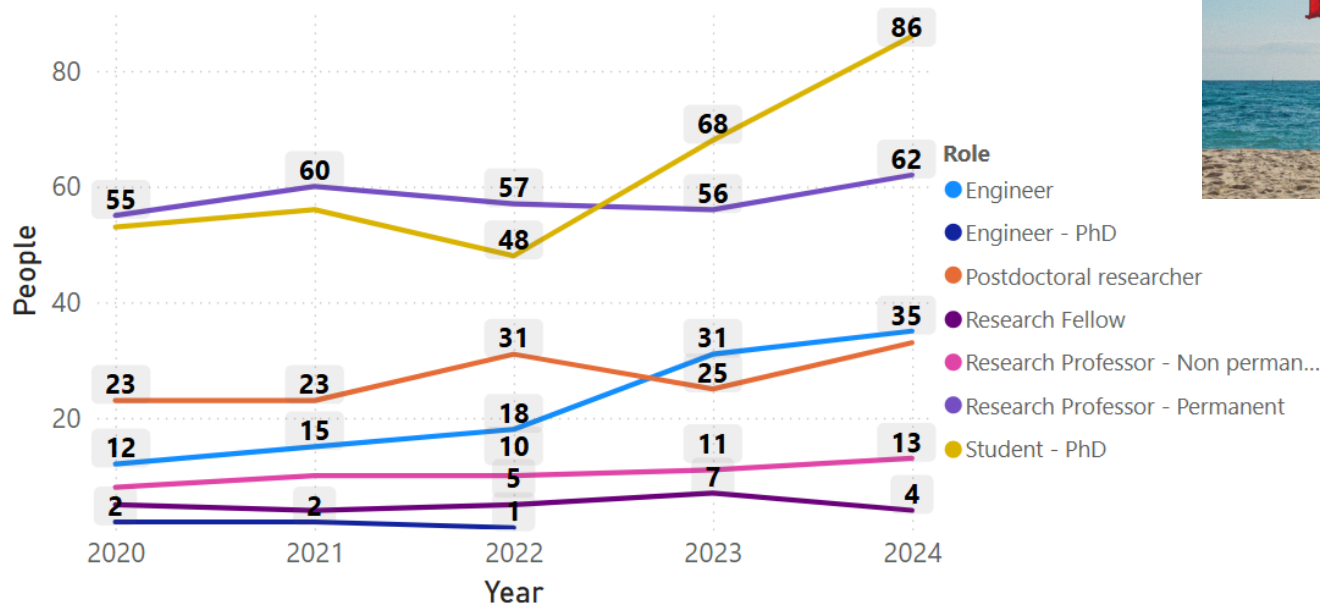
Deadline: 30/11/2025

<https://icc.ub.edu/job-offers>

Maria de Maeztu Postdoctoral position in Quantum Resources for Science and Technology



Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA



Fellowships



Fundación "la Caixa"



Nuclear Physics in Barcelona

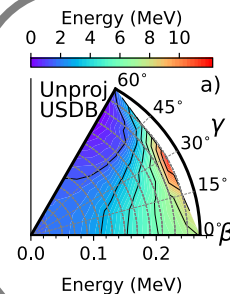
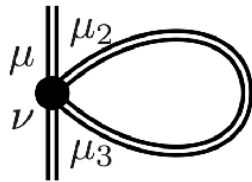
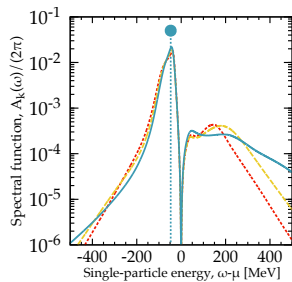
Open Postdoc & PhD opportunities

Deadline: 30/11/2025

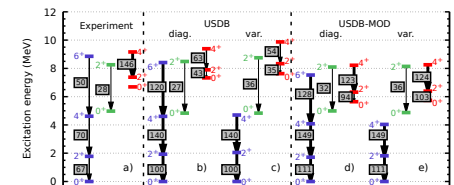
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Maria de Maeztu Postdoctoral position in Quantum Resources for Science and Technology

Dense matter

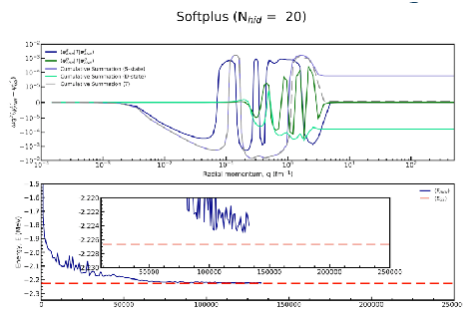


Nuclear structure

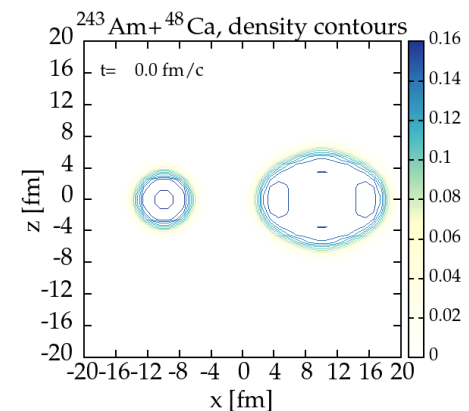


Frycz et al PRC 110, 054326 (2024)

Machine learning



DFT



Fellowships



Fundación "la Caixa"



• Nuclear shell model

• VQEs for nuclei

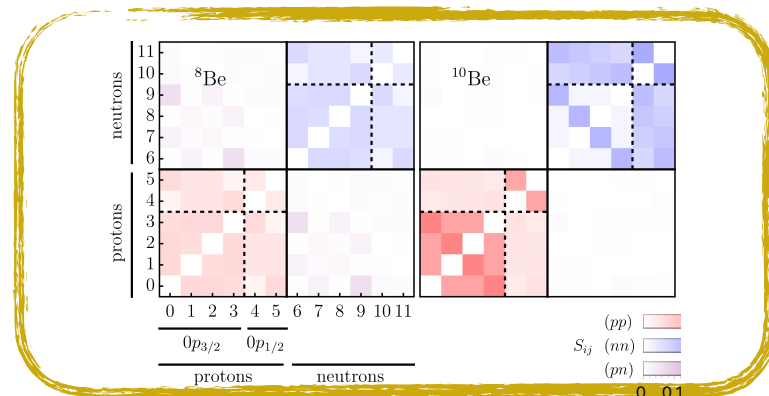
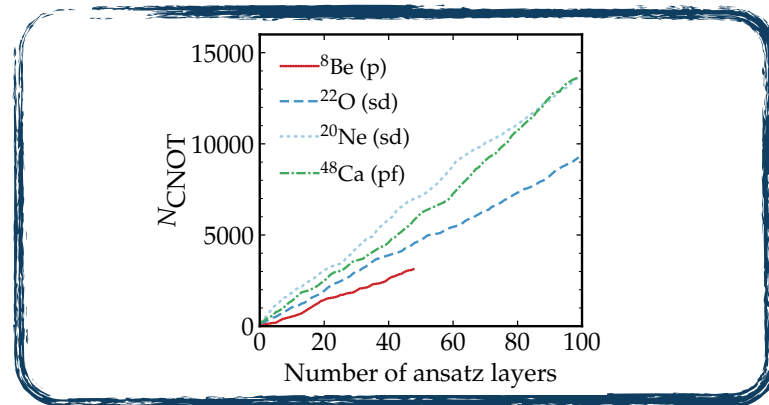
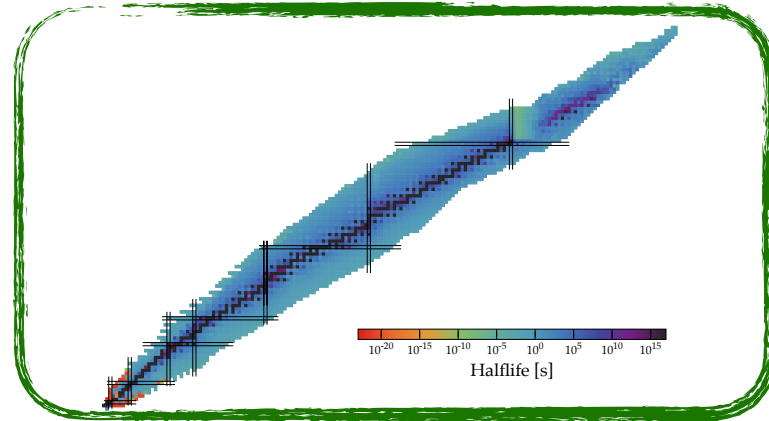
[Scientific Reports **13**, 12291 \(2023\)](#)

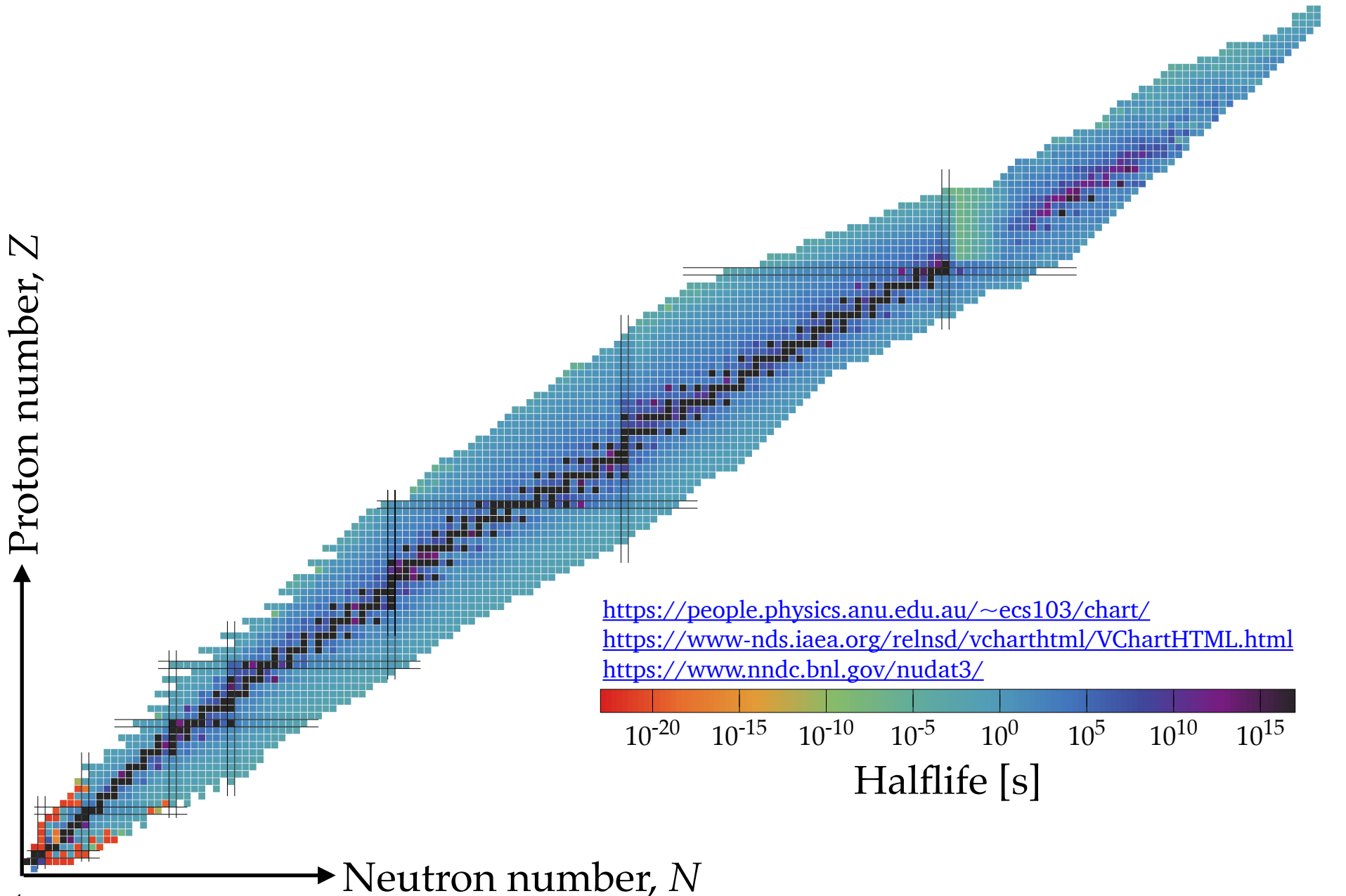
[EPJA **59**, 240 \(2023\)](#)

+ [arXiv:2409.04510](#) + [arXiv:2507.13819](#)

• Entanglement forging

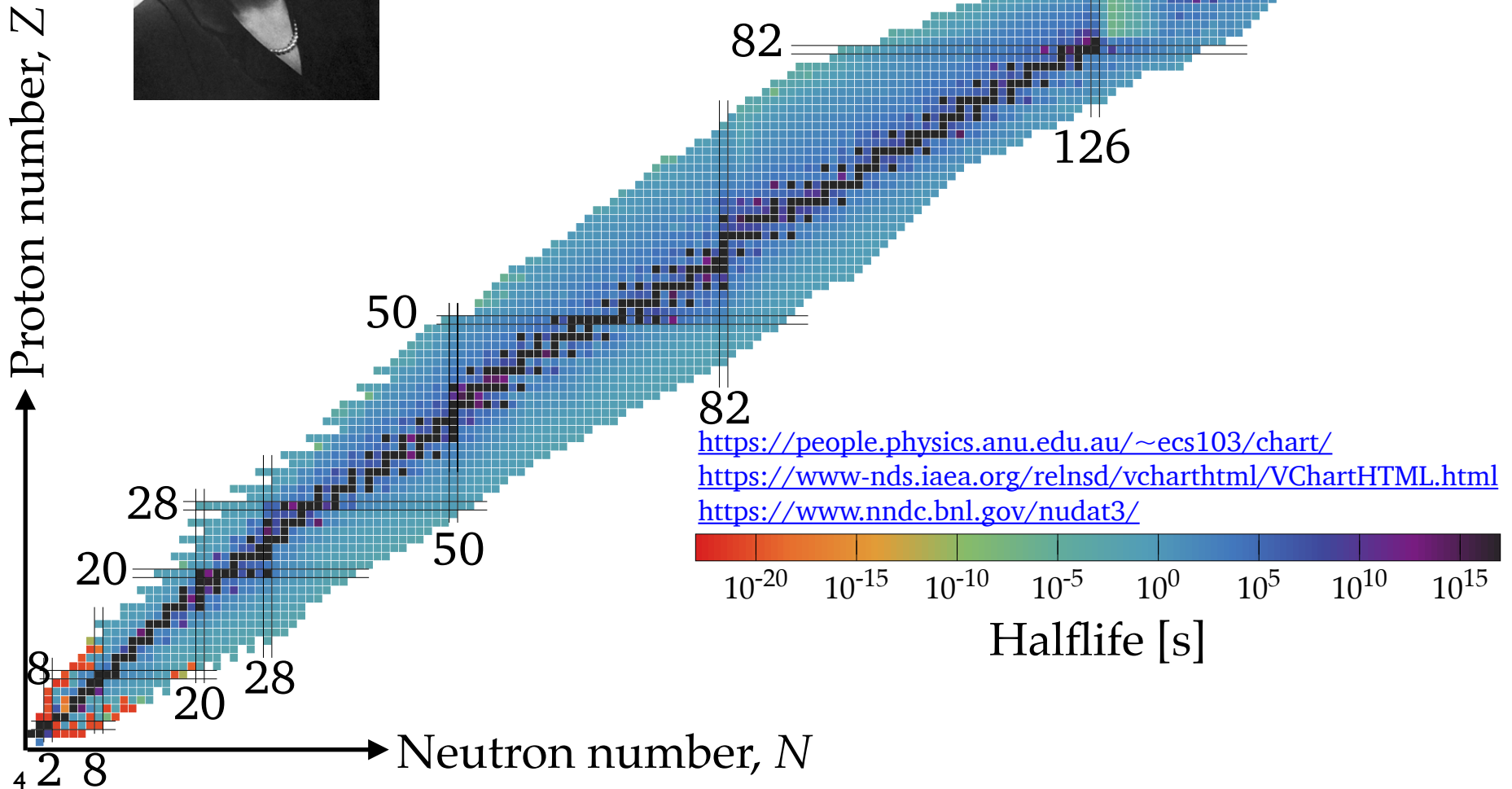
[arXiv:2411.06954](#)







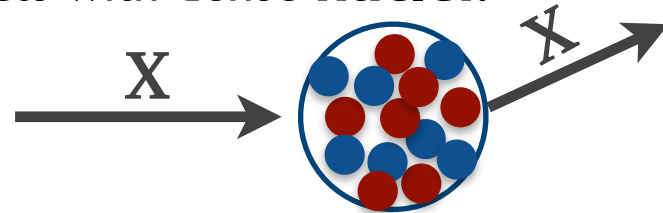
Maria Goeppert Mayer
Nobel Prize (1963)





- What is the nature of the **dark matter**?

- Dark matter interacts with dense **nuclei**!



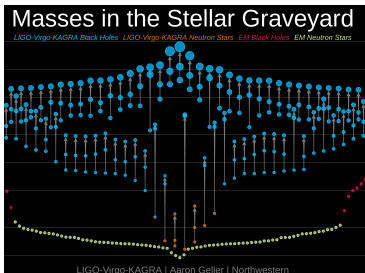
- What is the nature of the **neutrino**?

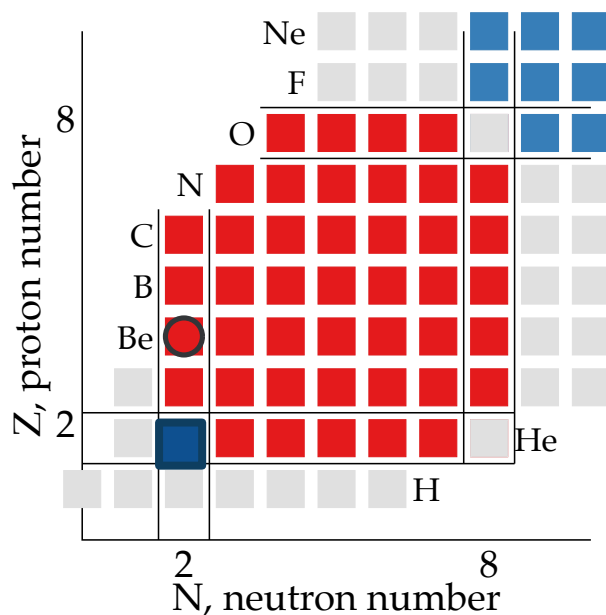
- Neutrinos interact with dense **nuclei**!
- Astrophysical neutrinos created in **Neutron Stars**



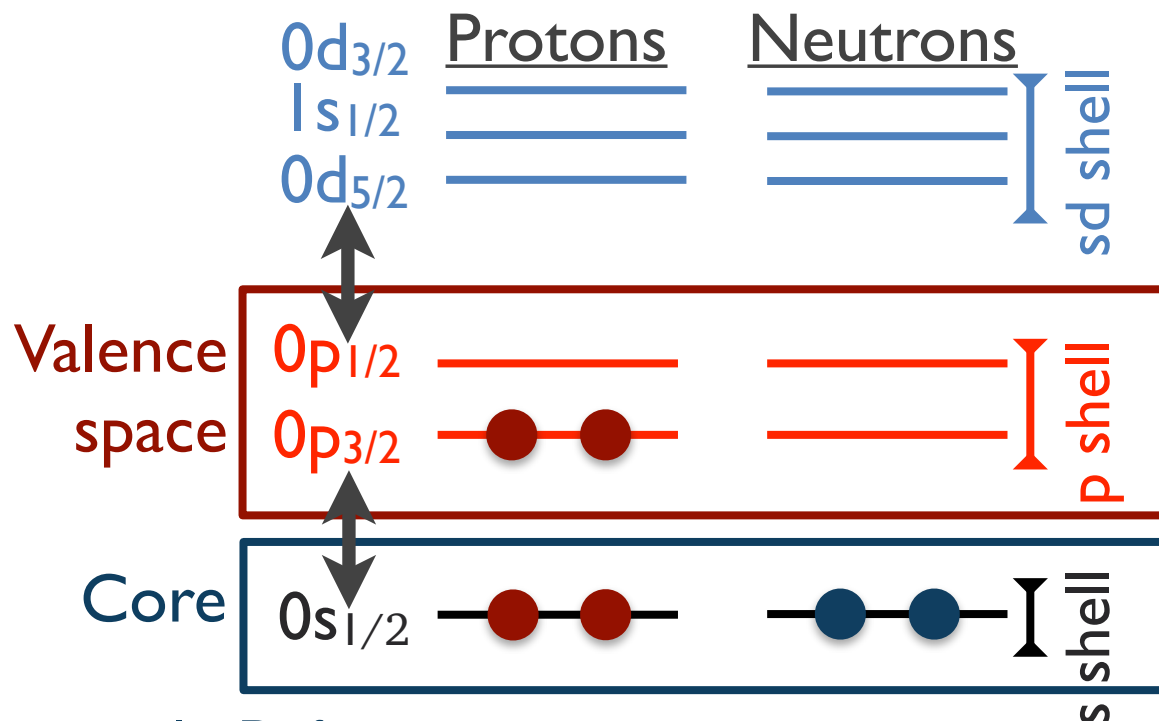
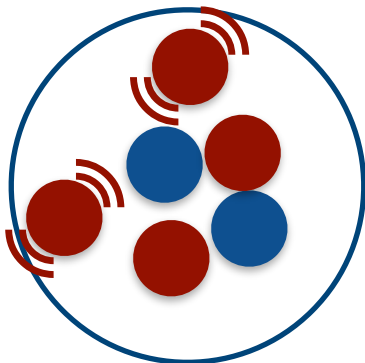
- What are the origins of **gravitational waves**?

- Nuclear fusion in stars
- r-process sites for **nucleosynthesis**



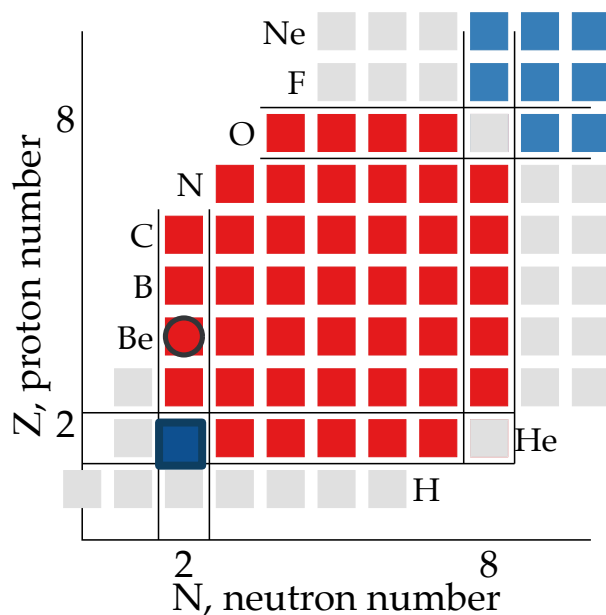
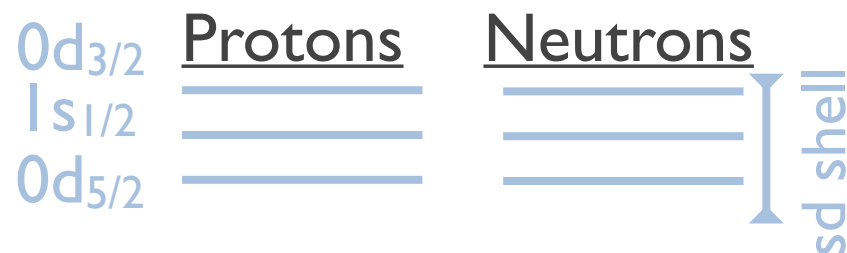
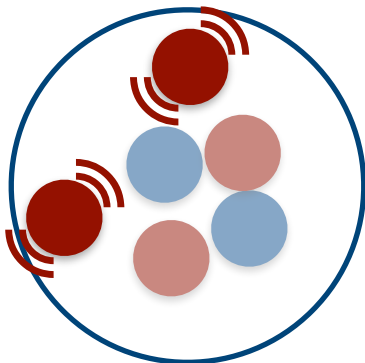


${}^6\text{Be}$

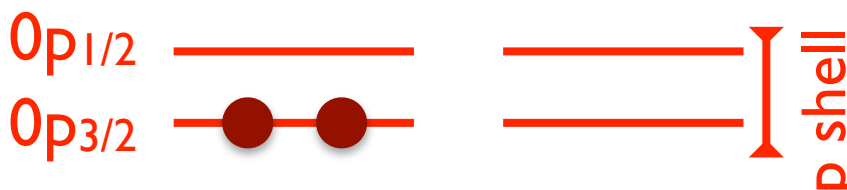


1. Define **core**
2. Define **valence space**
3. Use **effective Hamiltonian** in valence space
4. Generate **many-body basis** for system
5. Diagonalise **effective Hamiltonian matrix**

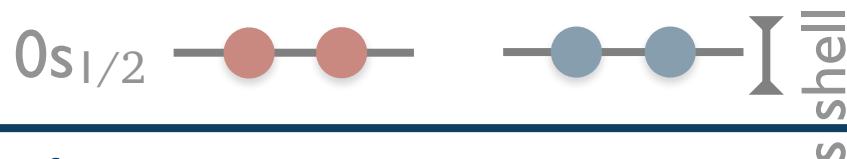
$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_p$$

 ${}^6\text{Be}$ 

Valence space



Core

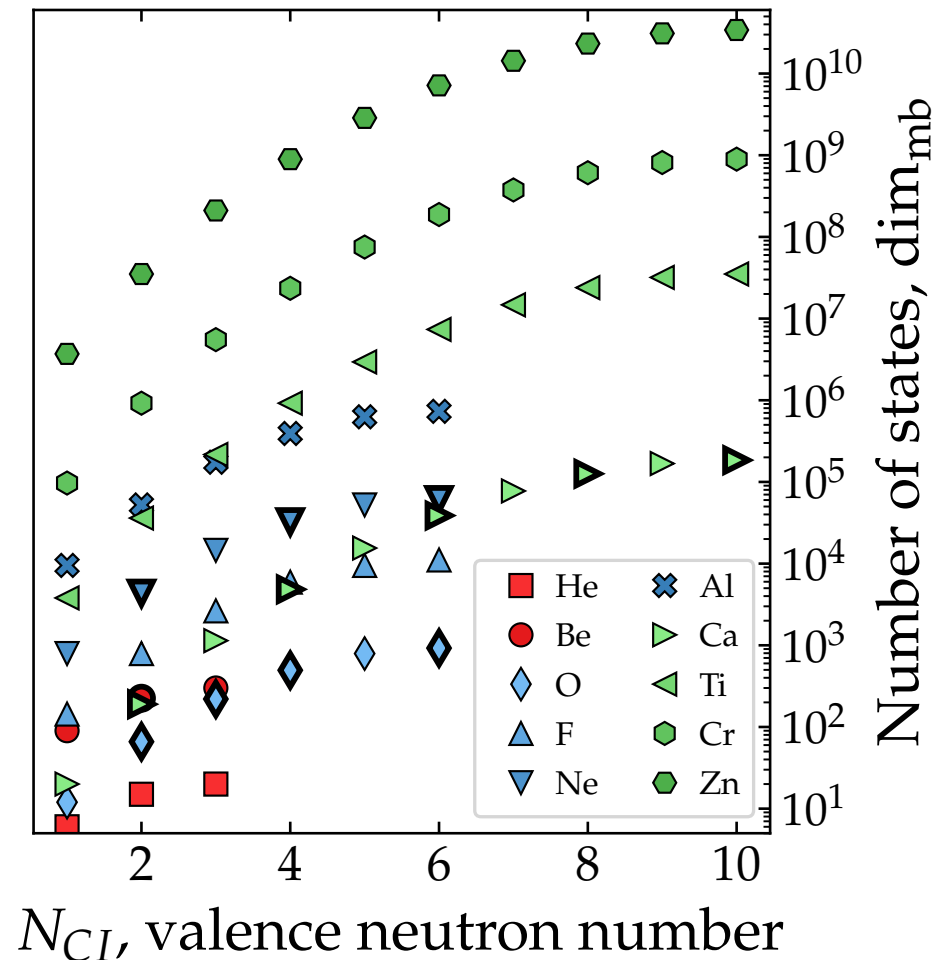
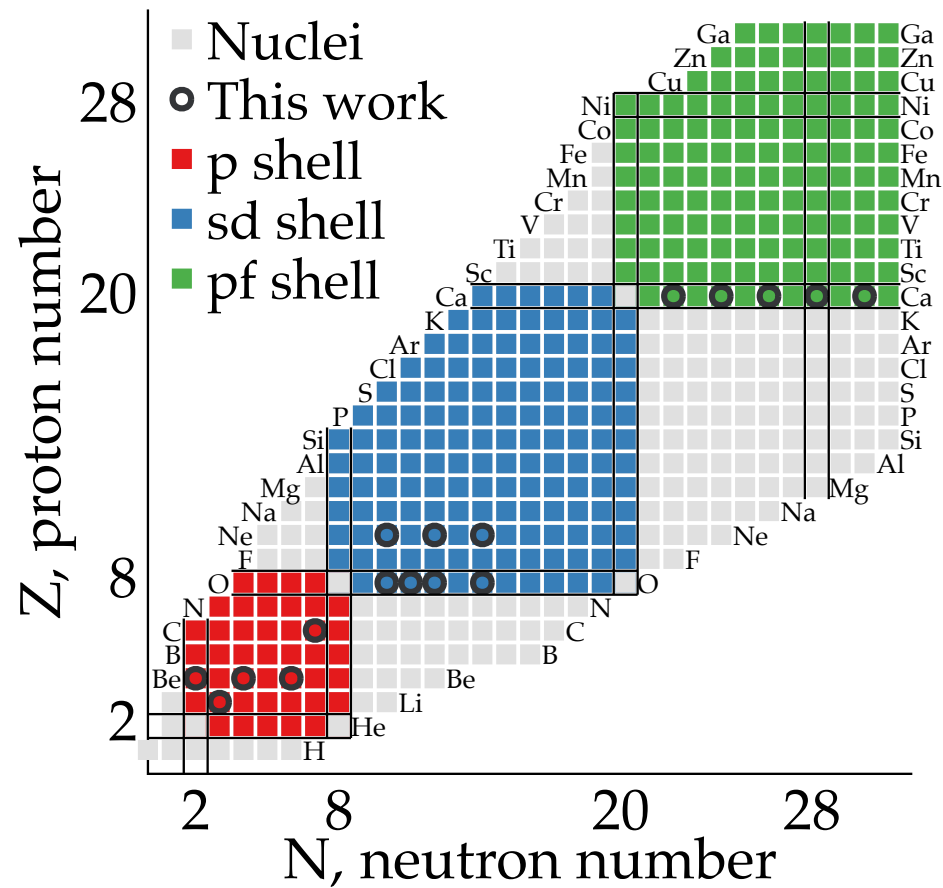


1. Define **core**
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5. Diagonalise **effective Hamiltonian matrix**

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

Shell model complexity

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



- Nuclear shell model

- VQEs for nuclei

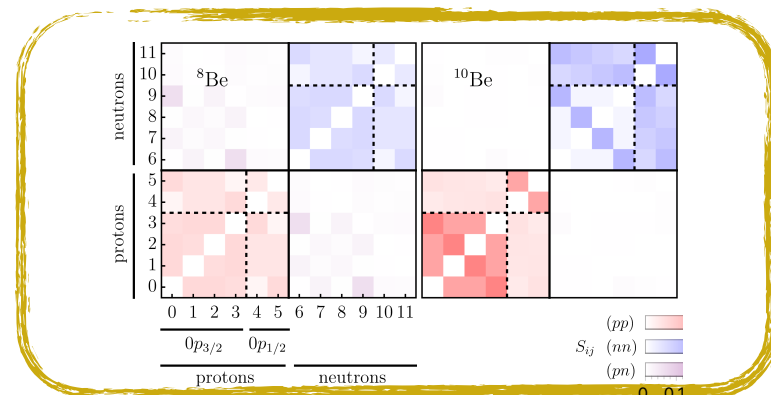
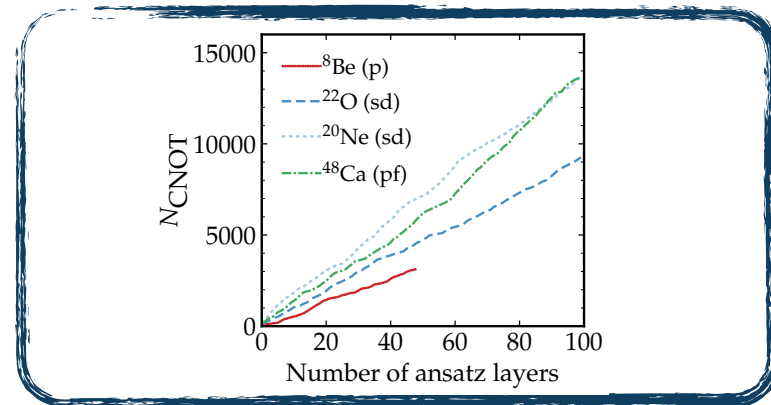
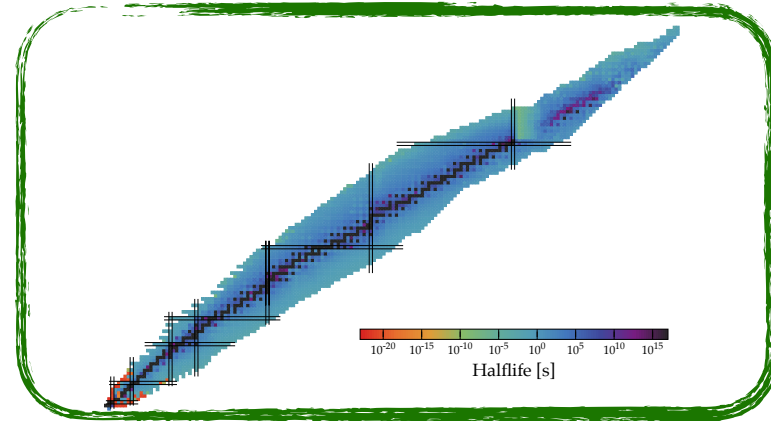
[Scientific Reports **13**, 12291 \(2023\)](#)

[EPJA **59**, 240 \(2023\)](#)

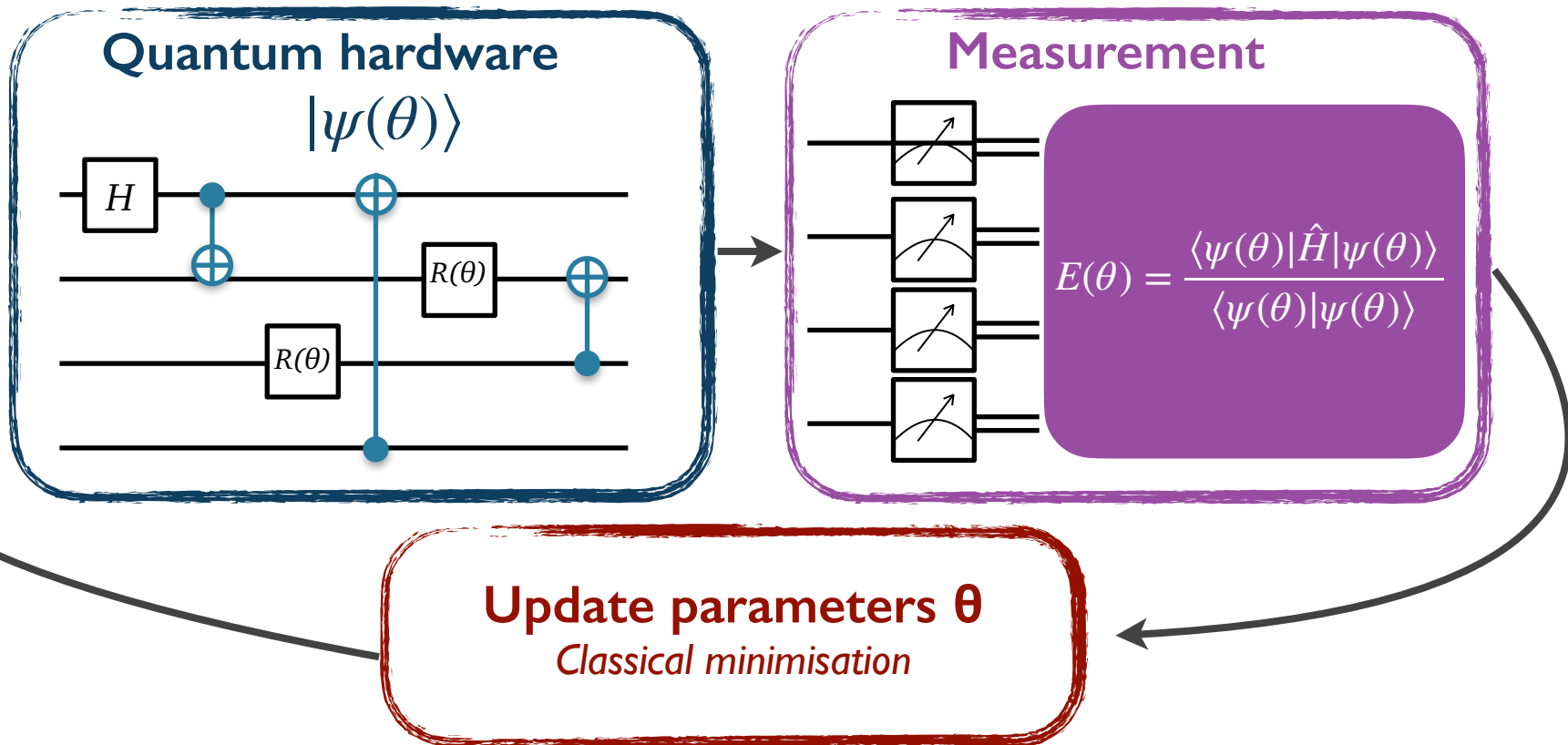
+ [arXiv:2409.04510](#) + [arXiv:2507.13819](#)

- Entanglement forging

[arXiv:2411.06954](#)



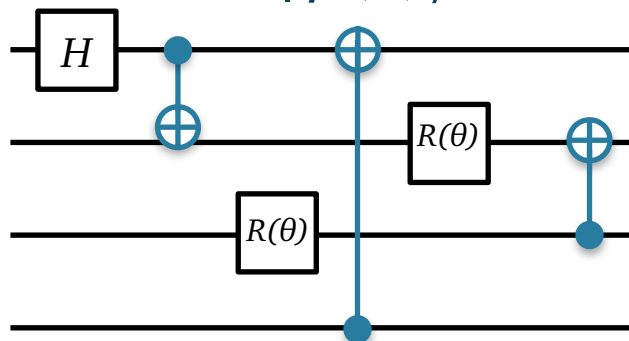
Variational Quantum Eigensolver



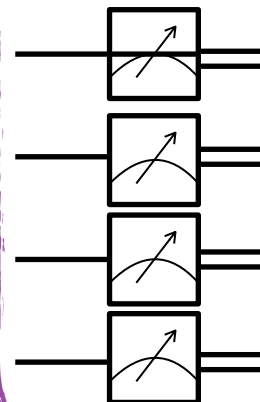
Variational Quantum Eigensolver

Quantum hardware

$|\psi(\theta)\rangle$



Measurement

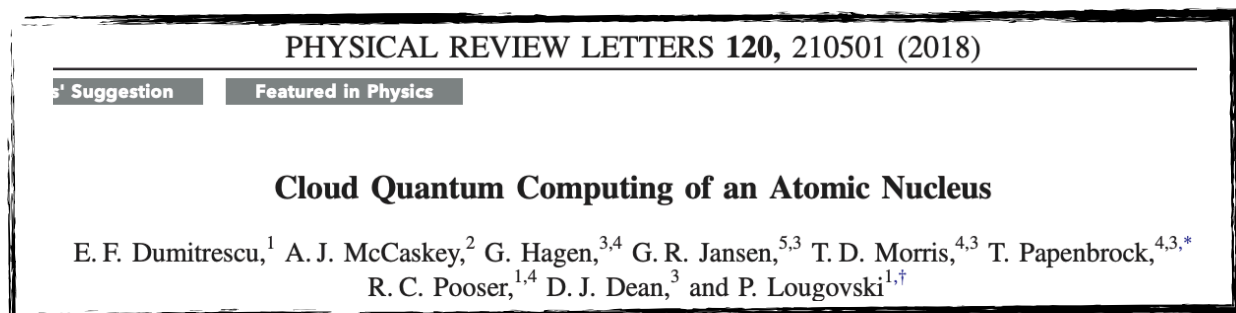


$$E(\theta) = \frac{\langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle}$$

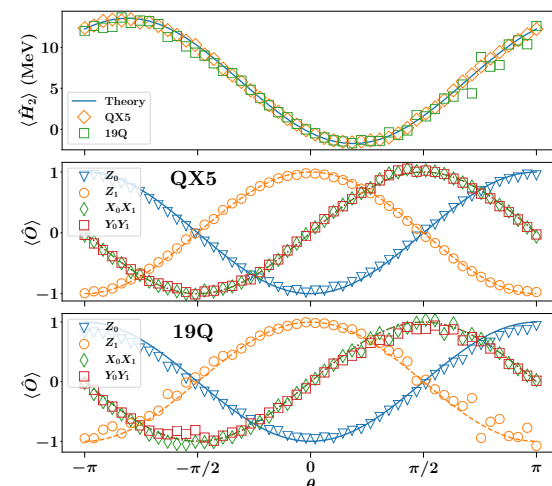
Update parameters θ
Classical minimisation



VQE: Variational Quantum Eigensolver,
Arnau Rios@Quantum Spain
<https://www.youtube.com/watch?v=lgqiDfpGg90>



Phys. Rev. Lett. **120** 210501 (2018)



• Initial work on nuclear structure (before '20)

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

Stetcu, Baroni, Carlson, Phys. Rev. C **105** 064308 (2022)

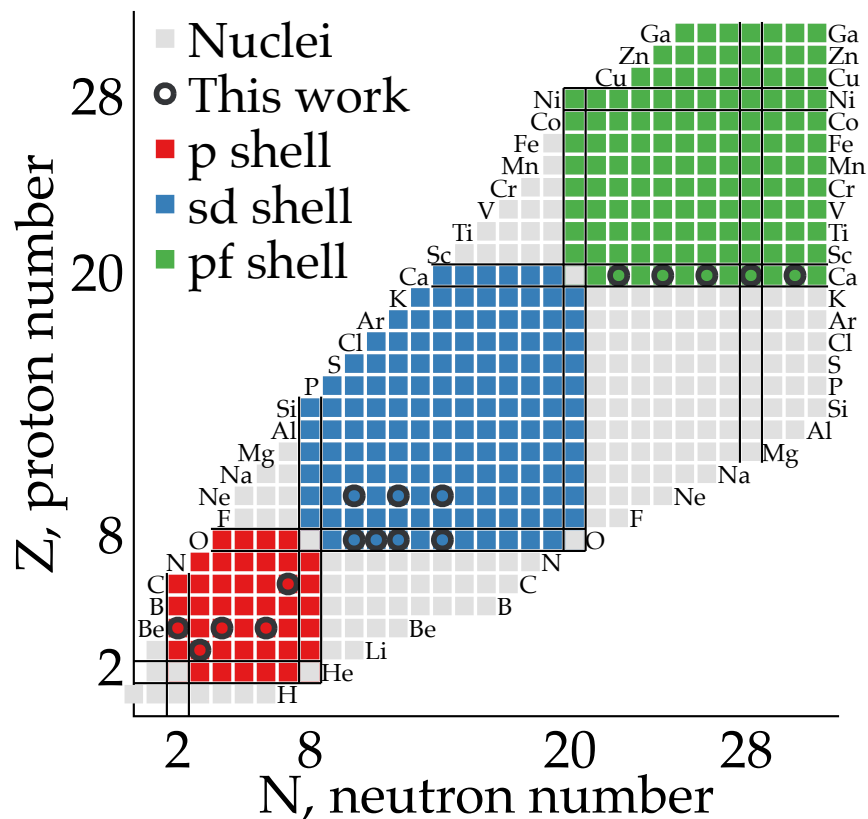
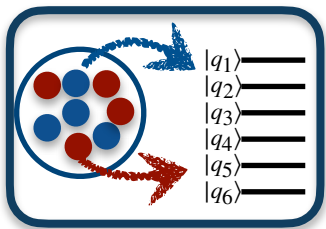
Kiss, Papenbrock et al Phys. Rev. C **106** 034325 (2022)

Lacroix et al, Quantum computing with and for many-body physics, EPJA **59** 227 (2023)

• Our strategy

- Can we **beat exponential scaling**?
- Does it work **across shells**?
- **Quantify** resources with **classical** simulations

Jordan-Wigner mapping



$$|0_\alpha\rangle \mapsto n_\alpha = 0 \quad |1_\alpha\rangle \mapsto n_\alpha = 1$$

$0f_{5/2}$	<u>19</u>	<u>18</u>	<u>17</u>	<u>16</u>	<u>15</u>	<u>14</u>	
$1p_{1/2}$			<u>13</u>	<u>12</u>			
$1p_{3/2}$		<u>11</u>	<u>10</u>	<u>9</u>	<u>8</u>		
$0f_{7/2}$	<u>7</u>	<u>6</u>	<u>5</u>	<u>4</u>	<u>3</u>	<u>2</u>	<u>1</u> <u>0</u>

pf

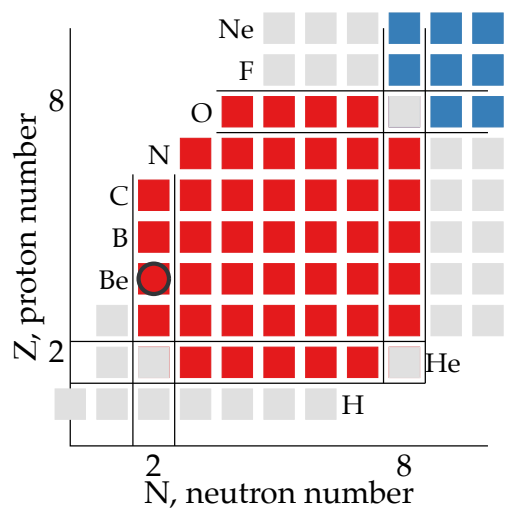
$0d_{3/2}$		<u>11</u>	<u>10</u>	<u>9</u>	<u>8</u>		
$1s_{1/2}$			<u>7</u>	<u>6</u>			
$0d_{5/2}$	<u>5</u>	<u>4</u>	<u>3</u>	<u>2</u>	<u>1</u>	<u>0</u>	

sd

$0p_{1/2}$			<u>5</u>	<u>4</u>			
$0p_{3/2}$		<u>3</u>	<u>2</u>	<u>1</u>	<u>0</u>		
m	$-\frac{7}{2}$	$-\frac{5}{2}$	$-\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{5}{2}$ $\frac{7}{2}$

p

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


 ${}^6\text{Be}$

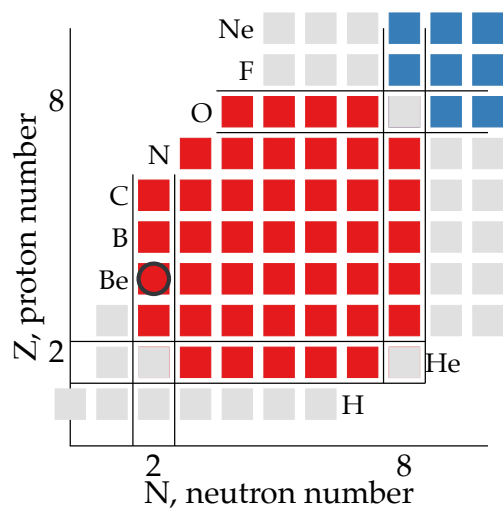
$$\begin{array}{l}
 |0_0\rangle \\
 |0_1\rangle \\
 |0_2\rangle \\
 |0_3\rangle \\
 |0_4\rangle \\
 |0_5\rangle
 \end{array}
 \begin{array}{c}
 \boxed{X} \\
 \\
 \\
 \boxed{X} \\
 \\
 \\
 \end{array}
 \begin{array}{l}
 |1_1\rangle \\
 \\
 \\
 |1_4\rangle \\
 \\
 \\
 \end{array}$$

$$|100100\rangle$$

$0p_{1/2}$		5	4	
$0p_{3/2}$	2	2	1	0
m	$-\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$

- **Minimum energy** Slater determinant
- Other options: Hartree-Fock state or random (see later)

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


 ${}^7\text{Be}$

$$|0_0\rangle \xrightarrow{\boxed{X}} |1_1\rangle$$

$$|0_1\rangle \xrightarrow{\quad} \quad$$

$$|0_2\rangle \xrightarrow{\quad} \quad$$

$$|0_3\rangle \xrightarrow{\boxed{X}} |1_4\rangle$$

$$|0_4\rangle \xrightarrow{\quad} \quad$$

$$|0_5\rangle \xrightarrow{\boxed{\text{Gaussian}}} \quad$$

$$|100101\rangle$$

$0p_{1/2}$		5	4	
$0p_{3/2}$	2	2	1	0
m	$-\frac{3}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{3}{2}$

- **Minimum energy** Slater determinant
- Other options: Hartree-Fock state or random (see later)

PHYSICAL REVIEW LETTERS **120**, 210501 (2018)

Suggestion

Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,¹ A. J. McCaskey,² G. Hagen,^{3,4} G. R. Jansen,^{5,3} T. D. Morris,^{4,3} T. Papenbrock,^{4,3,*}
R. C. Pooser,^{1,4} D. J. Dean,³ and P. Lougovski^{1,†}Operator pool

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

 Δ operators (respecting symmetry)

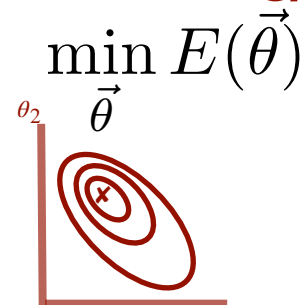
Nucleus	Z	N	Z _{val}	N _{val}	dim($\mathcal{H}$)	Δ
⁶ He	2	4	0	2	5	8
⁶ Be	4	2	2	0		
⁶ Li	3	3	1	1	10	45
⁸ Li	3	5	1	3	28	129
⁸ B	5	3	3	1		
⁸ Be	4	4	2	2	51	145
¹⁰ Li	3	7	1	5	10	49
¹⁰ N	7	3	5	1		
¹⁰ Be	4	6	2	4	51	145
¹⁰ C	6	4	4	2		
¹⁰ B	5	5	3	3	84	145

1. Ansatz

$$|\psi(\vec{\theta})\rangle = e^{i \sum_{m=1}^{\Delta} \theta_m \hat{A}_m} |\psi_0\rangle$$

2. Choose ordering & Trotterize

$$|\psi(\vec{\theta})\rangle \approx \Pi_{m=1}^{\Delta} e^{i\theta_m \hat{A}_m} |\psi_0\rangle$$

3. Minimise the Δ -dim energy (classically)

PHYSICAL REVIEW LETTERS **120**, 210501 (2018)

Suggestion

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 Δ operators (respecting symmetry)

1. Ansatz

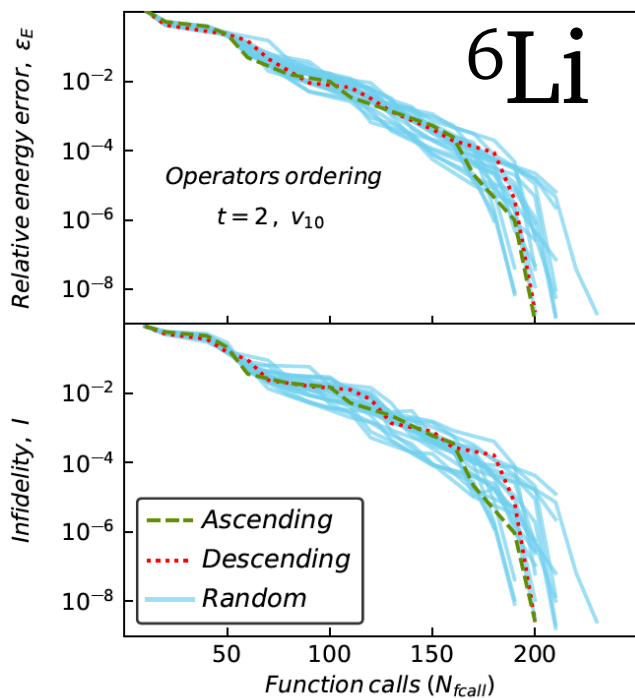
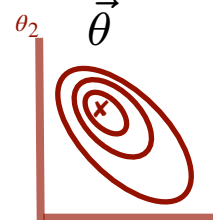
$$|\psi(\vec{\theta})\rangle = e^{i \sum_{m=1}^{\Delta} \theta_m \hat{A}_m} |\psi_0\rangle$$

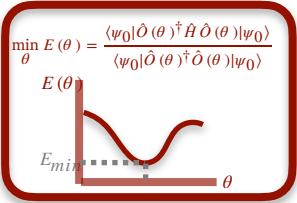
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$$|\psi(\vec{\theta})\rangle \approx \Pi_{m=1}^{\Delta} e^{i \theta_m \hat{A}_m} |\psi_0\rangle$$

3. Minimise the Δ -dim energy (classically)

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





Layer I

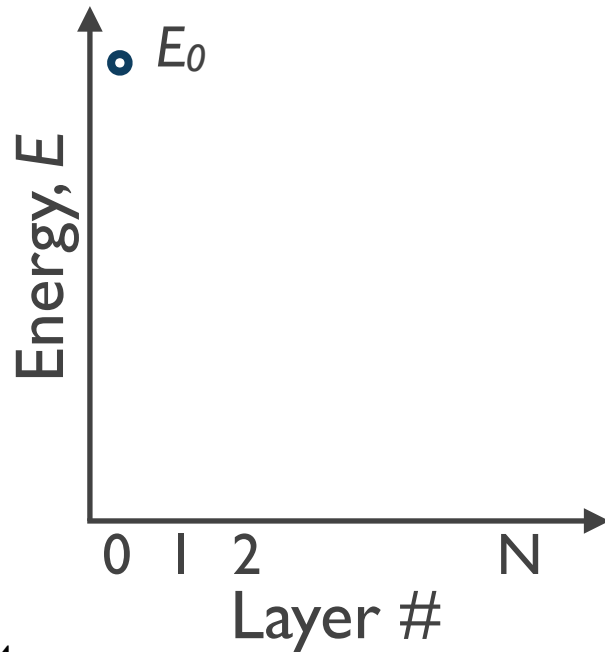
I. Ansatz

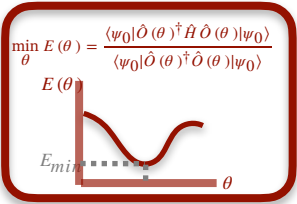
$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_k} |\psi_0\rangle$$

Operator pool

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

Δ operators (respecting symmetry)



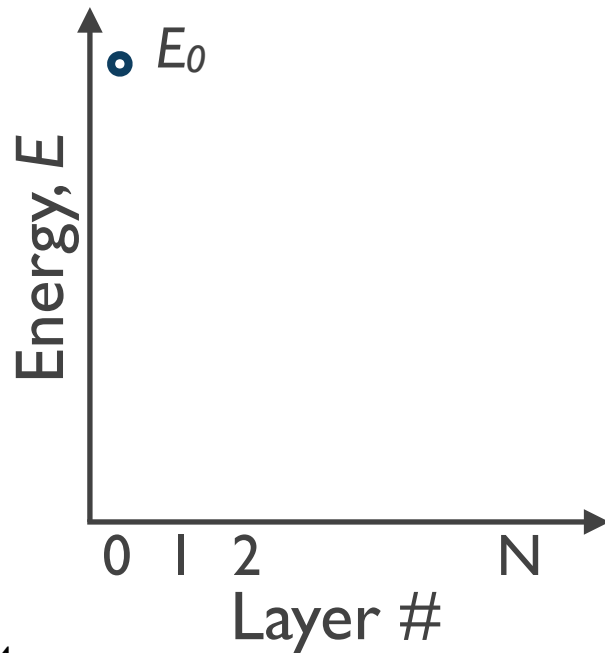


Layer I

Operator pool

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

Δ operators (respecting symmetry)



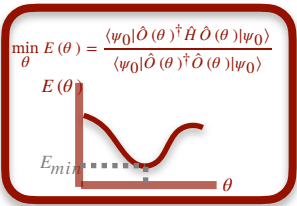
1. Ansatz

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

2. Compute gradients

for $k=1, \Delta$:

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

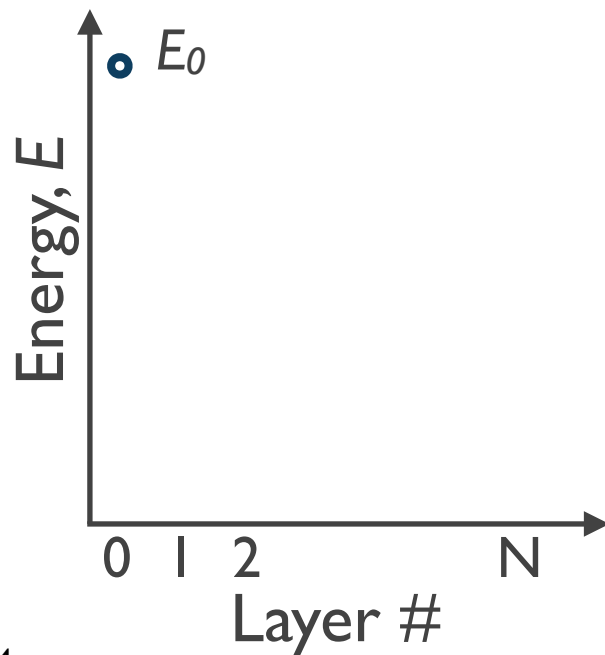


Layer 1

Operator pool

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

Δ operators (respecting symmetry)



1. Ansatz

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

2. Compute gradients

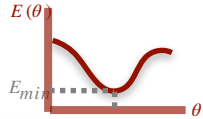
for $k=1, \Delta$:

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

3. Keep the operator with largest gradient

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

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

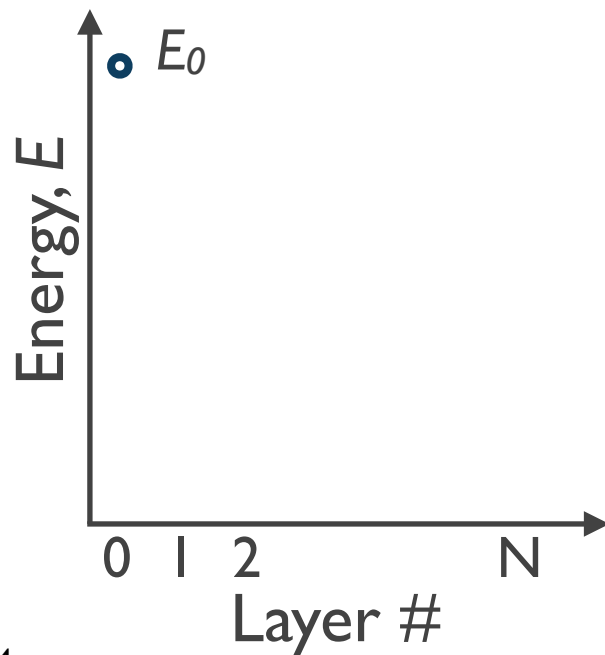


Layer I

Operator pool

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

Δ operators (respecting symmetry)



1. Ansatz

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

2. Compute gradients

for $k=1, \Delta$:

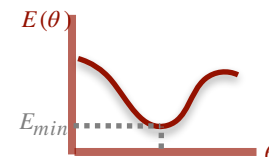
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

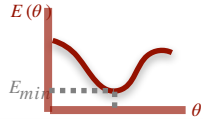
$$|\psi_1(\theta_1)\rangle = e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

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



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

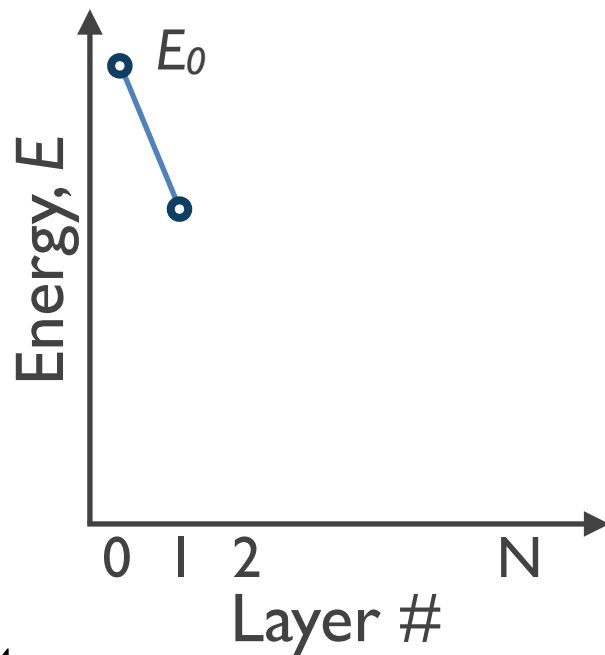


Layer 1

Operator pool

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

Δ operators (respecting symmetry)



1. Ansatz

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

2. Compute gradients

for $k=1, \Delta$:

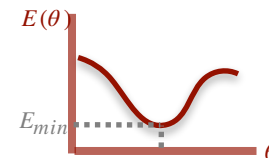
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

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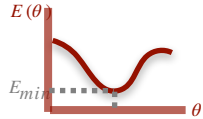
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4. Minimise the energy (classically)

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

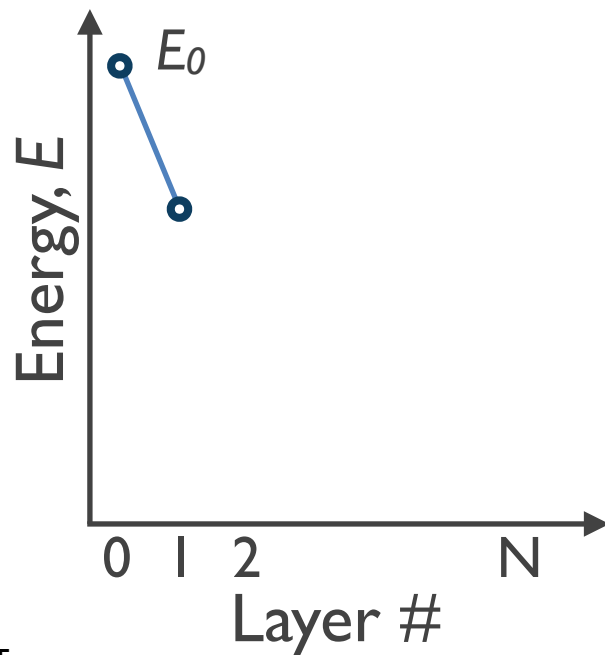


Layer 2

Operator pool

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

Δ operators (respecting symmetry)



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 $k=1, \Delta$:

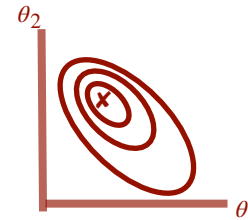
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

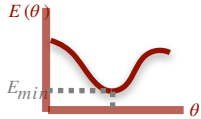
$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

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



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

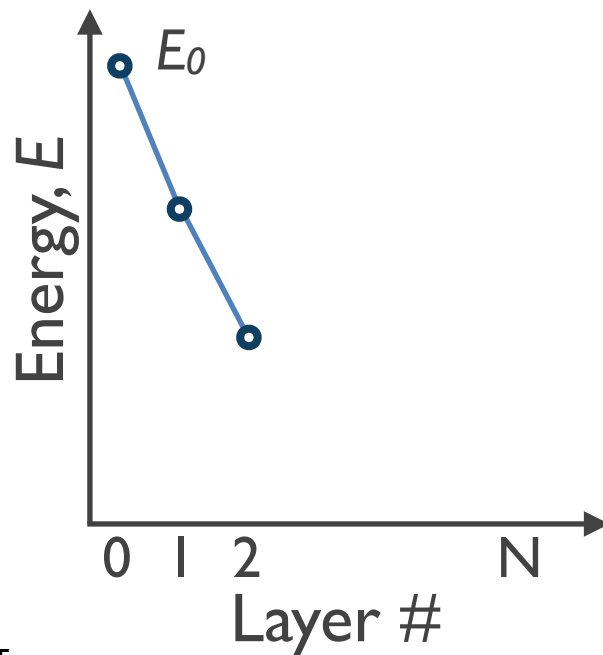


Layer 2

Operator pool

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

Δ operators (respecting symmetry)



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 $k=1, \Delta$:

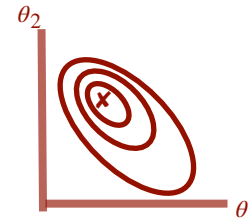
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

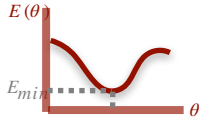
$$|\psi_2(\theta_1, \theta_2)\rangle = e^{i\theta_2 \hat{A}_{k_2}} e^{i\theta_1 \hat{A}_{k_1}} |\psi_0\rangle$$

4. Minimise the energy (classically)

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



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

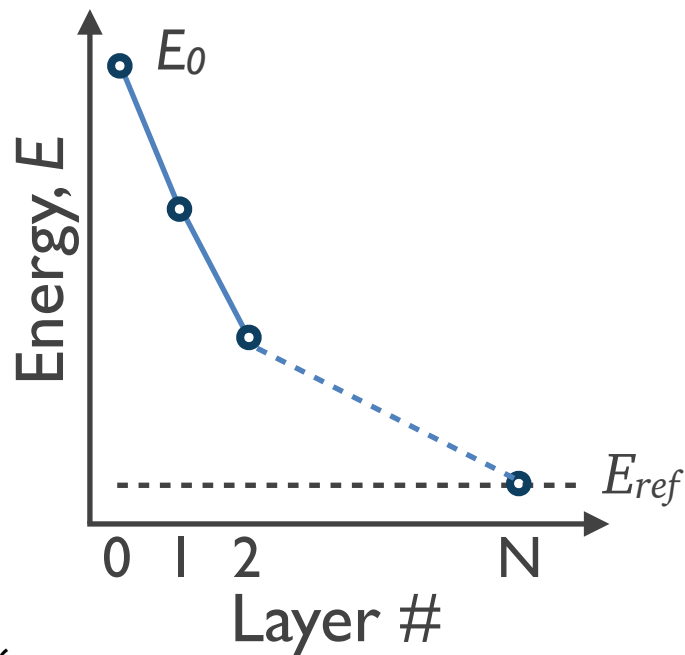


Layer N

Operator pool

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

Δ operators (respecting symmetry)



1. Ansatz

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

2. Compute gradients

for $k=1, M$:

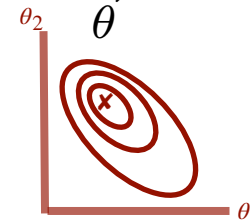
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

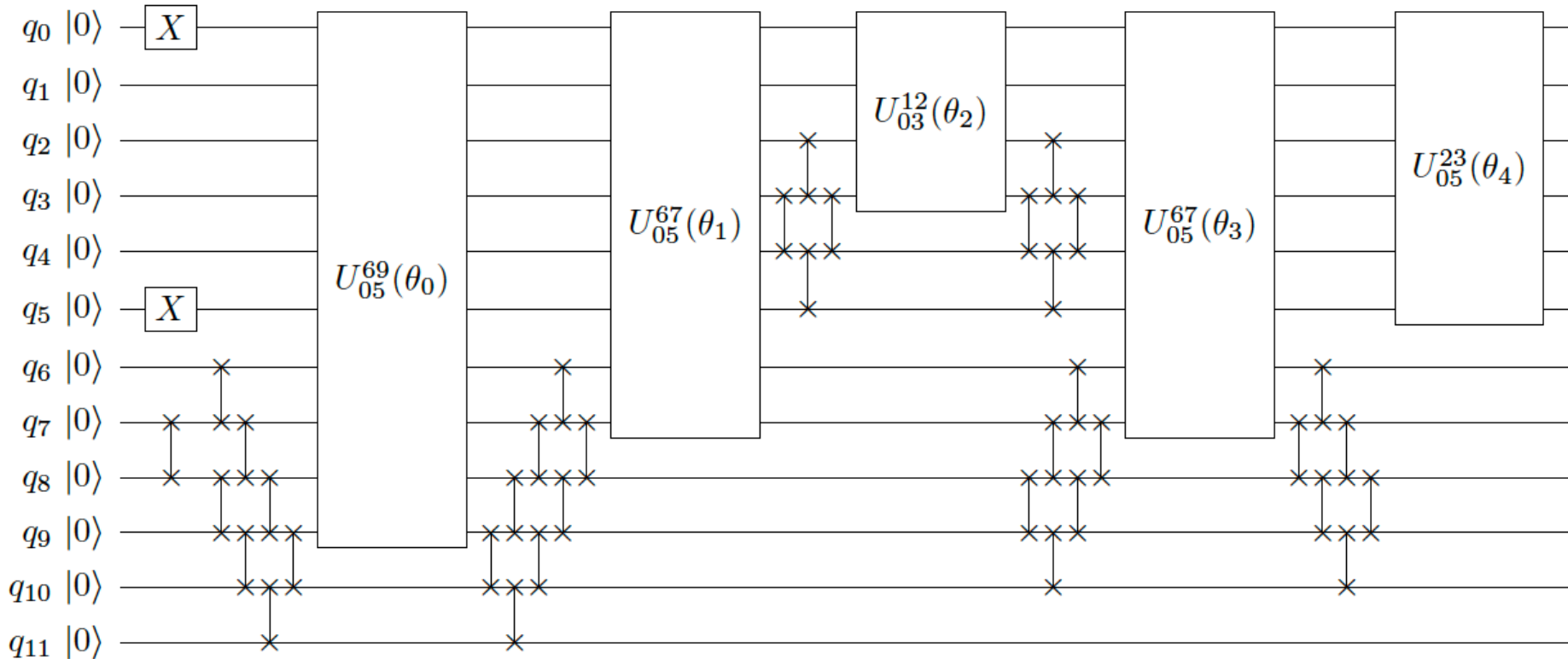
$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

4. Minimise the energy (classically)

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



Circuit for the ground state of ^{18}O



- 10^{-6} in energy with around 99 CNOTS/layer
- FSWAPS so operators act on adjacent qubits

1. Ansatz

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

2. Compute gradients

for $k=1, M$:

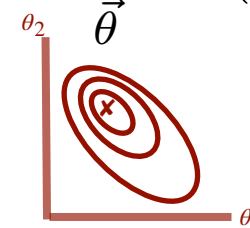
$$\left. \frac{\partial E}{\partial \theta_k} \right|_{\theta_k=0} = i \langle \psi(\theta) | [\hat{H}_{\text{eff}}, \hat{A}_k] | \psi(\theta) \rangle \Big|_{\theta_k=0}$$

3. Keep the operator with largest gradient

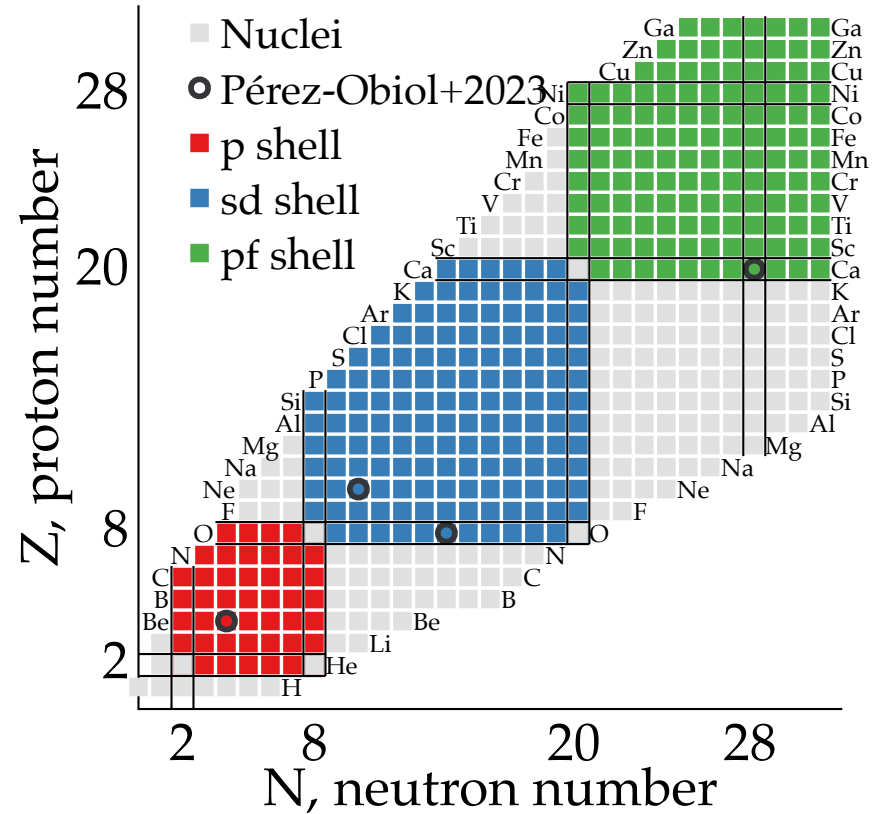
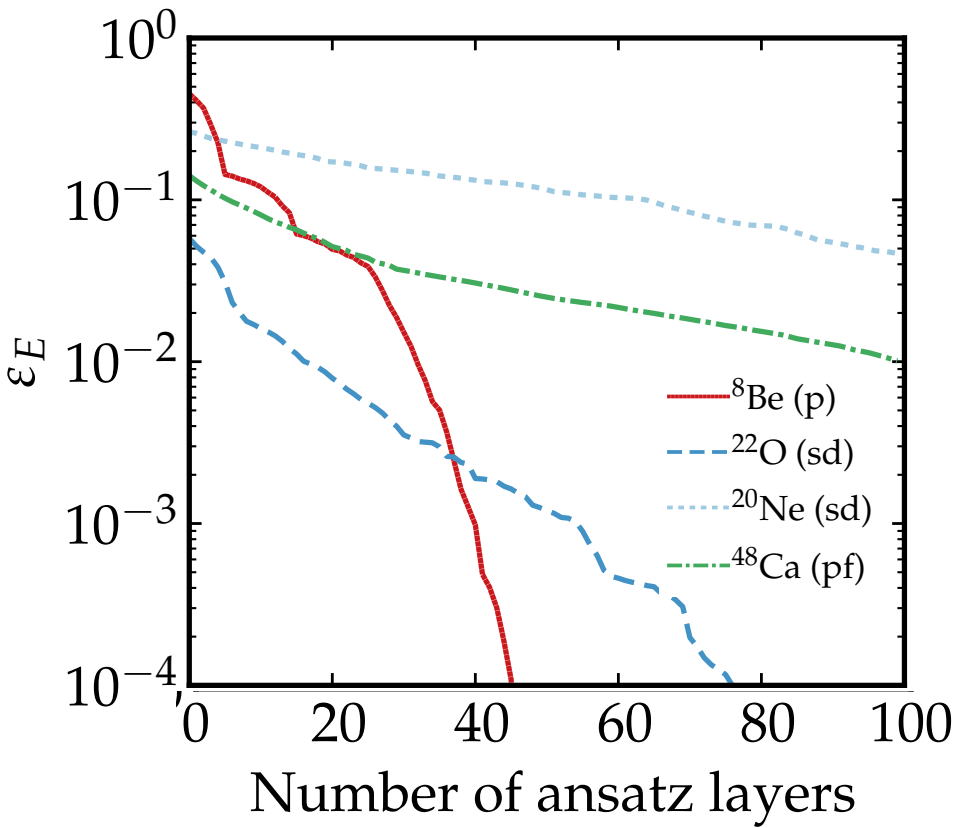
$$|\psi_N(\vec{\theta})\rangle = e^{i\theta_M \hat{A}_{k_N}} |\psi_{N-1}(\vec{\theta})\rangle$$

4. Minimise the energy (classically)

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

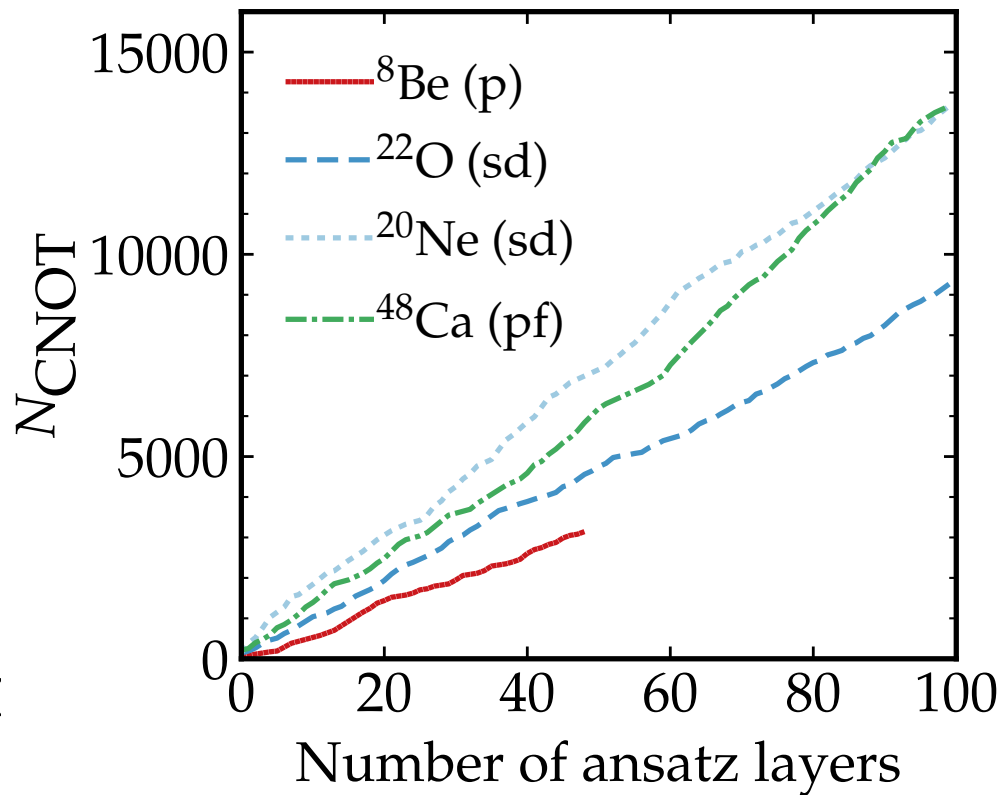
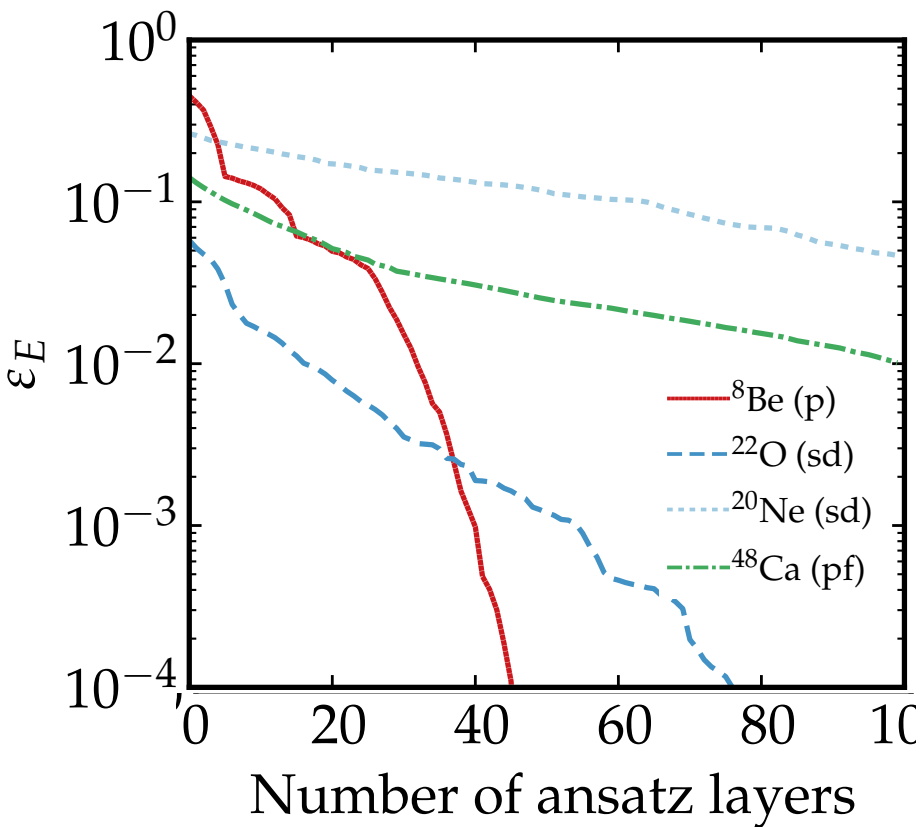


`scipy.optimize.
minimize`



Relative Energy

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

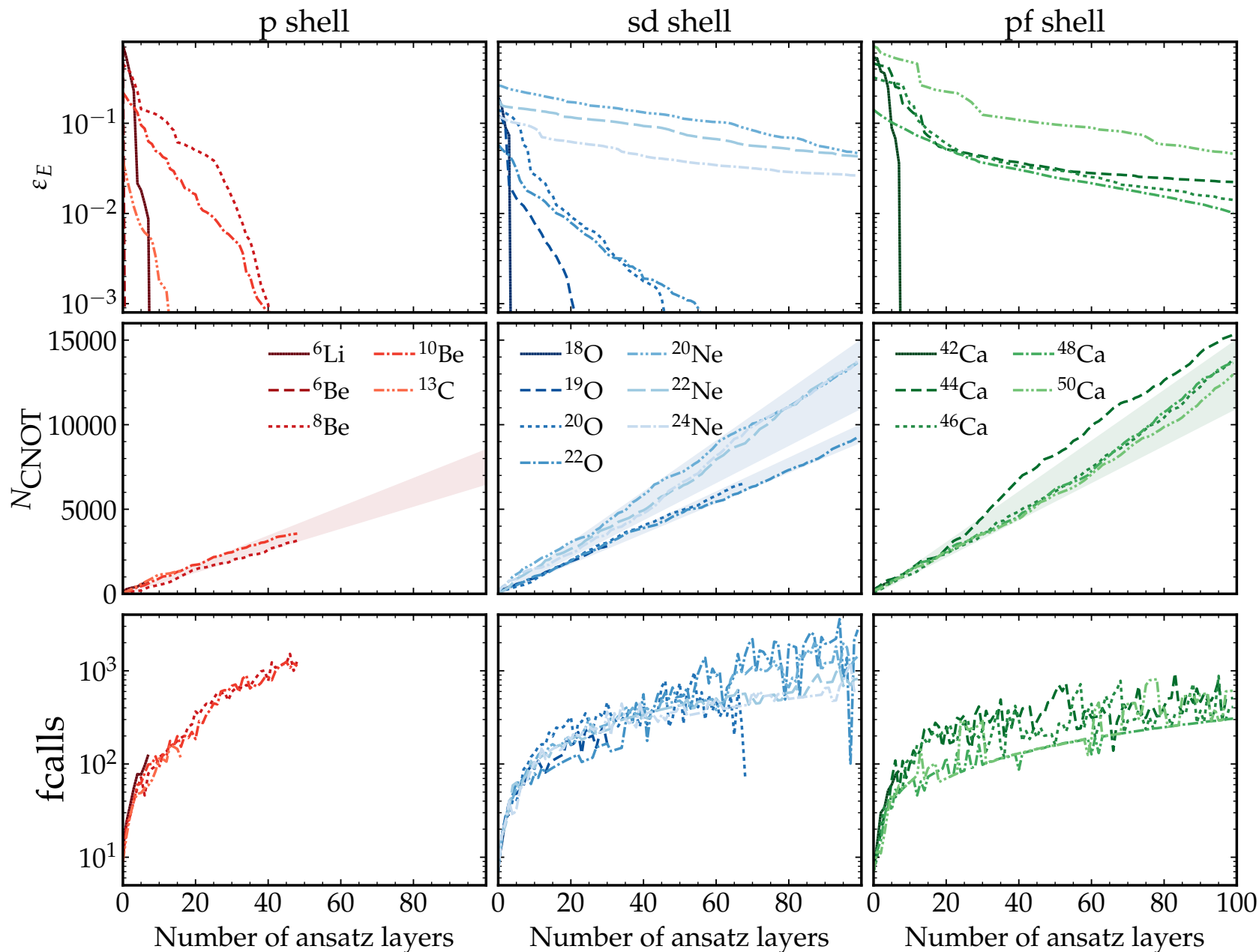


Relative Energy

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

N_{CNOT} is proxy for circuit depth
But also quantum complexity

Results: resources across shells



Number of operations

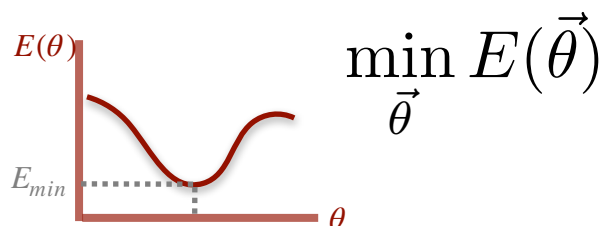
- What algorithm **costs more** in terms of quantum resources?
- Heuristic number of operations

ADAPT

- Δ operators (respecting symmetry)
- Layer I: requires I operators

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

- Layer I: I-dim minimisation



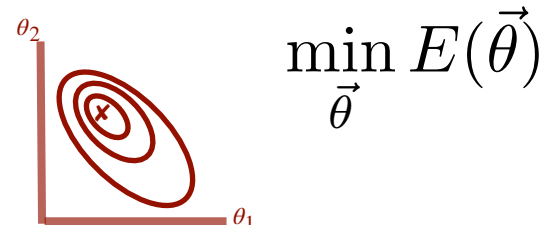
$$N_{\text{op}}^{\text{ADAPT}} = \text{fcalls}_1$$

UCC

- Δ operators (respecting symmetry)
- Ansatz requires Δ operators

$$|\psi(\vec{\theta})\rangle \approx \prod_{m=1}^{\Delta} e^{i\theta_m \hat{A}_m} |\psi_0\rangle$$

- Each iteration is a Δ -dim minimisation



$$N_{\text{op}}^{\text{UCC}} = \text{fcalls} \times \Delta$$

Number of operations

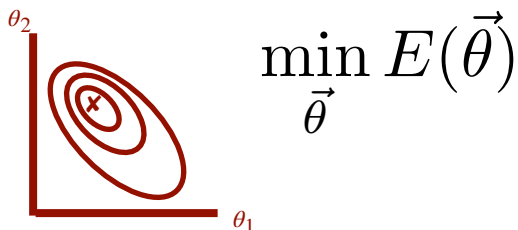
- What algorithm **costs more** in terms of quantum resources?
- Heuristic number of operations

ADAPT

- Δ operators (respecting symmetry)
- Layer 2: requires 2 operators

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

- Layer 2: 2-dim minimisation



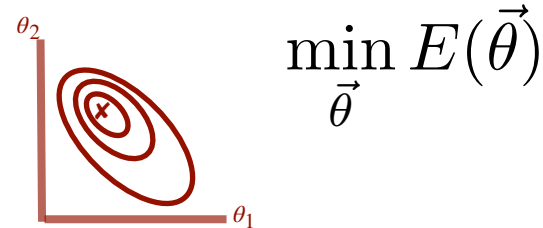
$$N_{\text{op}}^{\text{ADAPT}} = \sum_{i=1}^{N_{\text{layers}}} \text{fcalls}_i \times i$$

UCC

- Δ operators (respecting symmetry)
- Ansatz requires Δ operators

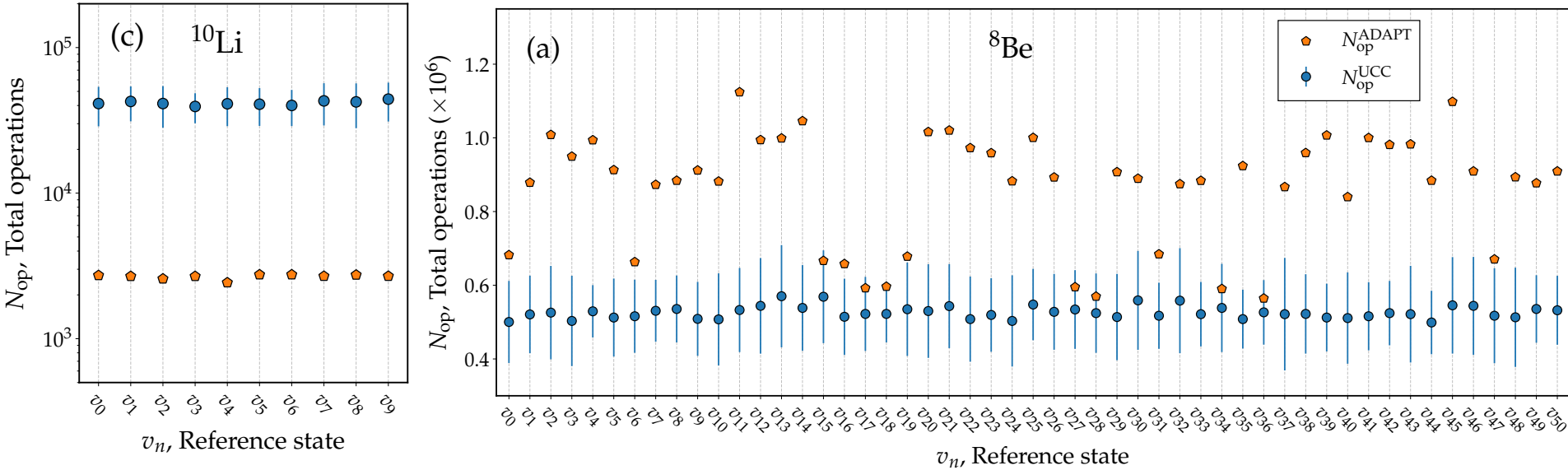
$$|\psi(\vec{\theta})\rangle \approx \prod_{m=1}^{\Delta} e^{i\theta_m \hat{A}_m} |\psi_0\rangle$$

- Each iteration is a Δ -dim minimisation



$$N_{\text{op}}^{\text{UCC}} = \text{fcalls} \times \Delta$$

Results: UCC vs ADAPT



Number of operations

$$N_{\text{op}}^{\text{ADAPT}} = \sum_{i=1}^{N_{\text{iter}}} \text{fcalls}_i \times i$$

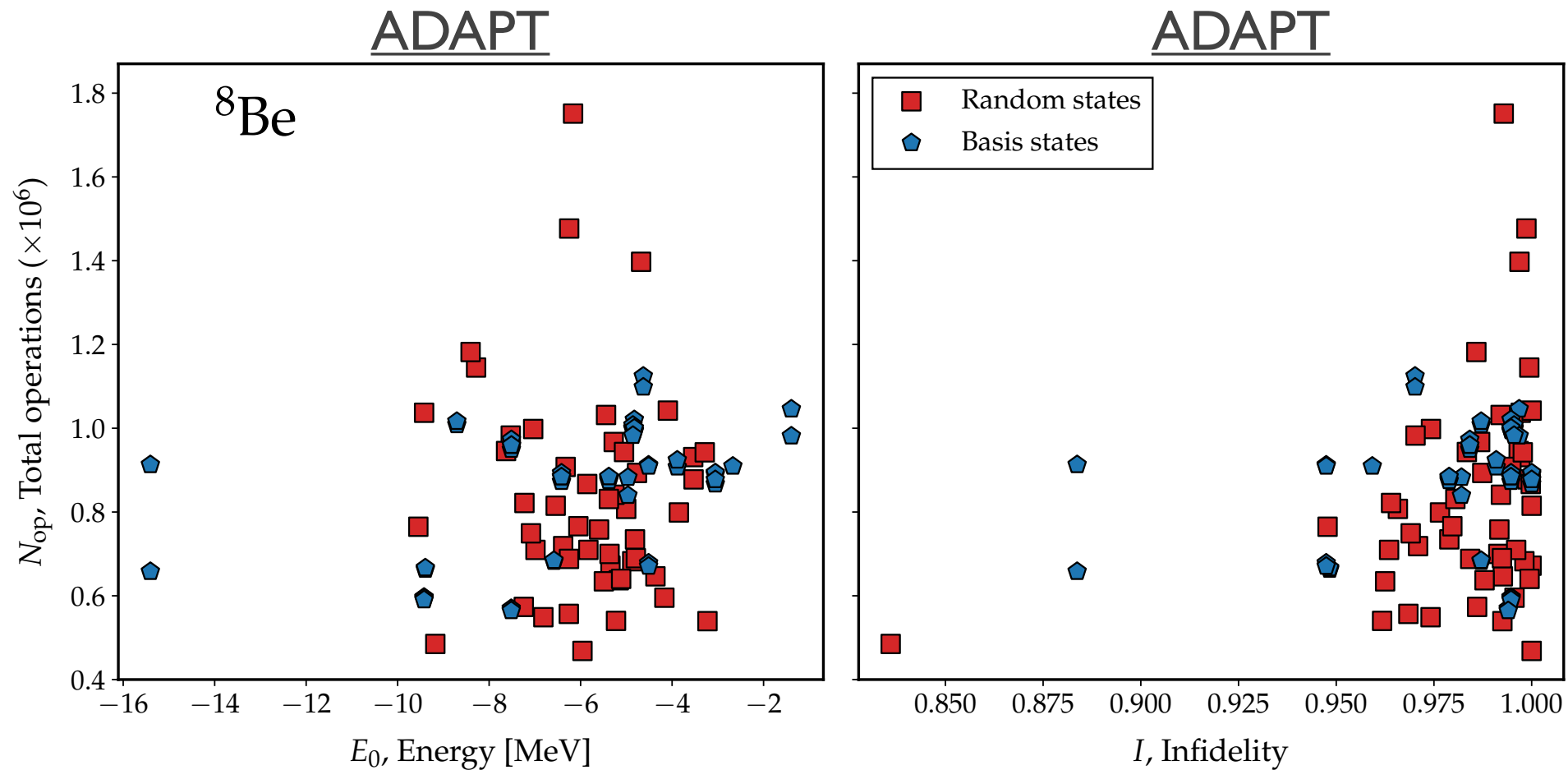
$$N_{\text{op}}^{\text{UCC}} = \text{fcalls} \times \Delta$$

- Dependence on reference state
- UCC: average over orderings and initialization



M Carrasco-Codina

Results: ADAPT reference state

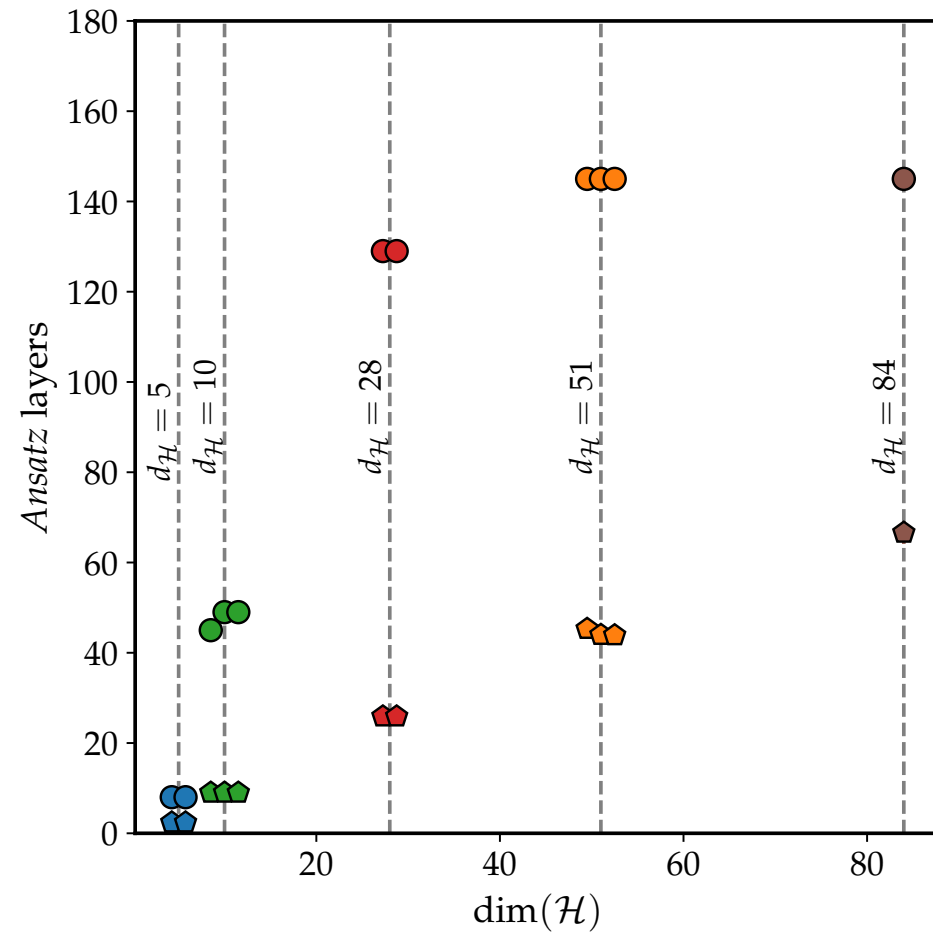
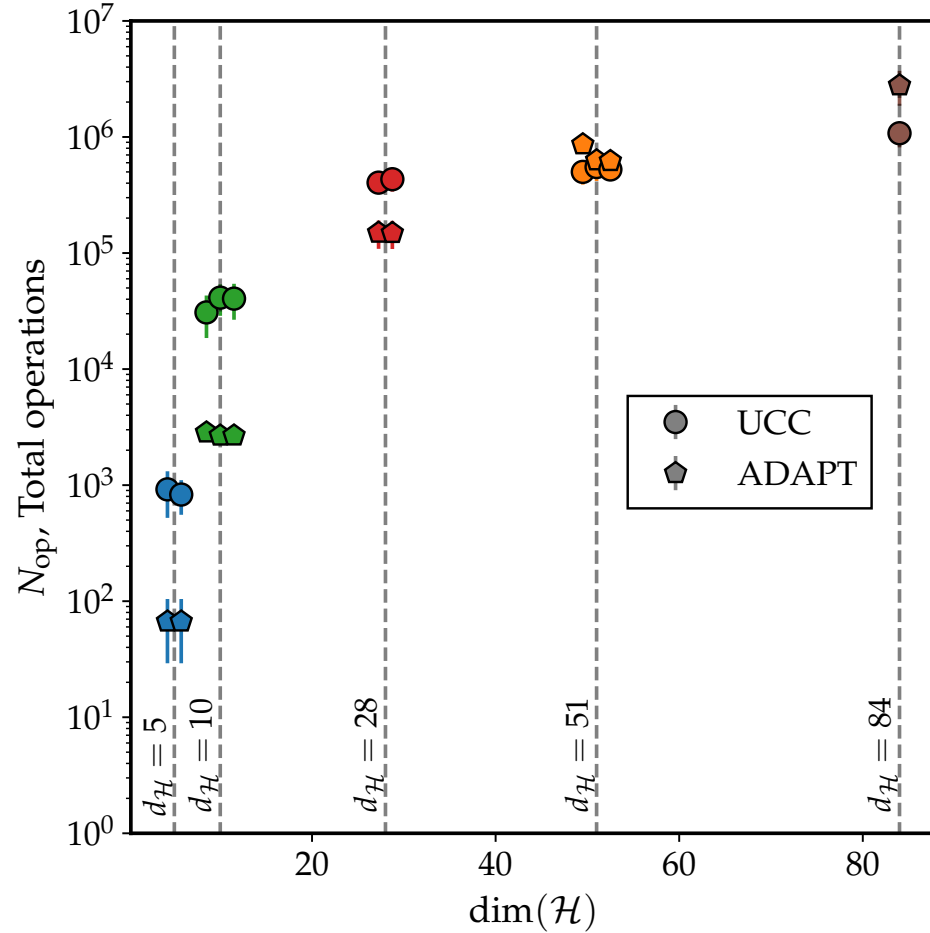


- No strong dependence with:
 - Reference state energy
 - Reference state overlap with benchmark



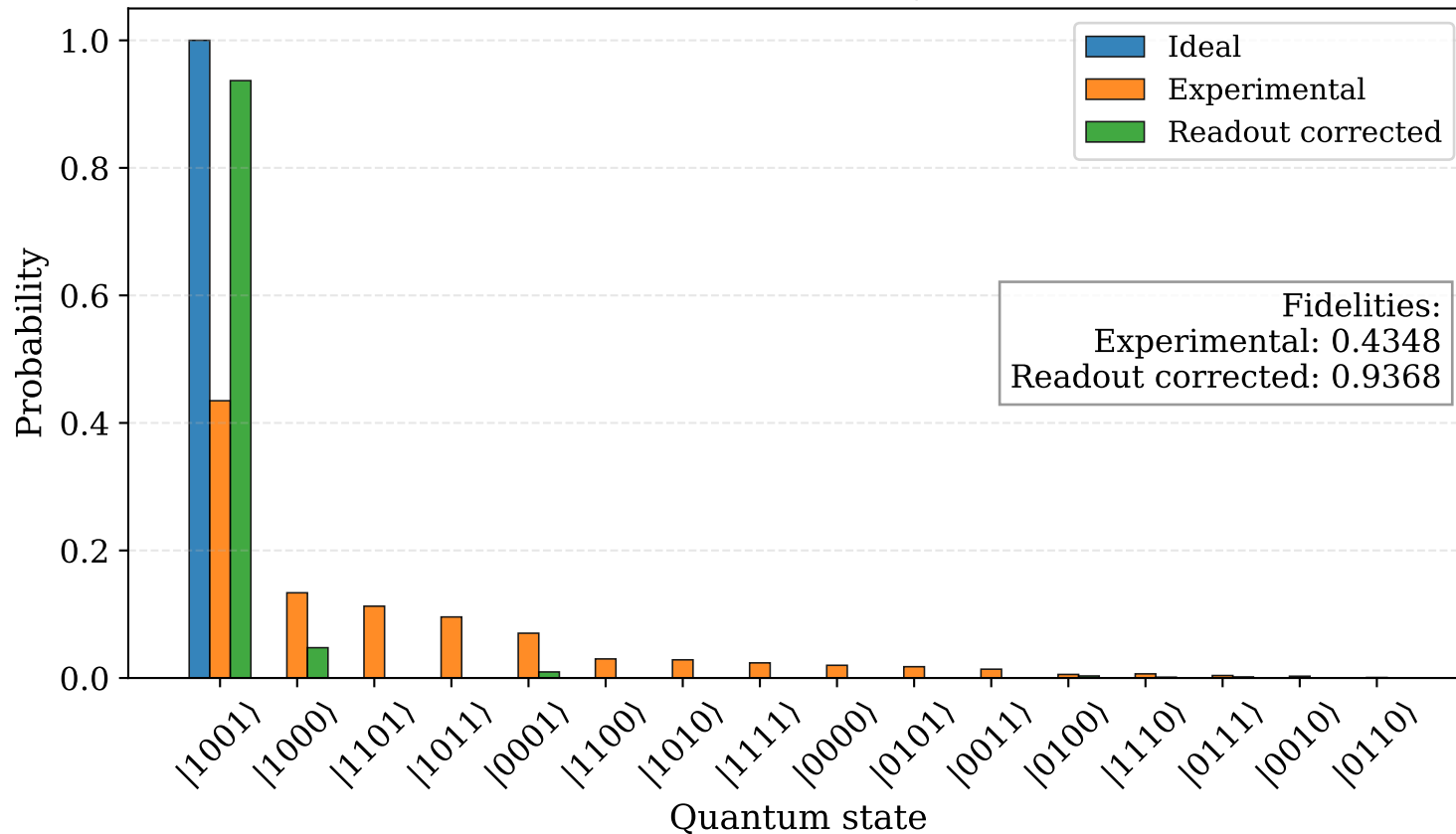
M Carrasco-Codina

Results: UCC vs ADAPT



Near closed shell: ADAPT **costs less** than UCC

Near mid-shell: UCC **costs less** than ADAPT

Reference state ${}^6\text{Be}$ reduced system ($1p_{3/2}$) (BSC Quantum Blue data)

MareNostrum Ona@BSC



A. Morón

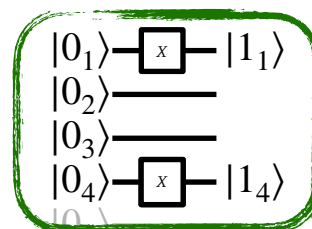
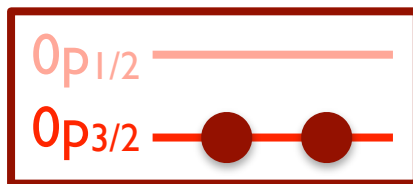


J. Ainaud

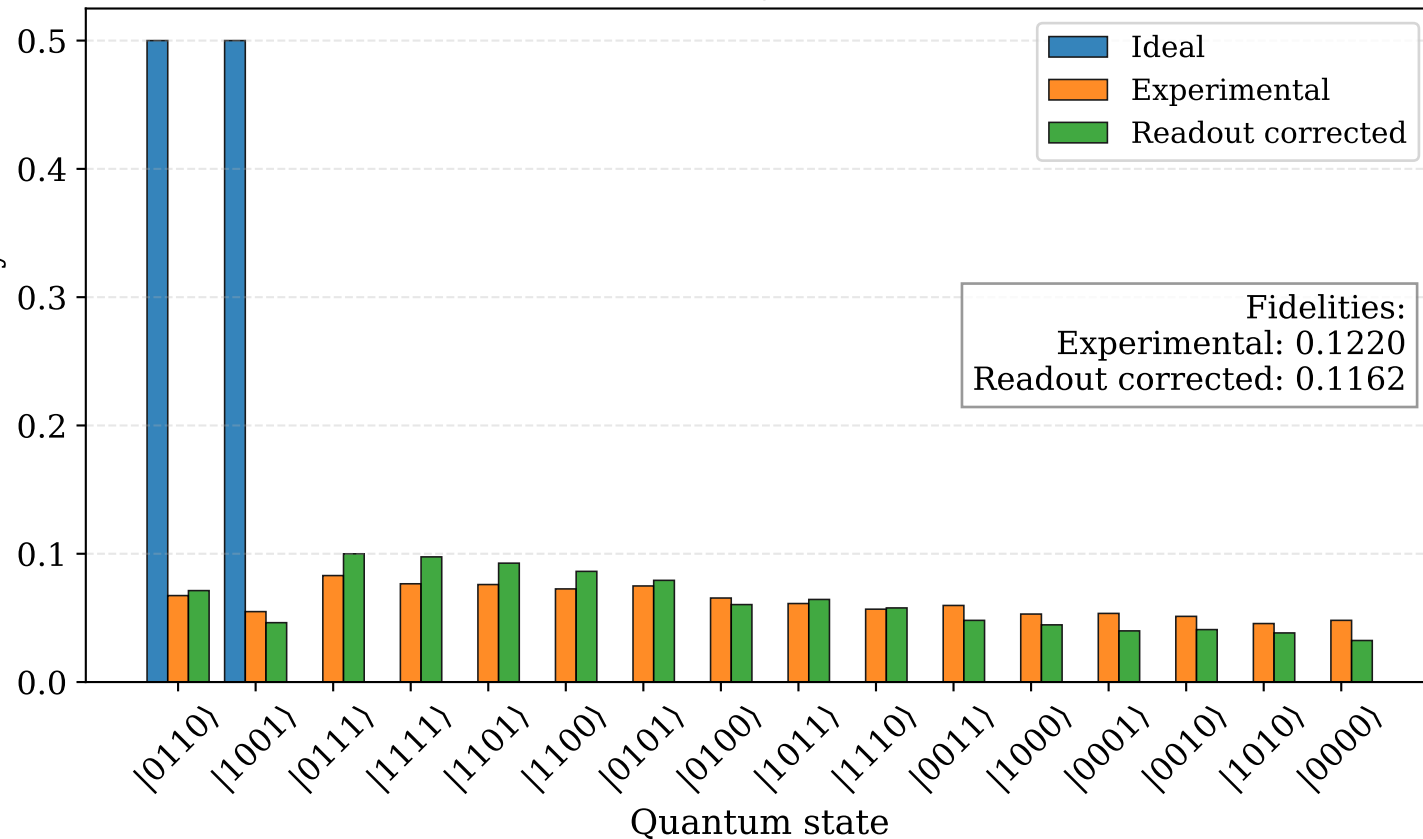


K. Gallego

Master's thesis, Arnau Morón (ongoing)

 ${}^6\text{Be}$ Valence
space $|1001\rangle$ $|06\rangle$

1 Layer ADAPT ^6Be reduced system ($1p_{3/2}$) opt. circuit (BSC Quantum Blue data MareNostrum Ona@BSC)



A. Morón



J. Ainaud

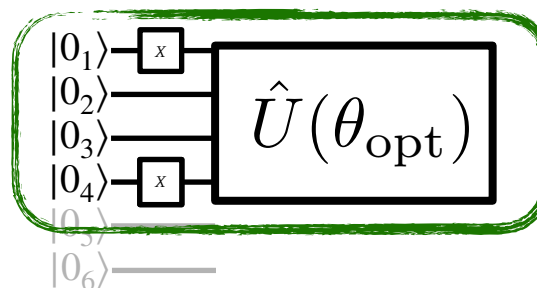
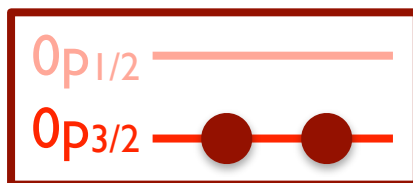


K. Gallego

Master's thesis, Arnau Morón (ongoing)

^6Be

Valence
space



- Nuclear shell model

- VQEs for nuclei

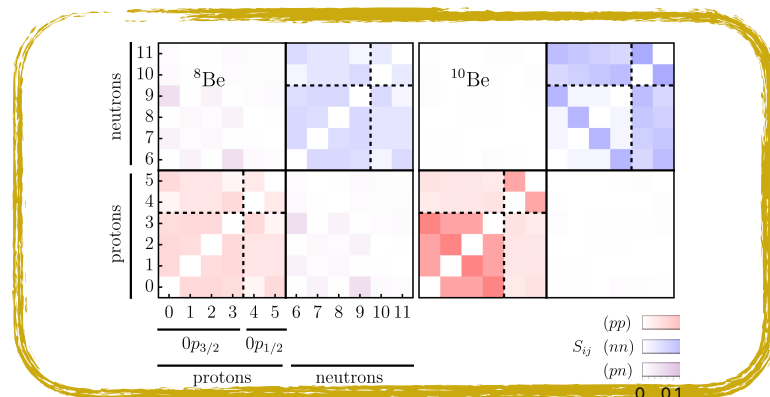
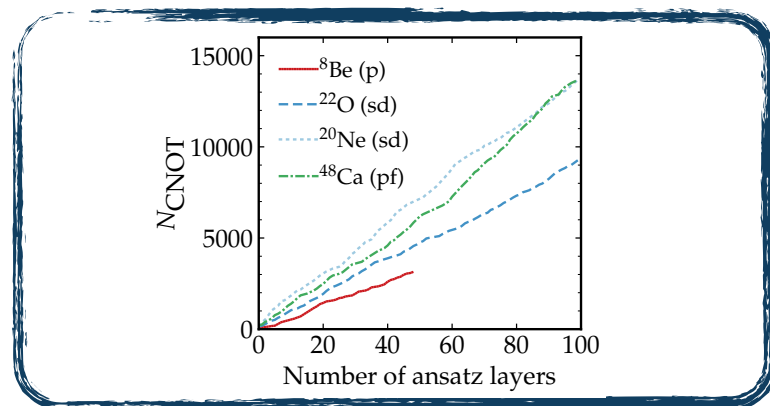
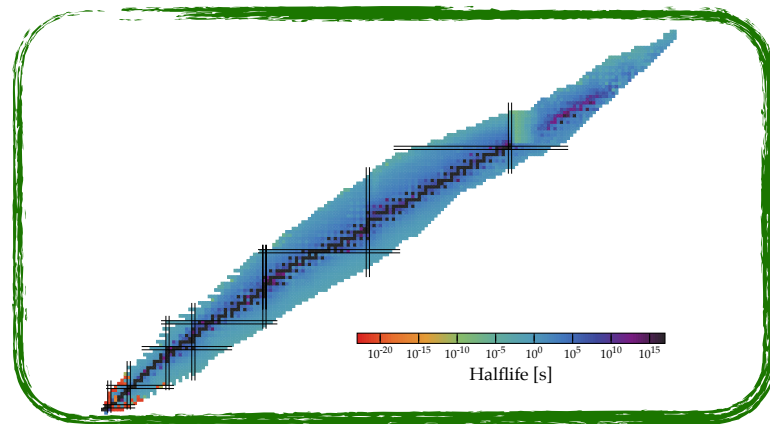
[Scientific Reports **13**, 12291 \(2023\)](#)

[EPJA **59**, 240 \(2023\)](#)

+ [arXiv:2409.04510](#) + [arXiv:2507.13819](#)

- Entanglement forging

[arXiv:2411.06954](#)



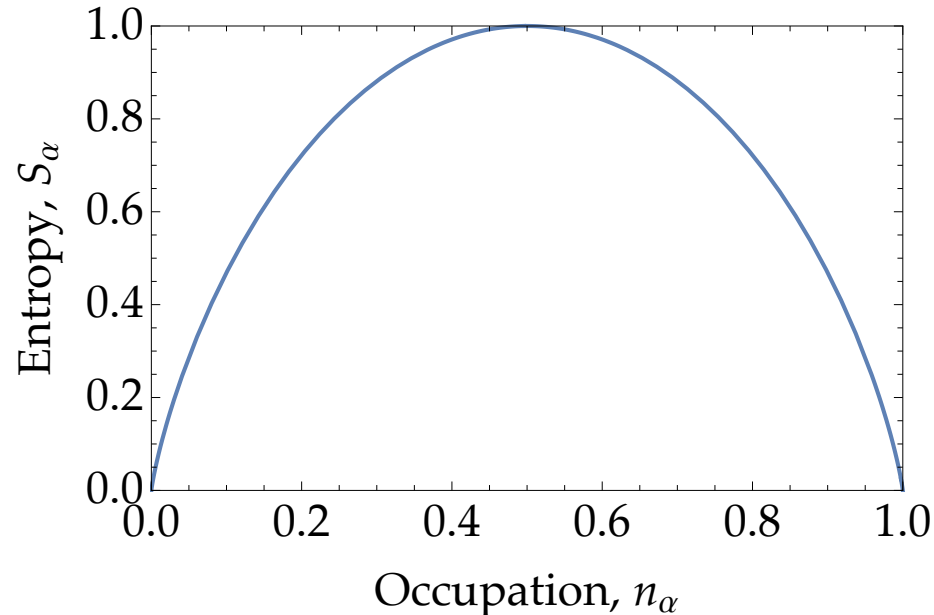
Single-orbital entanglement

- A is single-nucleon basis states
- B all other states

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

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

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



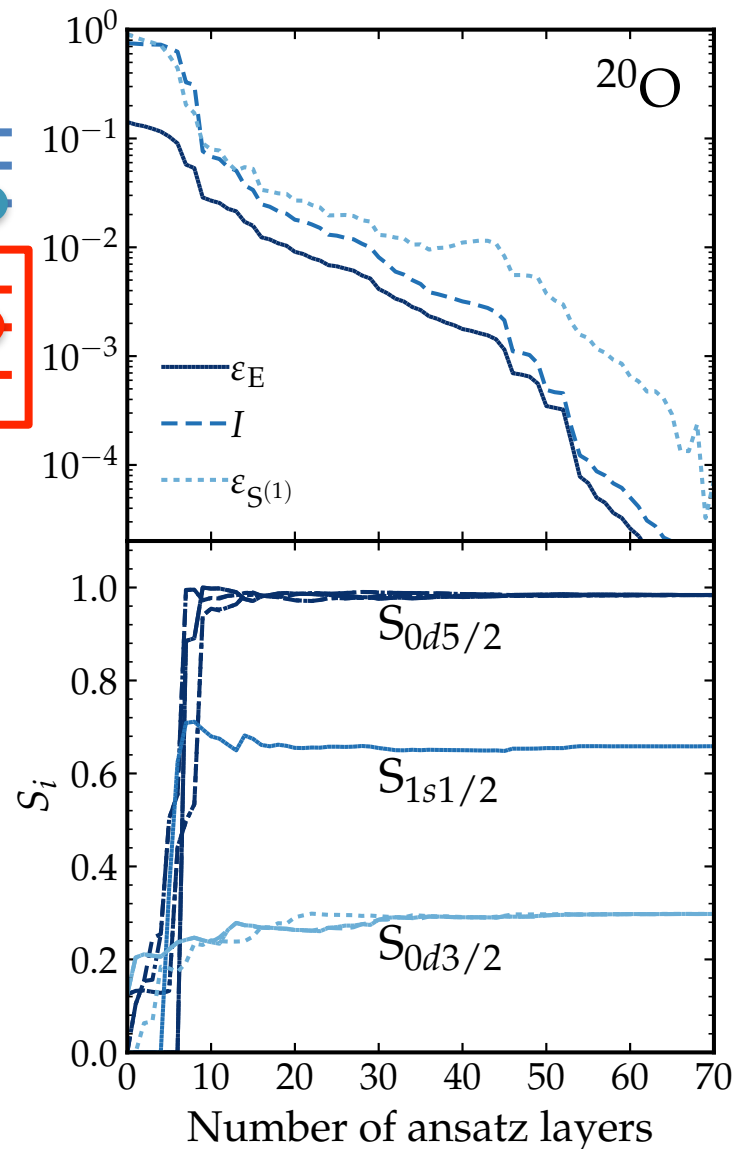
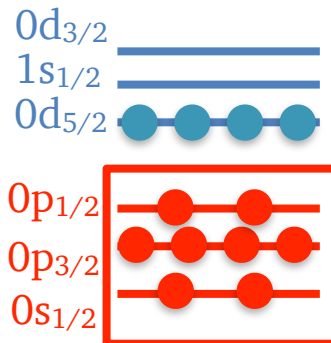
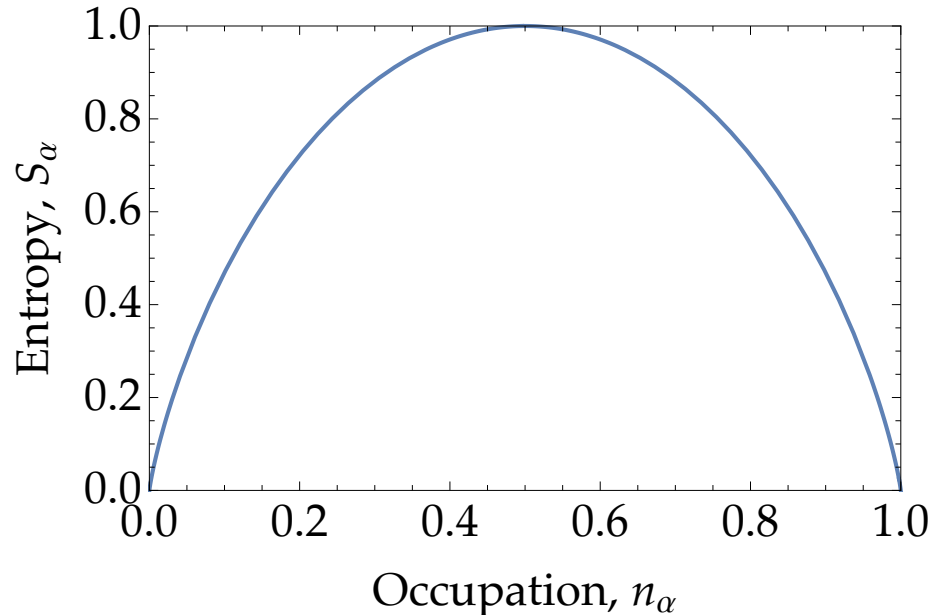
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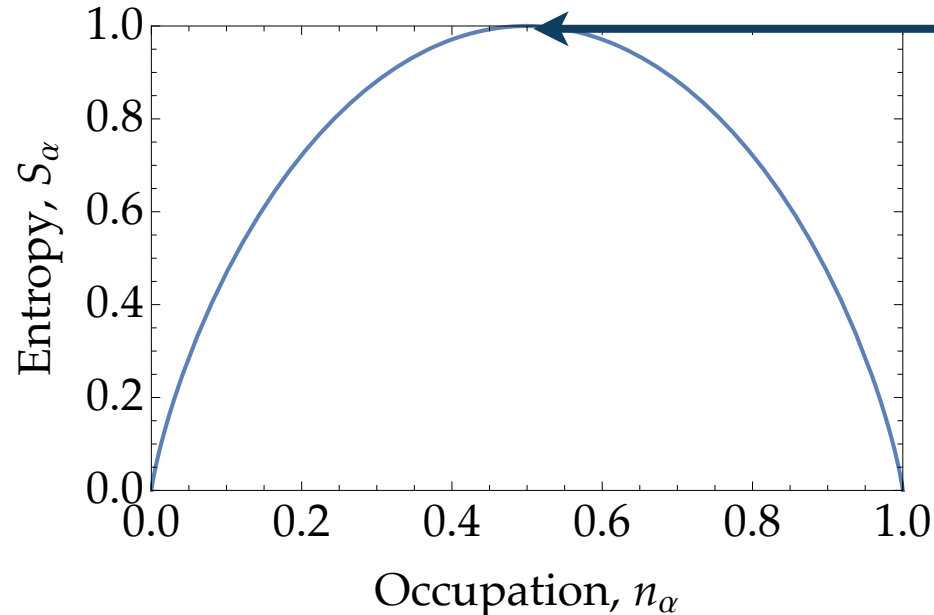
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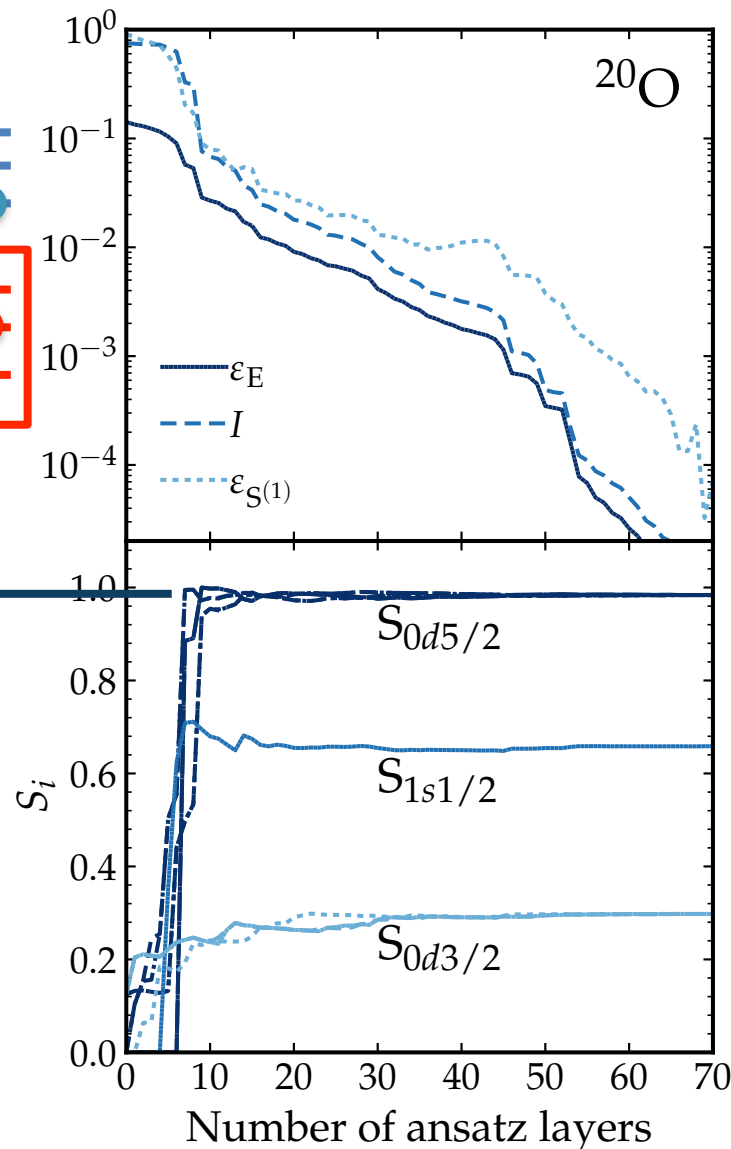
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$0d_{3/2}$
 $1s_{1/2}$
 $0d_{5/2}$

$0p_{1/2}$
 $0p_{3/2}$
 $0s_{1/2}$



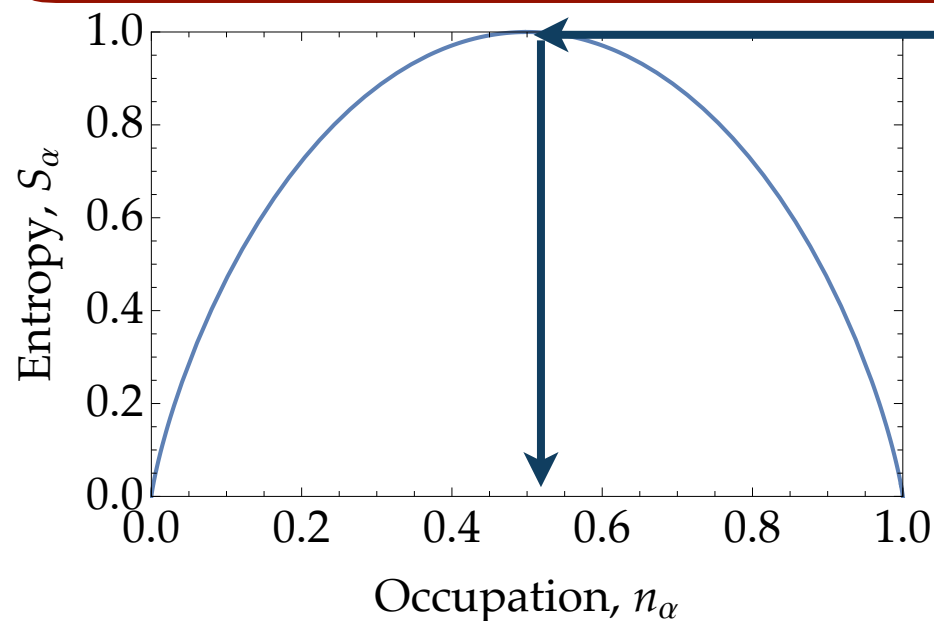
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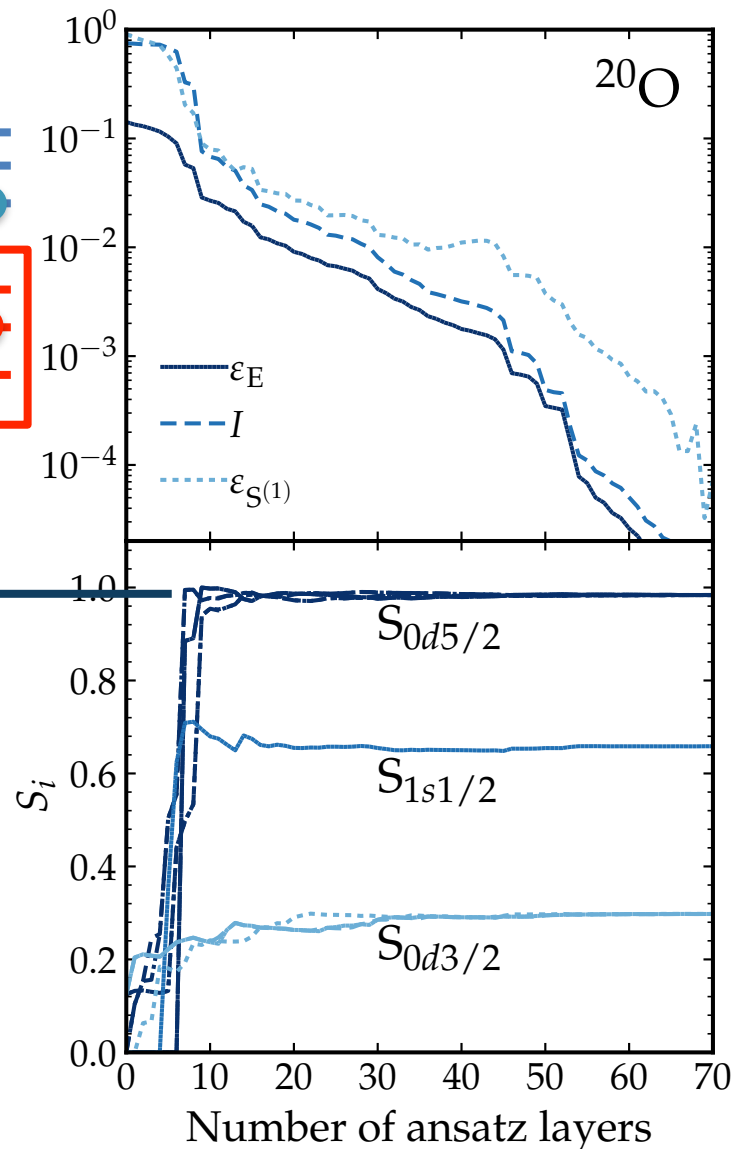
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$0d_{3/2}$
 $1s_{1/2}$
 $0d_{5/2}$

$0p_{1/2}$
 $0p_{3/2}$
 $0s_{1/2}$



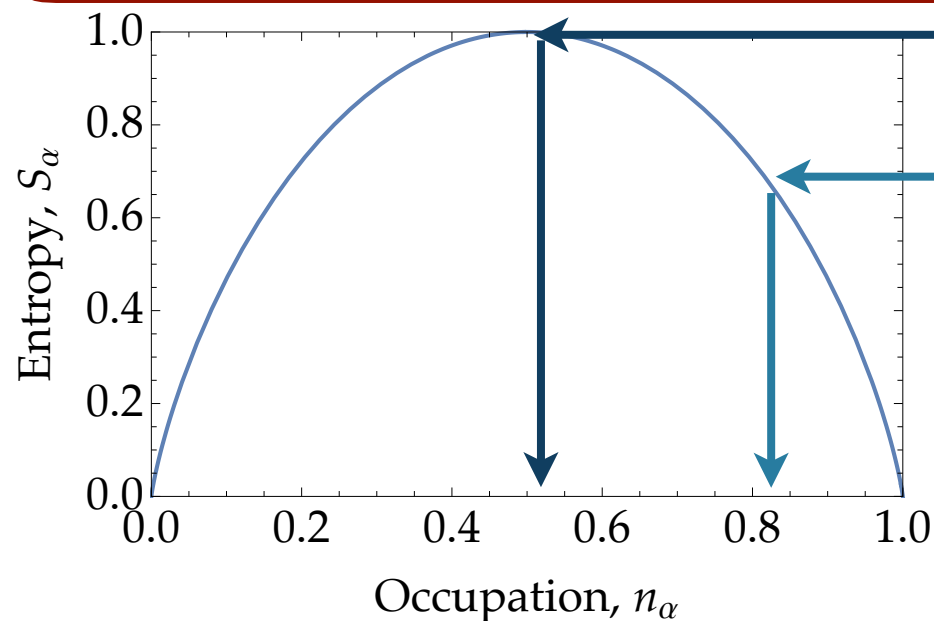
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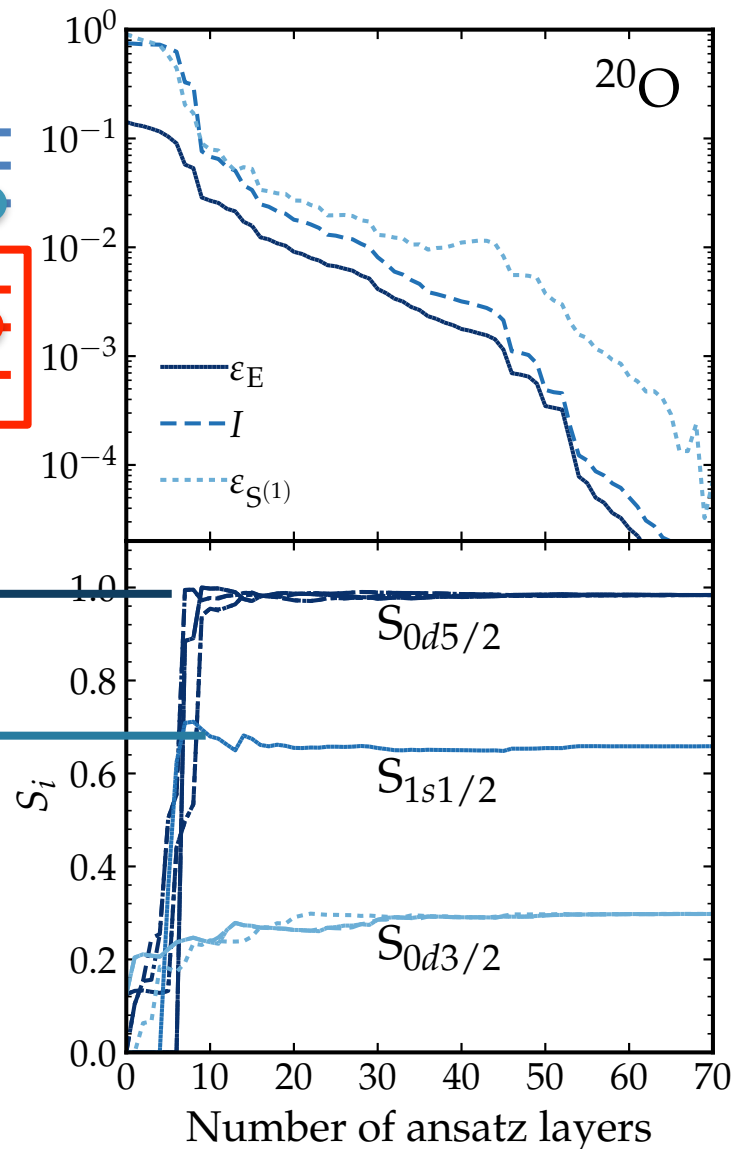
$$S(\hat{\rho}_A) = -\text{Tr} \hat{\rho}_A \log \hat{\rho}_A$$

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



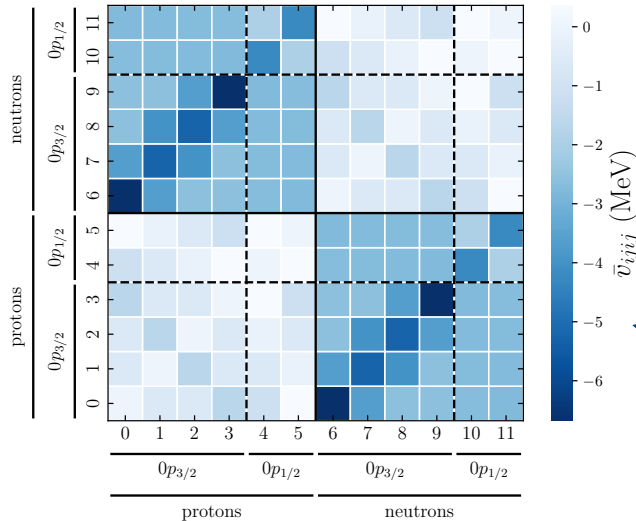
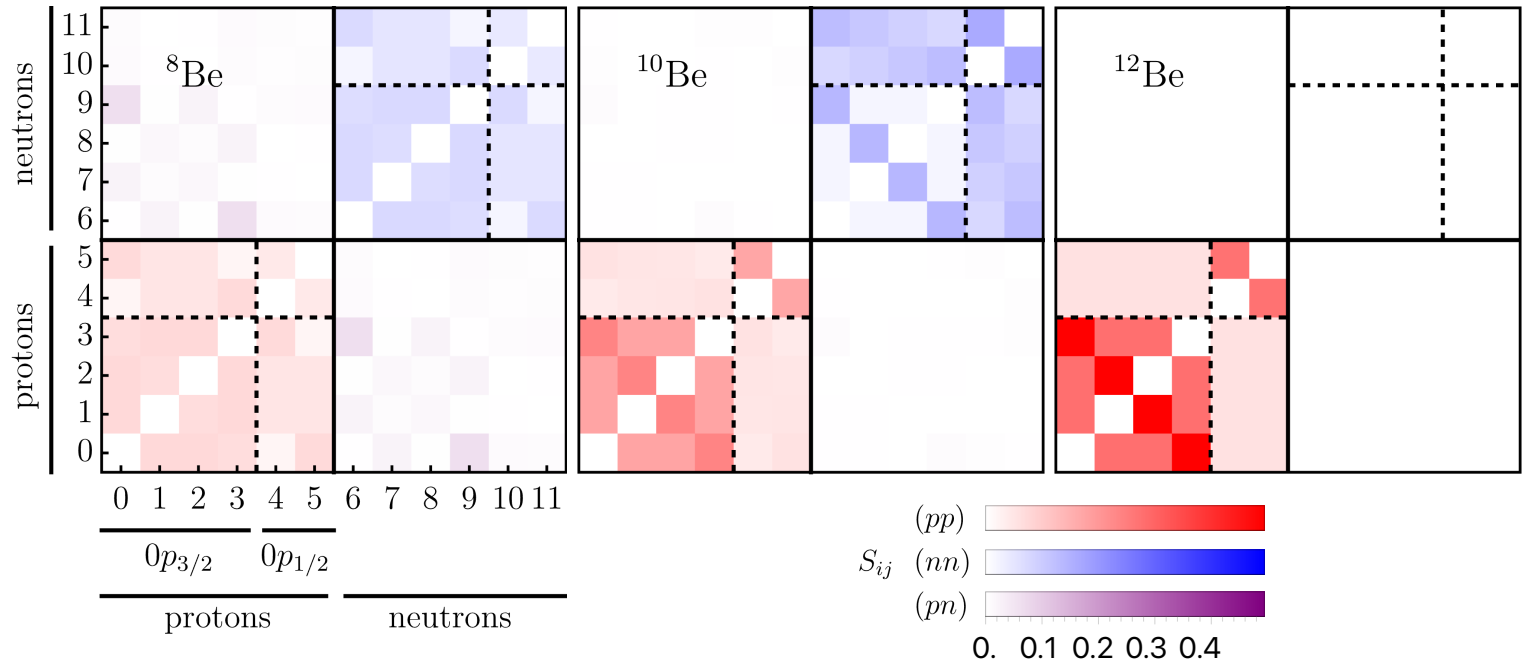
$0d_{3/2}$
 $1s_{1/2}$
 $0d_{5/2}$

$0p_{1/2}$
 $0p_{3/2}$
 $0s_{1/2}$



Mutual information

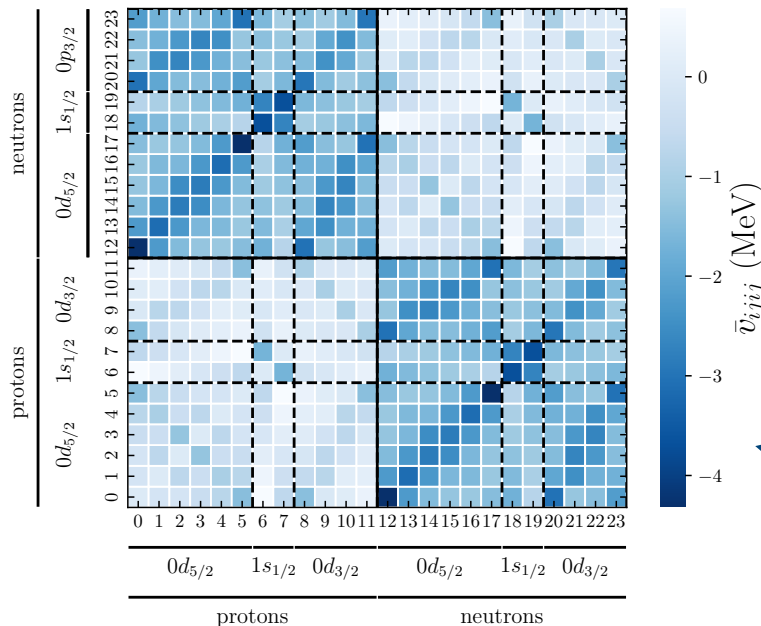
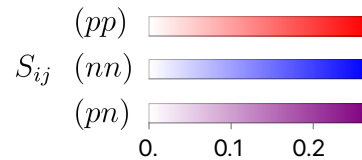
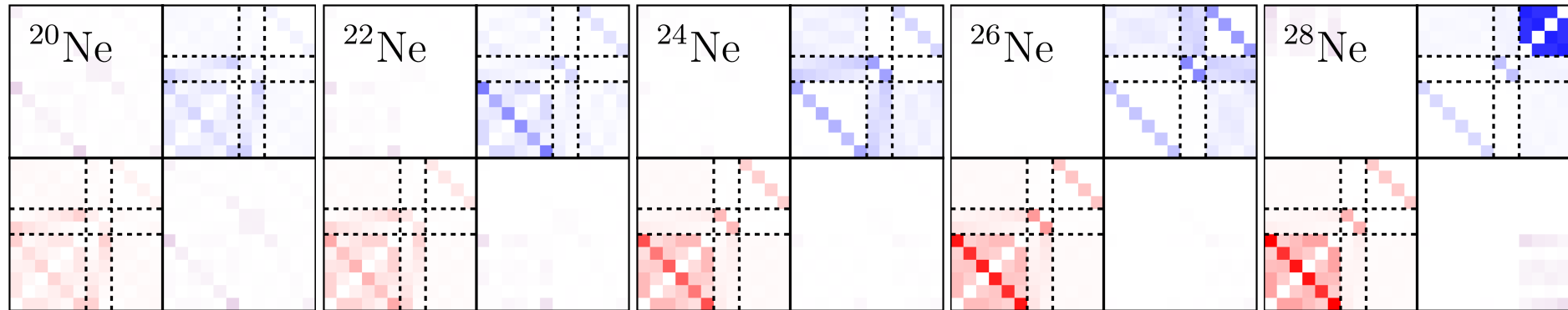
$$S(A; B) = S(A) - S(A|B) = S(A) + S(B) - S(AB)$$



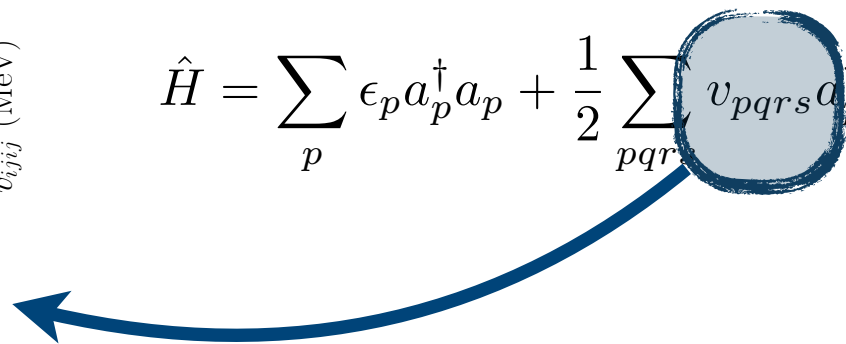
$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$$

Mutual information in nuclei

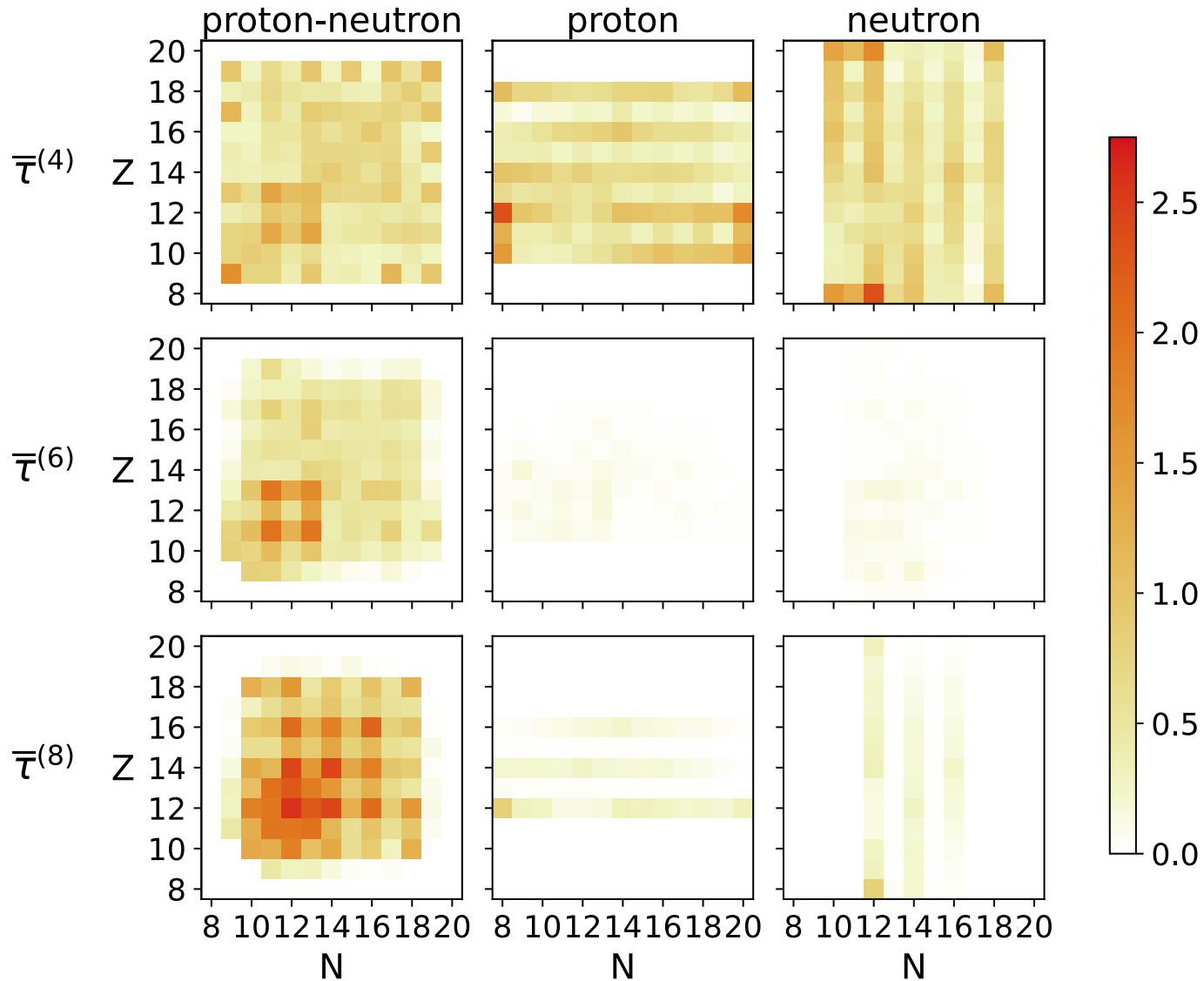
$$S(A; B) = S(A) - S(A|B) = S(A) + S(B) - S(AB)$$



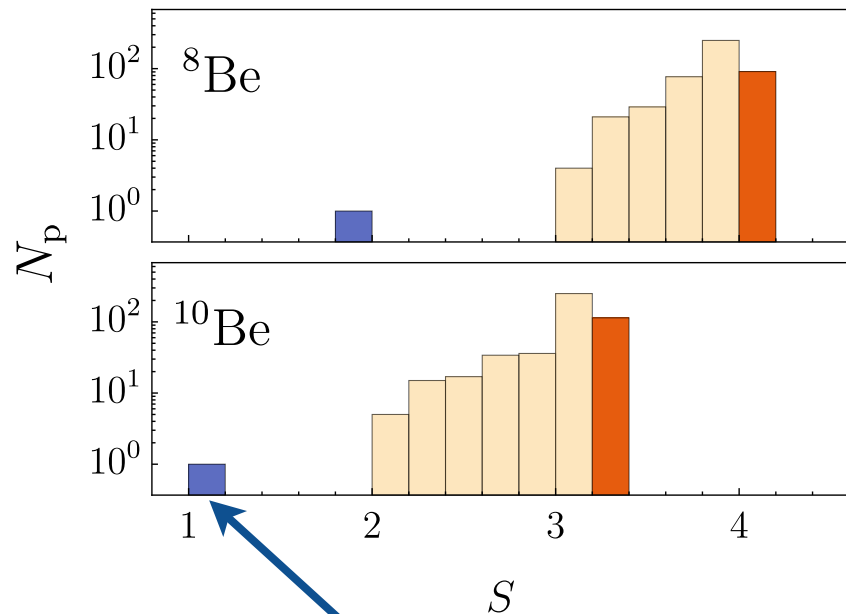
$$\hat{H} = \sum_p \epsilon_p a_p^\dagger a_p + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r$$



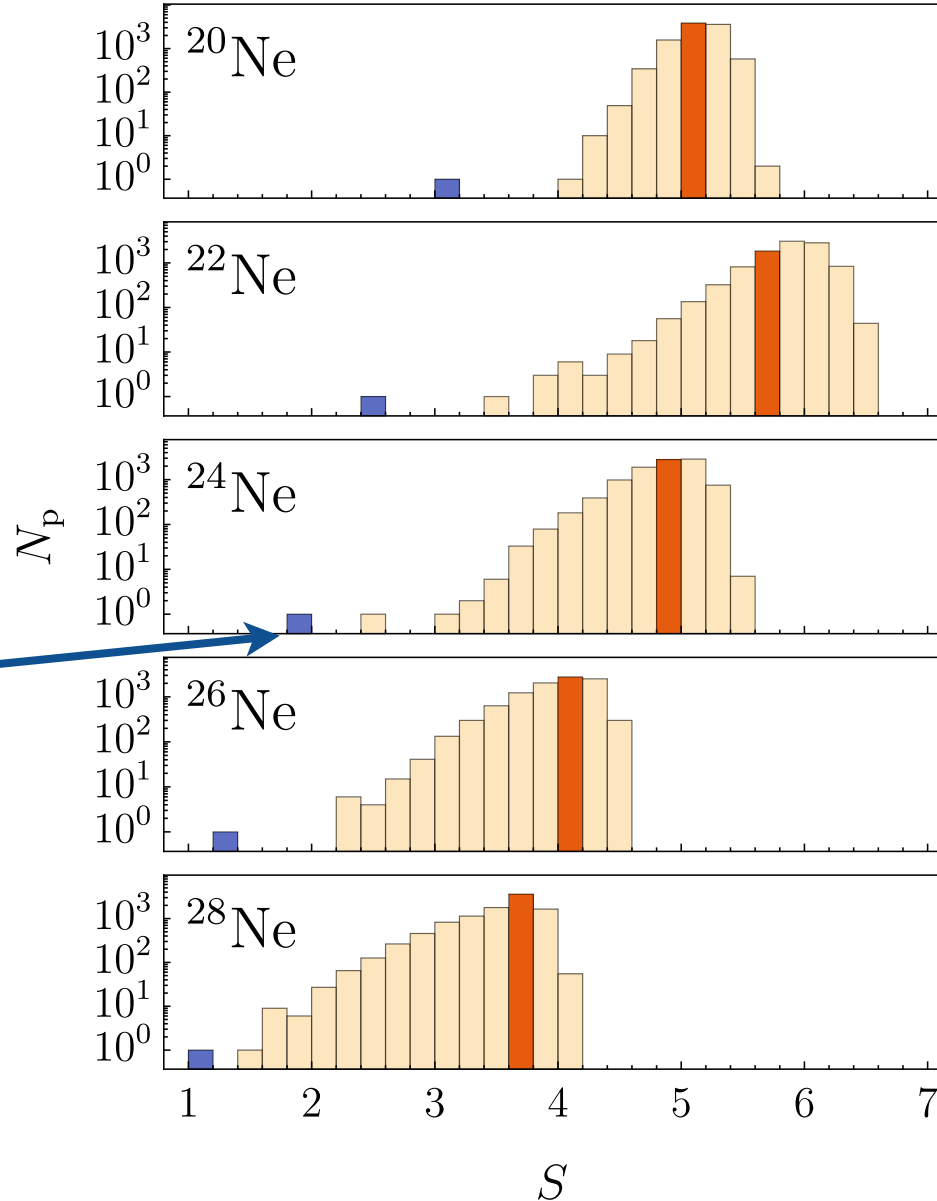
Other q complexity measures



Equipartition entropies

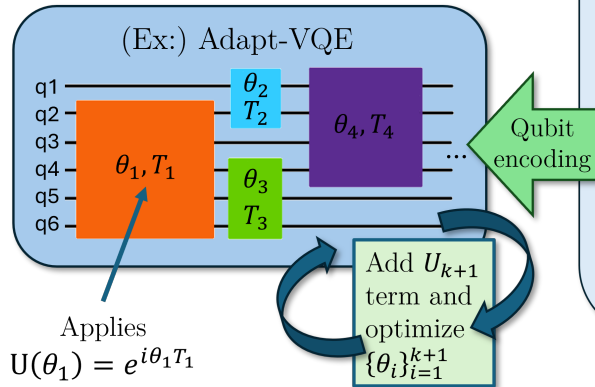


n/p partition



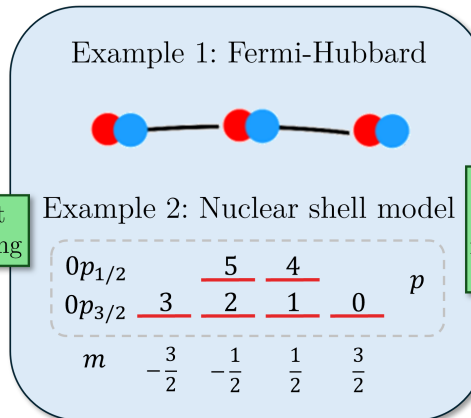
Variational quantum algorithm

- Finds $|\psi(\theta)\rangle$ by training θ



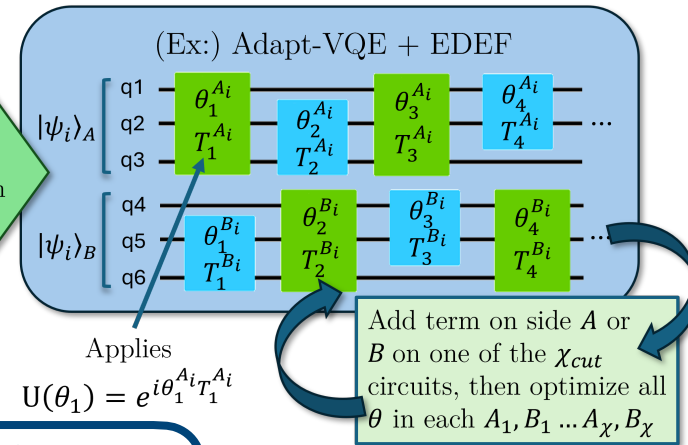
Physical system

- Describes $|\psi\rangle$



Reduced VQA using EDEF

- Finds $|\psi(\theta)\rangle = \sum_{i=1}^{\chi_{cut}} |\psi_i(\theta^{A_i})\rangle_A \otimes |\psi_i(\theta^{B_i})\rangle_B$ by training all $\theta^{A_i}, \theta^{B_i}$



Schmidt decomposition

$$|\psi\rangle = \sum_i^\chi \lambda_i |\psi_i\rangle_A \otimes |\psi_i\rangle_B$$

vN entropy of partition

$$S = - \sum_i \lambda_i^2 \log_2(\lambda_i^2)$$

Bound on # Schmidt terms

$$2^S \leq \chi \leq 2^{N_q/2}$$

Infidelity of circuit cut up to n

$$I_n = 1 - |\langle \psi_\chi | \psi_n \rangle|^2 = 1 - \sum_i^n \lambda_i^2$$

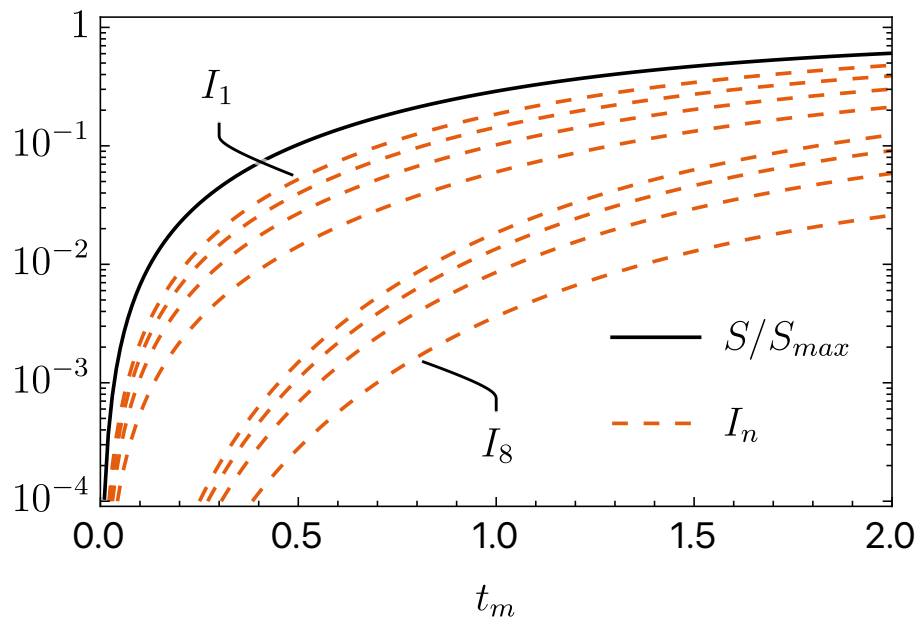
1D Fermi-Hubbard model

$$N_s = 8$$

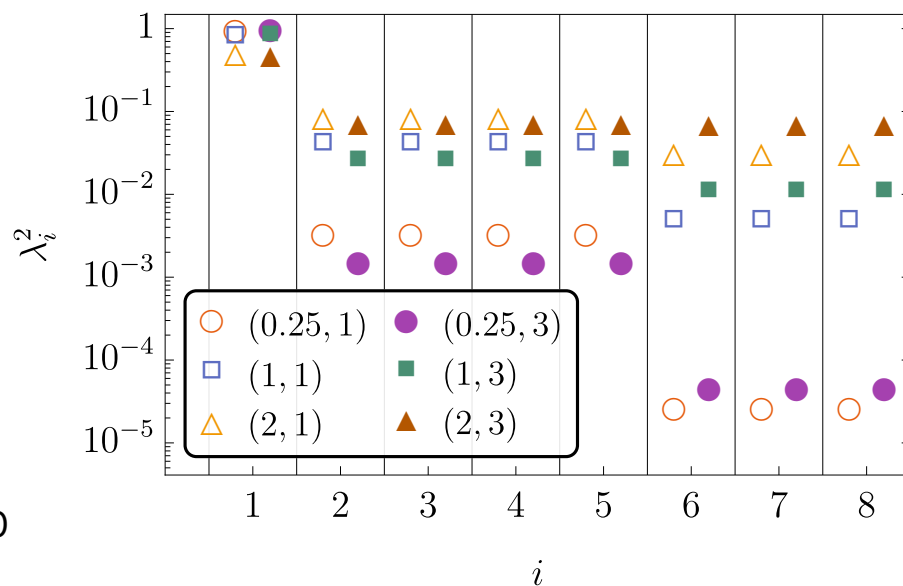


$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

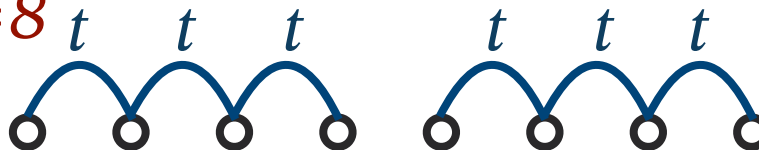
$N_s=4$, $U=t$, half-filling



$N_s=4$, half-filling

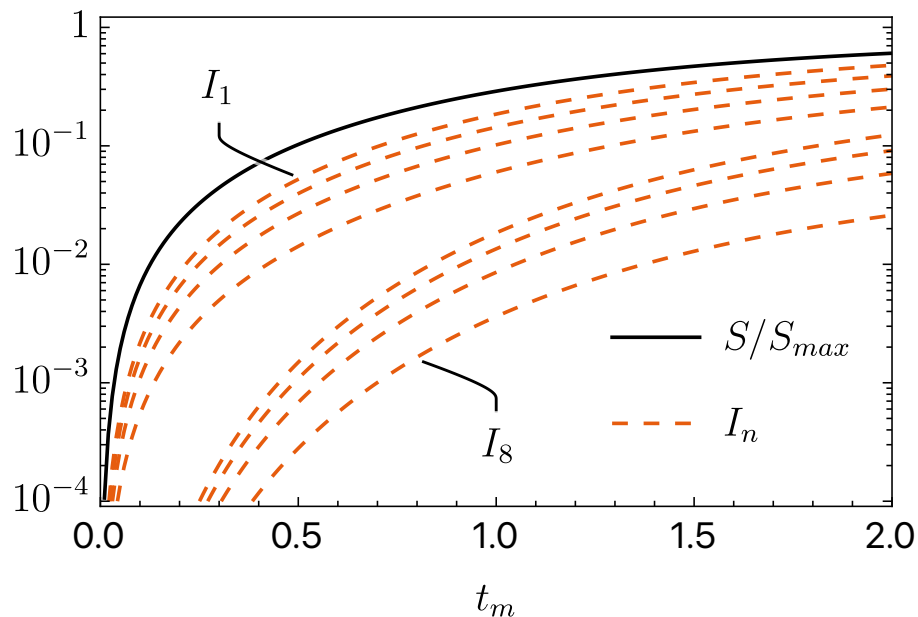


1D Fermi-Hubbard model

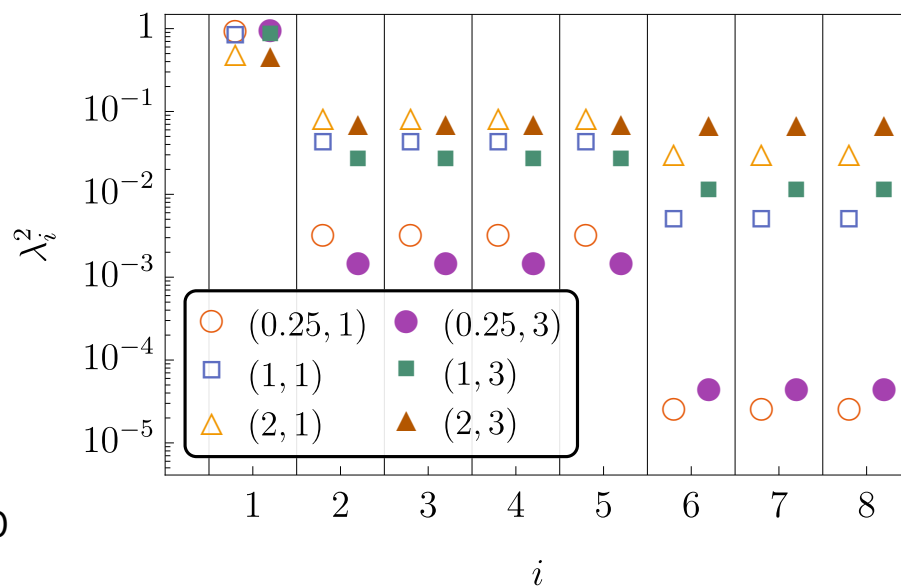
 $N_s = 8$


$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

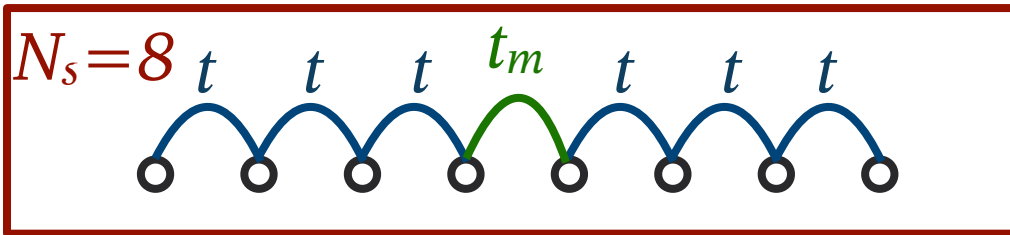
$N_s=4$, $U=t$, half-filling



$N_s=4$, half-filling

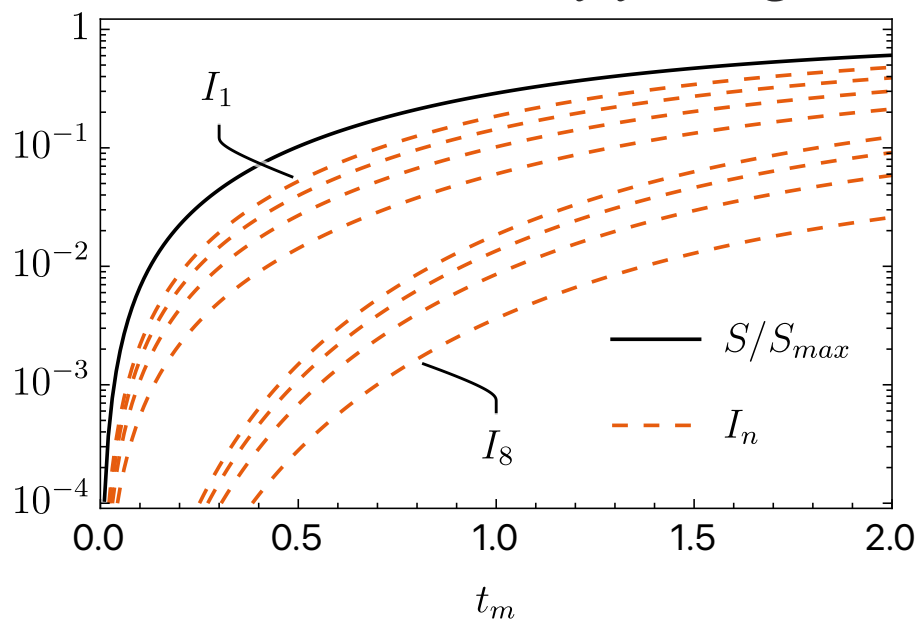


1D Fermi-Hubbard model

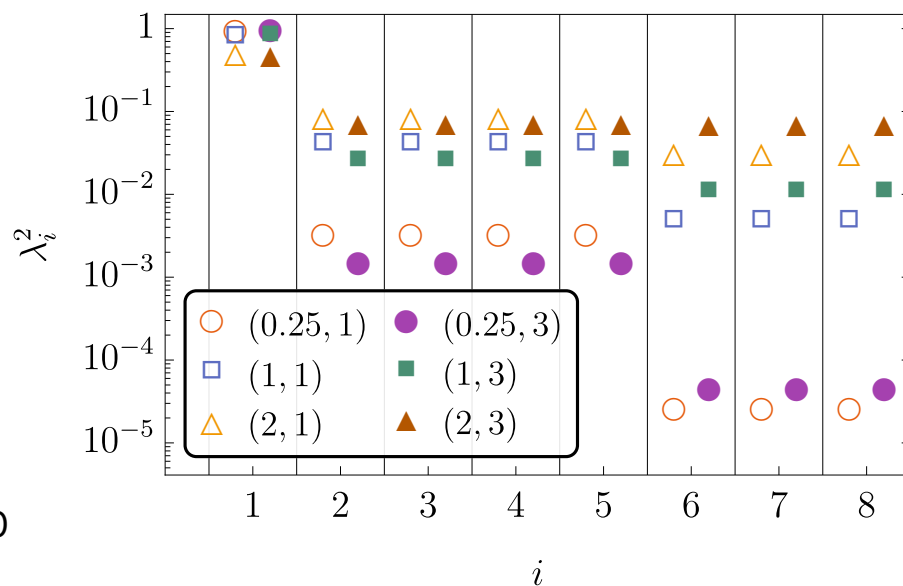


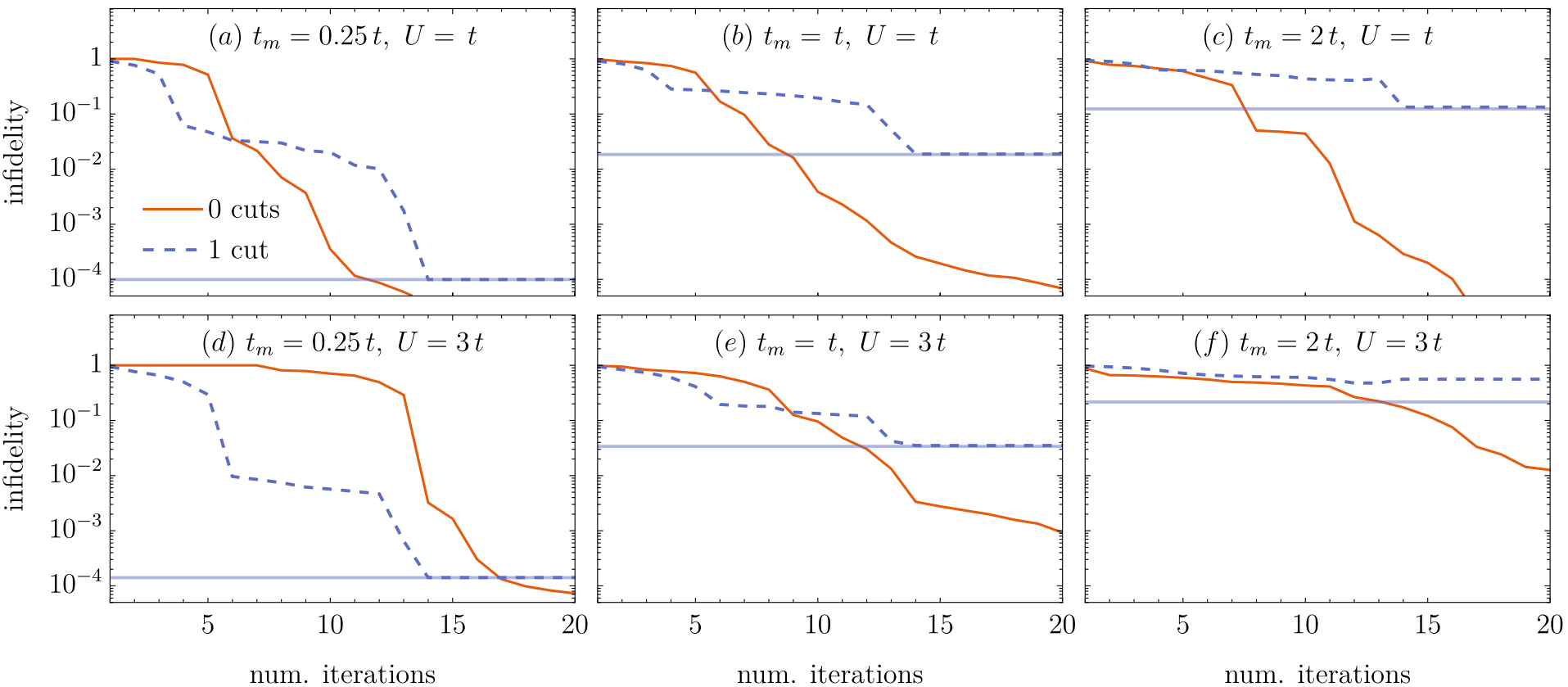
$$H = \boxed{t} \sum_{\langle i,j \rangle, \sigma} \left(a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ - \boxed{t_m - t} \sum_{\sigma} \left(a_{i_m\sigma}^\dagger a_{j_m\sigma} + a_{j_m\sigma}^\dagger a_{i_m\sigma} \right)$$

$N_s=4, U=t, \text{ half-filling}$

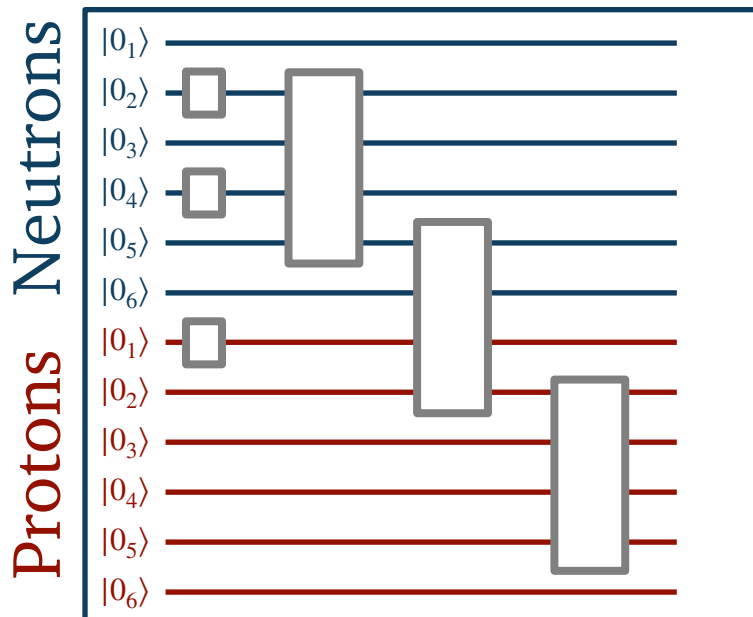
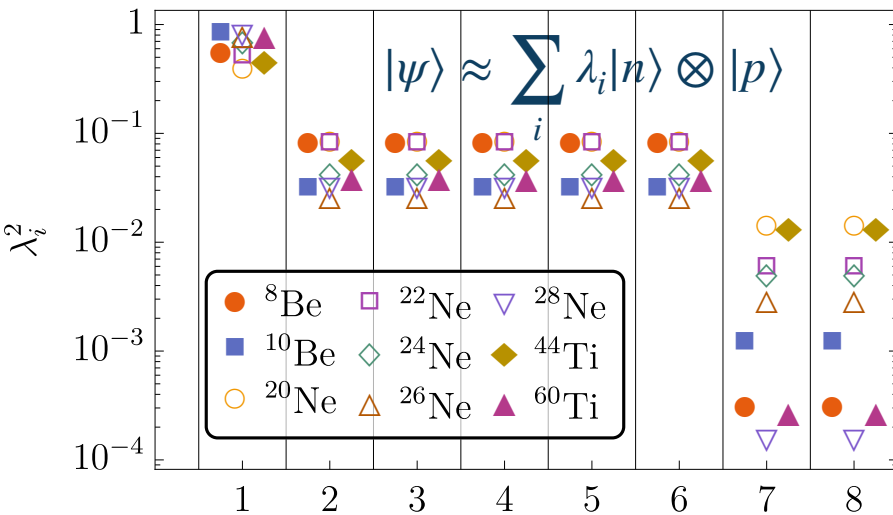


$N_s=4, \text{ half-filling}$

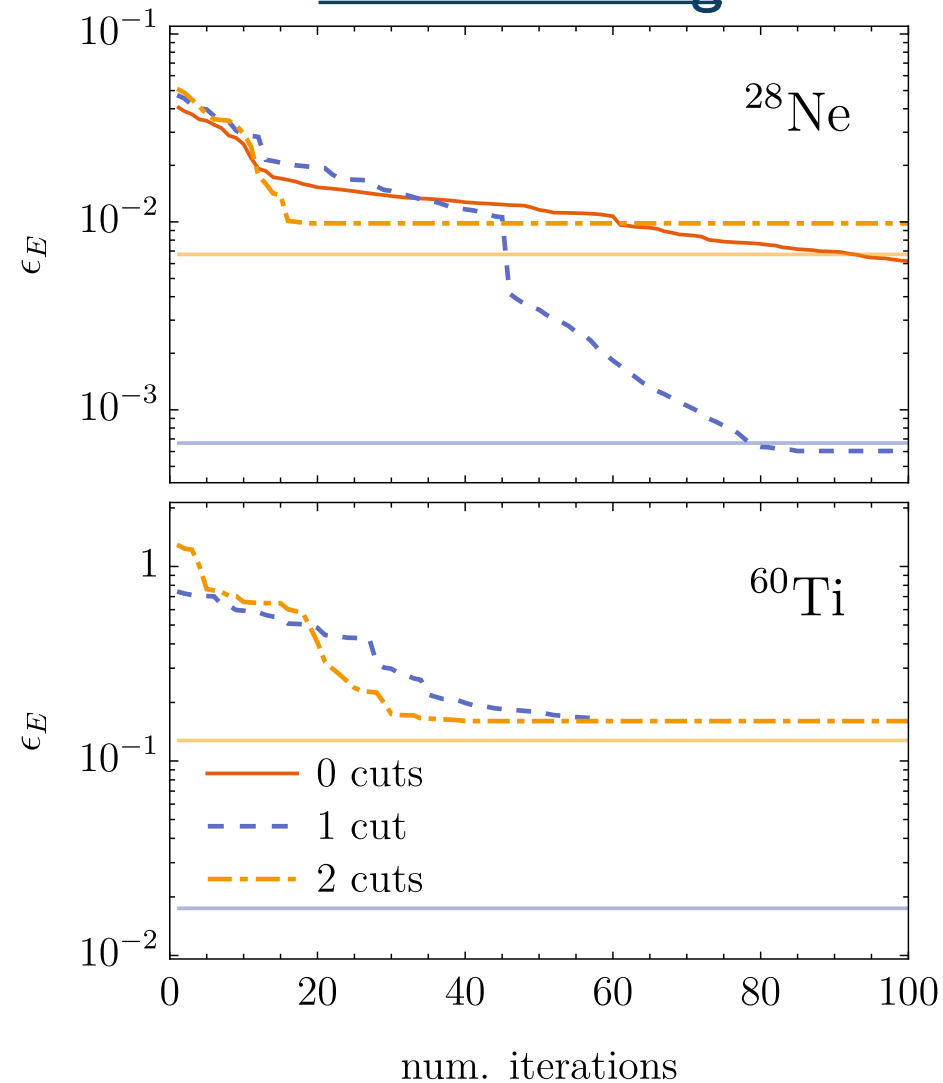




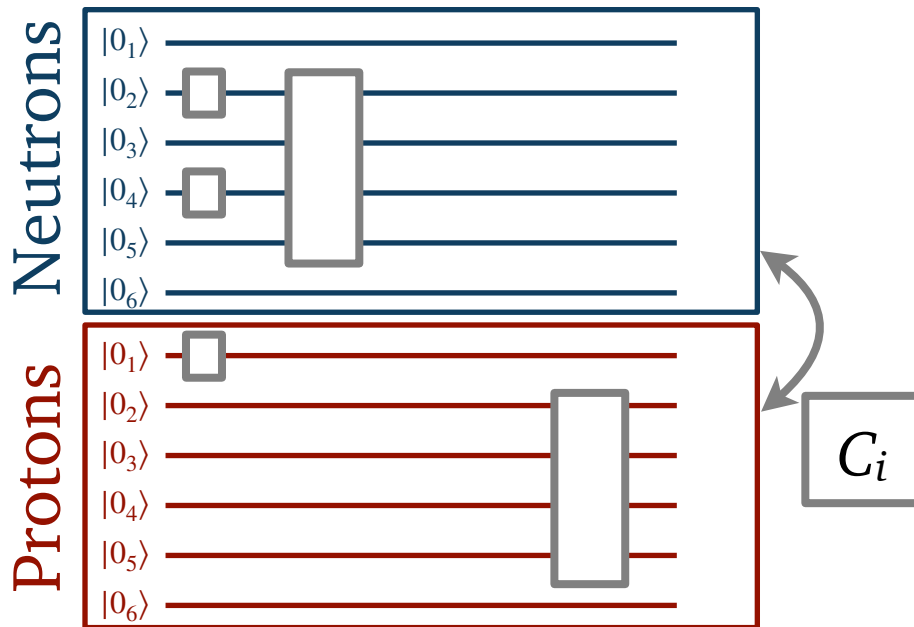
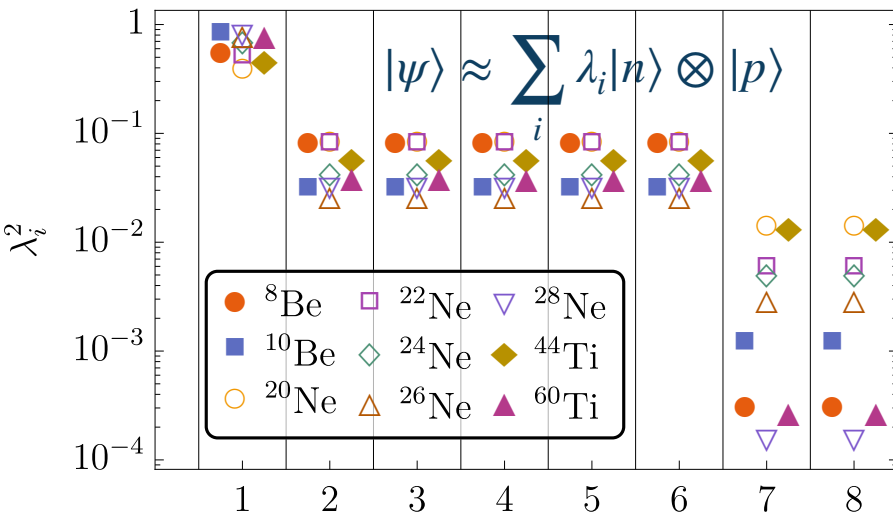
Schmidt decomposition



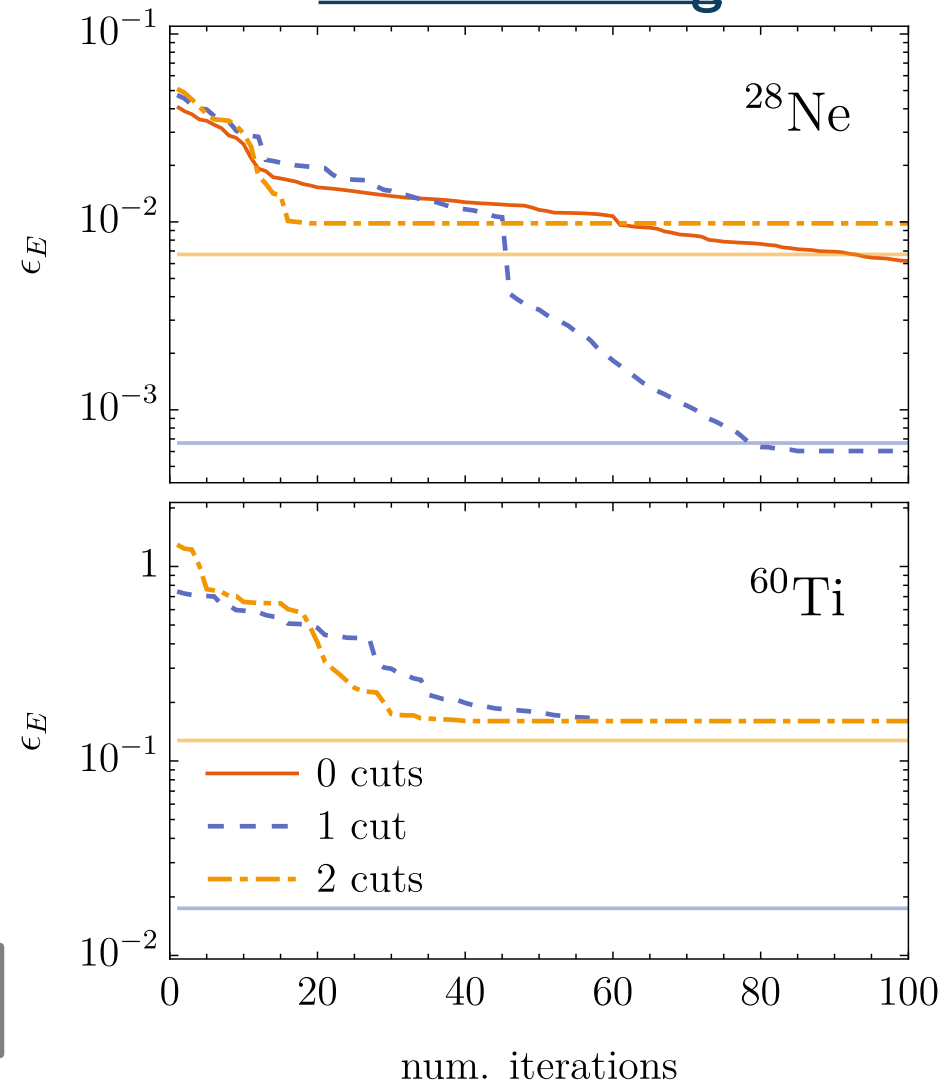
Circuit cutting

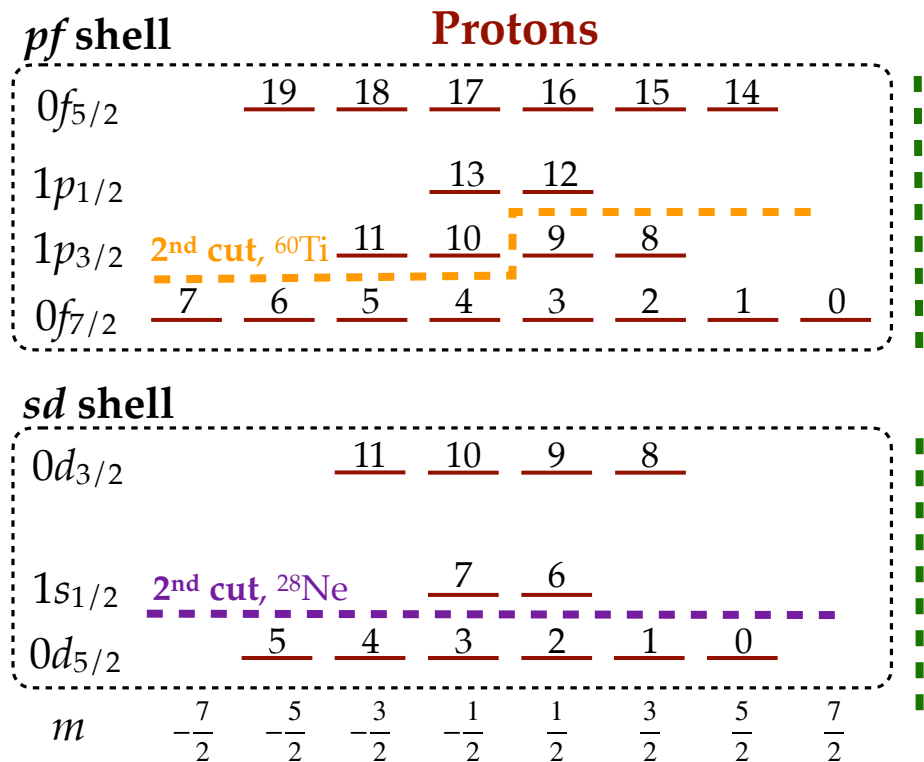


Schmidt decomposition



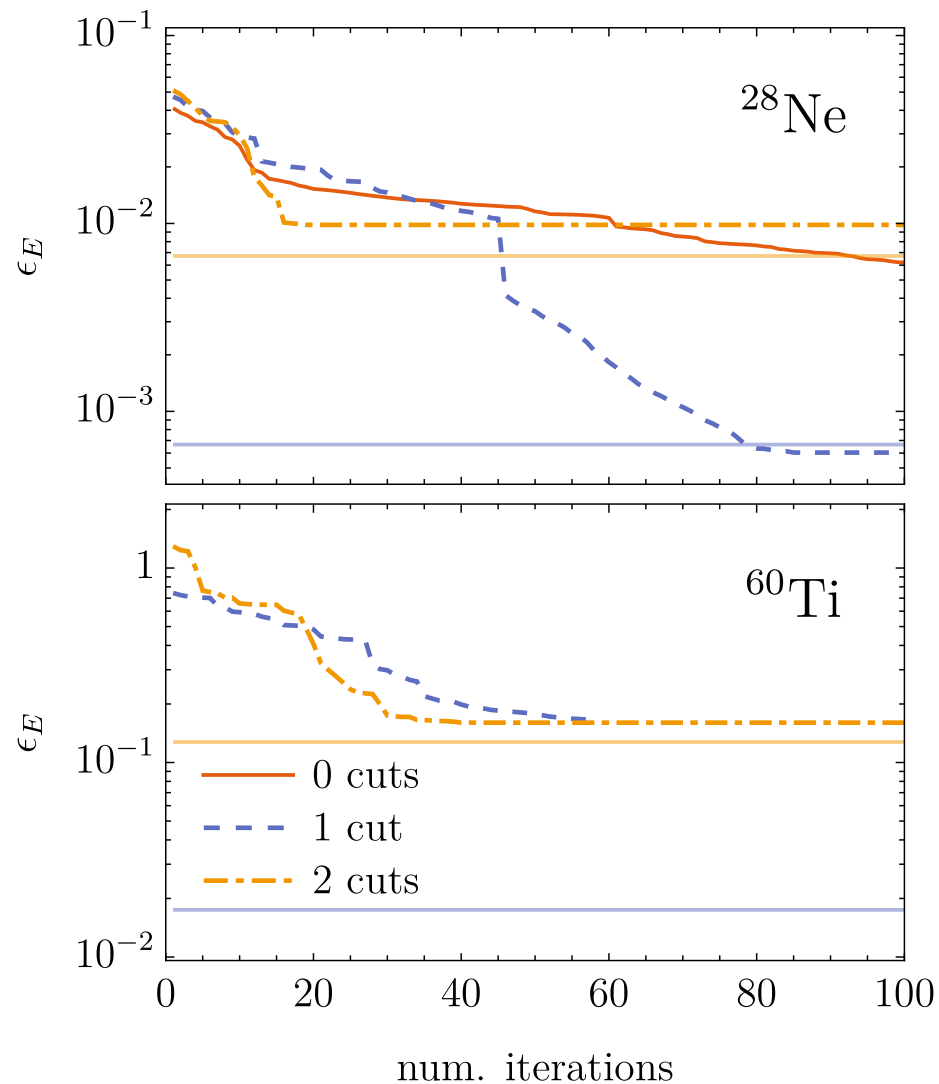
Circuit cutting

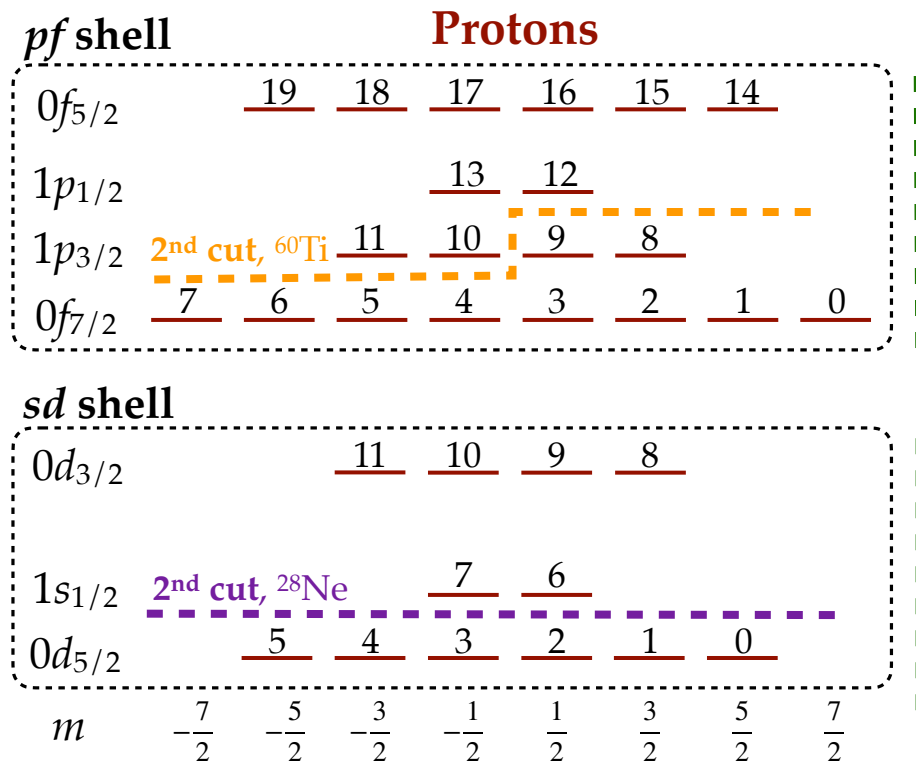




- Allows costly simulations
- Reduces quantum resources

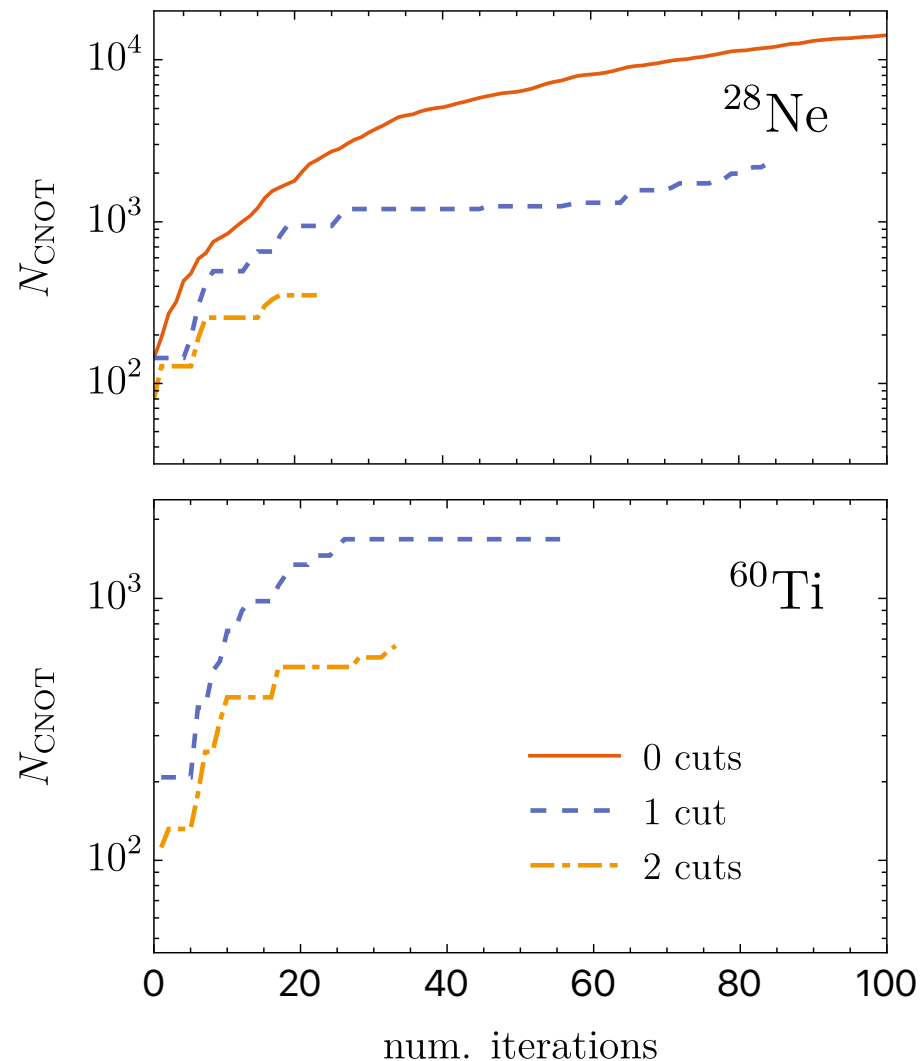
Circuit cutting





- Allows costly simulations
- Reduces quantum resources

Circuit cutting



Similar ideas in “standard” SM

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Journal of Physics G: Nuclear and Particle Physics

J. Phys. G: Nucl. Part. Phys. **50** (2023) 045110 (12pp)

<https://doi.org/10.1088/1361-6471/acbece>

Proton-neutron entanglement in the nuclear shell model

Calvin W Johnson^{*} and Oliver C Gorton[†]

PHYSICAL REVIEW C **110**, 034305 (2024)

Weak entanglement approximation for nuclear structure

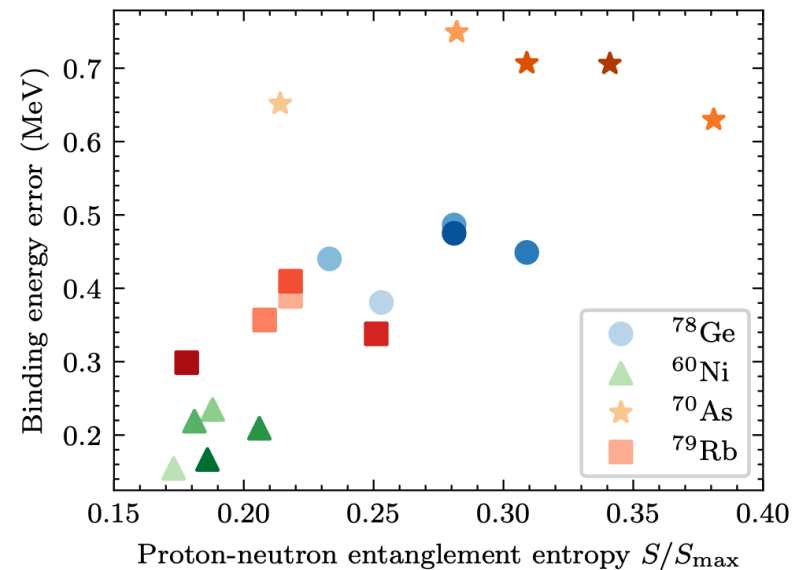
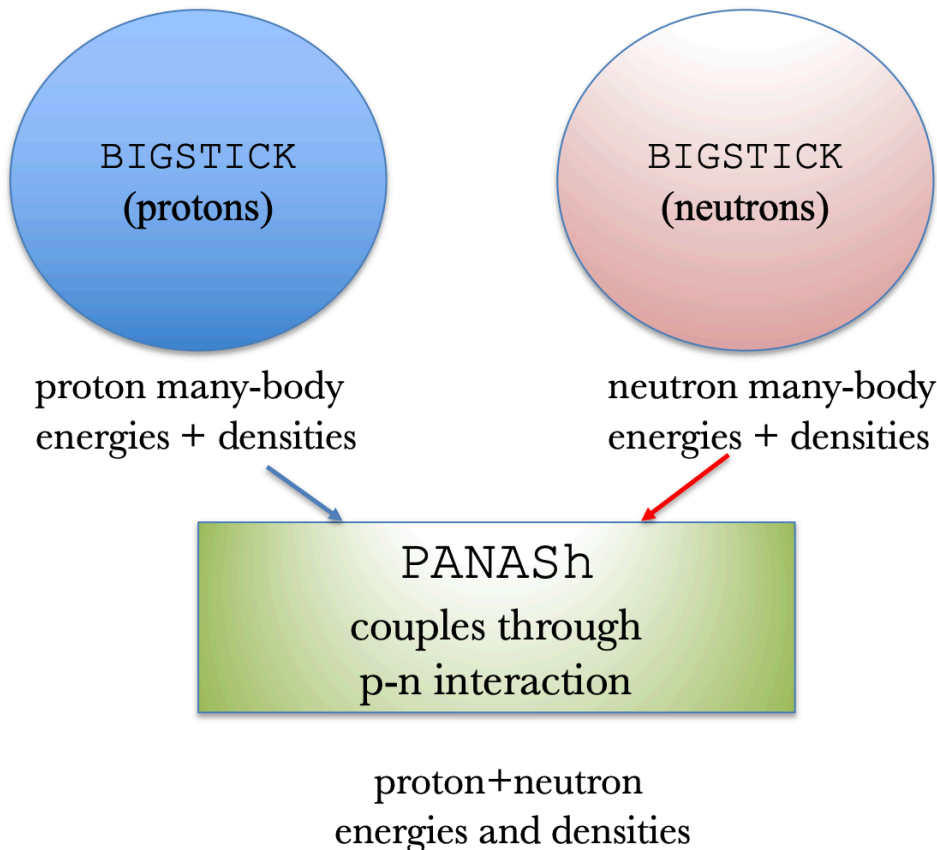
Oliver C. Gorton[†]

Lawrence Livermore National Laboratory, Livermore, California 94550, USA

and Department of Computational Science, San Diego State University, San Diego, California 92182, USA

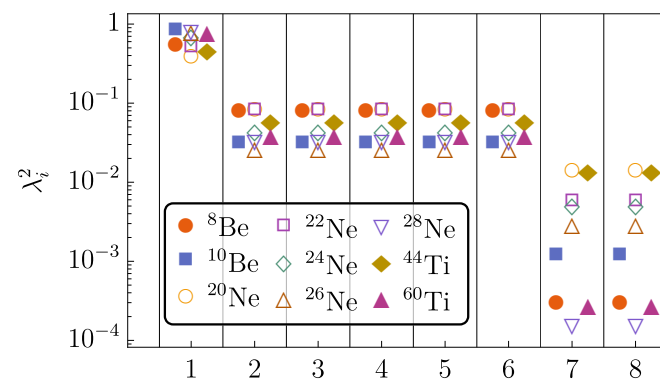
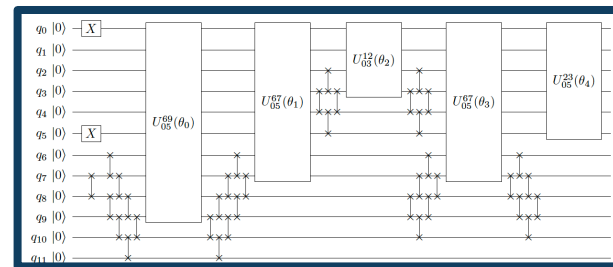
Calvin W. Johnson[†]

Department of Physics, San Diego State University, San Diego, California 92182, USA



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- VQEs can reproduce **shell model** wavefunctions
 - **Number of qubits** not an issue
 - Depth of circuit **is** an issue
 - ADAPT vs UCC quantification
 - Entanglement forging



MareNostrum Ona@BSC



To-Do List:

- Error mitigation
 - Simulations in real hardware
- Entanglement
 - Other quantifications
- Excited states & dynamics
 - Other quantifications

Thank you!

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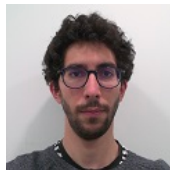
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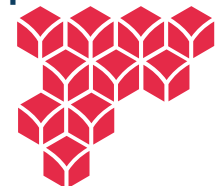
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