Exploiting low entanglement in nuclear shells

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Outline

1. Introduction: Entanglement, Shell model

2. Quantifying entanglement in the nuclear shell model

Pérez-Obiol, A., Masot-Llima, S., Romero, A.M. *et al.*
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Eur. Phys. J. A **59**, 240 (2023)

3. Harnessing low entanglement with entanglement forging

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Entanglement in many-body physics

Measures unseparability of quantum states:

$$|\psi\rangle \neq |\psi_1\rangle \otimes |\psi_2\rangle$$

Quantified with Von Neuman entropy:

$$S_{VN} = -Tr(\rho_A \log(\rho_A))$$

It's a relative concept

(particle/mode, basis, mapping, partition)

$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ → $a_\uparrow^\dagger a_\downarrow^\dagger |0\rangle$ → $|11\rangle$

1st quantization "entangled"

2nd quantization

Jordan-Wigner (not entangled)

Shell model

1. Single particle Schrodinger equation

H.O. potential + spin-orbit

$$V(r) = \frac{1}{2}\hbar\omega r^2 + D\vec{l}^2 + C\vec{l}\cdot\vec{s}$$

➡ Predicts magic numbers

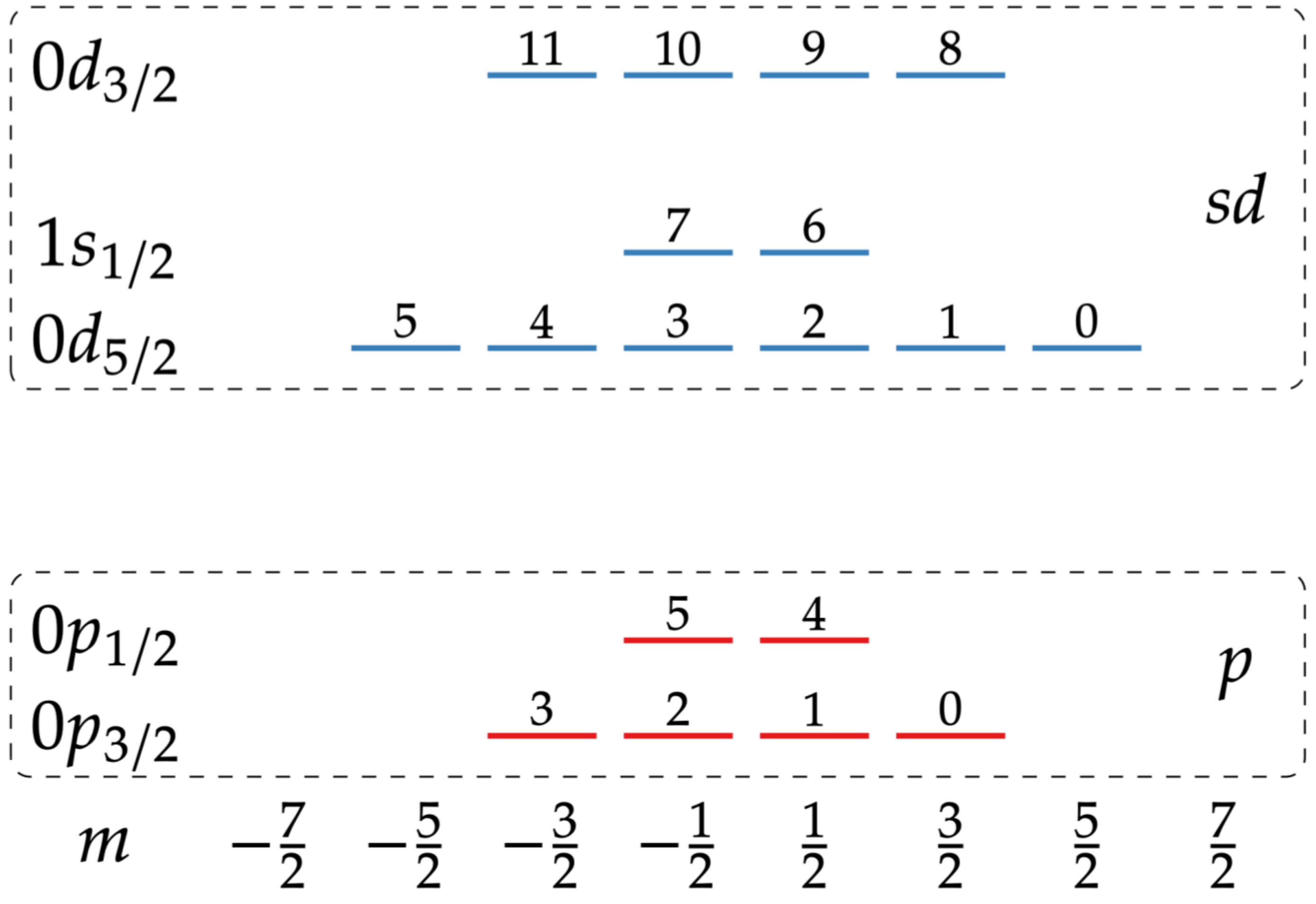
➡ Provides orbital/valence space

2. Interaction shell model:

➡ Mean field + residual two-body interactions:

$$\mathcal{H} = \sum_{ij} K_{ij} a_i^\dagger a_j + \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

➡ Diagonalization problem



Jordan-Wigner mapping:

$$a_j^\dagger = \prod_{k=0}^{j-1} Z_k \frac{X_j - iY_j}{2}$$

+ adapt-VQE

arXiv:2302.03641

3. Entanglement depends on:

➡ Basis chosen (M-scheme, J-scheme)

➡ fermion-qubit mappings (JW, BK, VC)

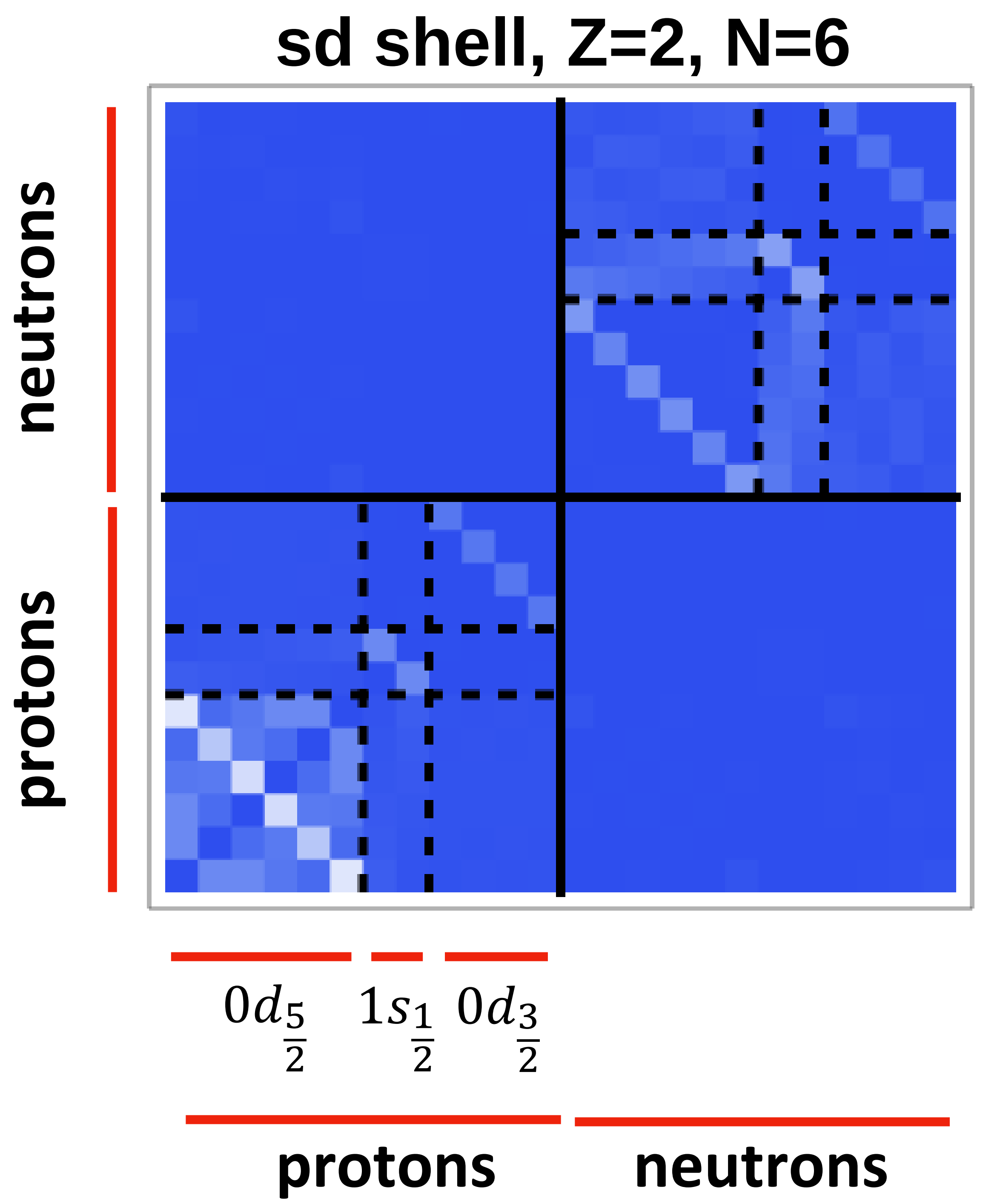
➡ Partition (1 orbital, 2 orbital, equipartition)

Single orbital & orbital-orbital entanglement

mutual information

$$S_i + S_j - S_{ij}$$

gives a good overall picture:



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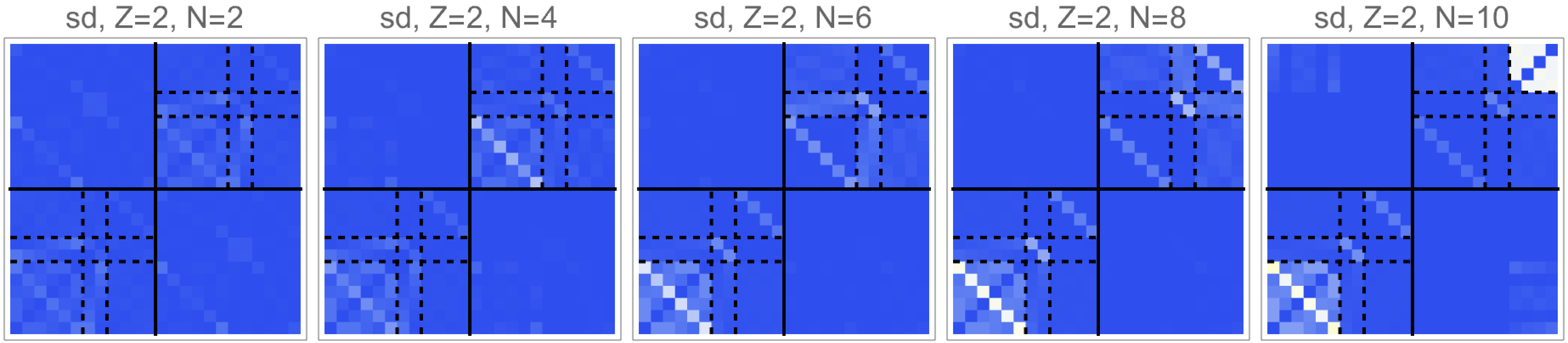
Mutual information across the sd shell



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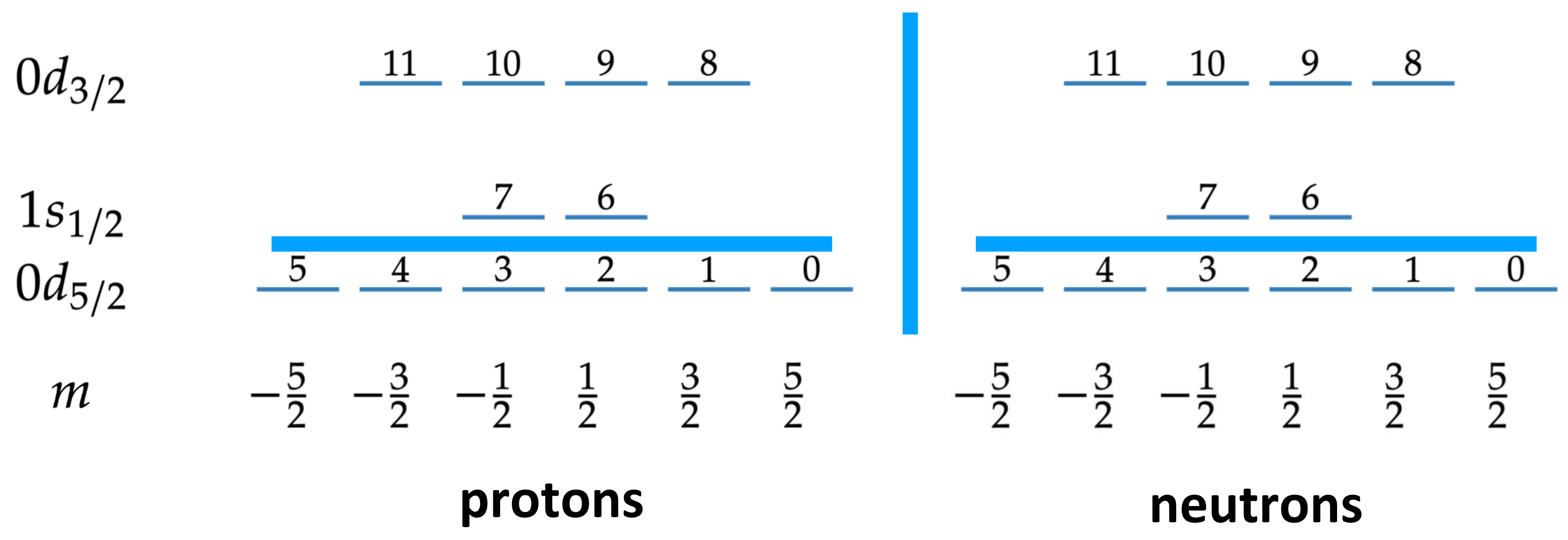
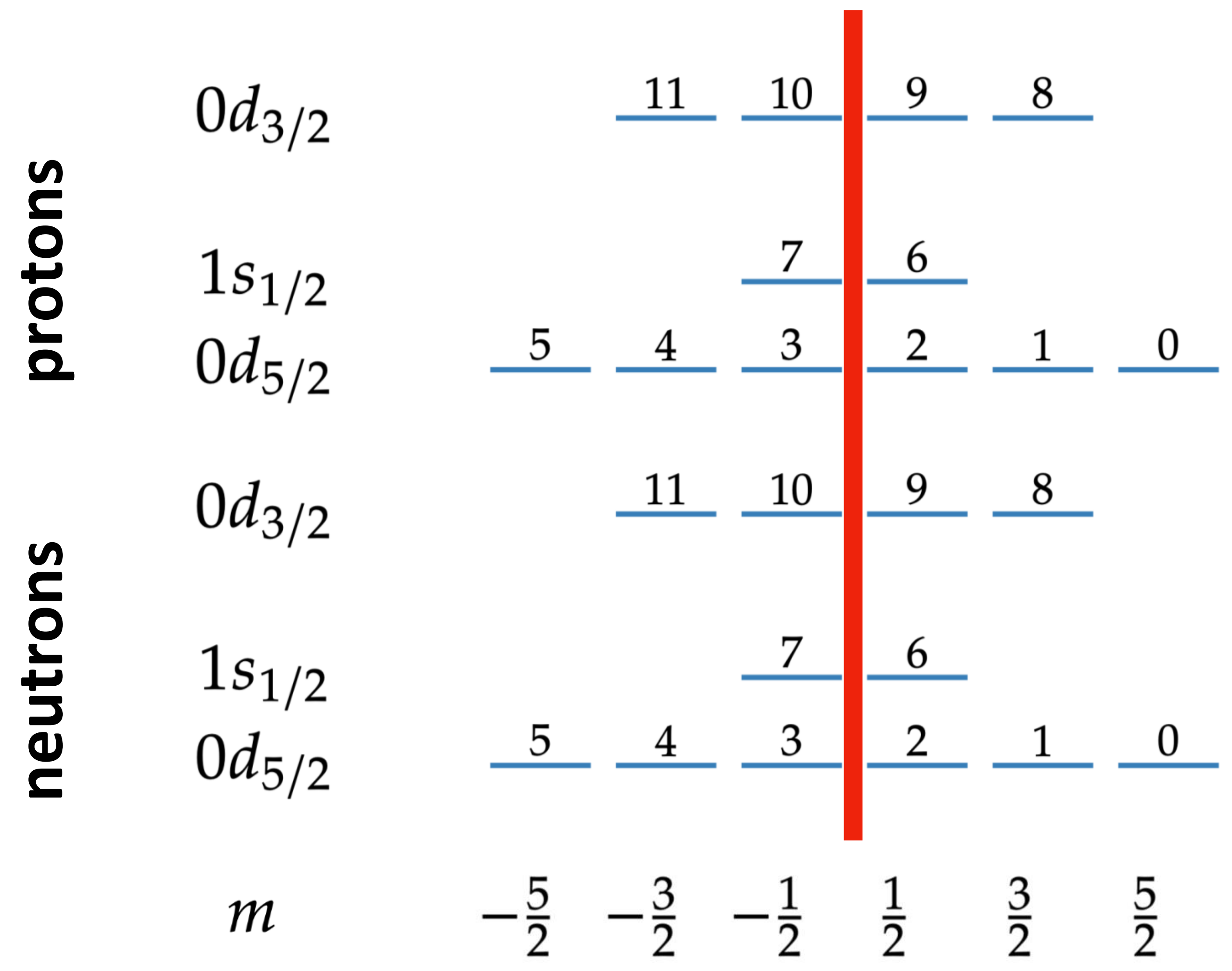
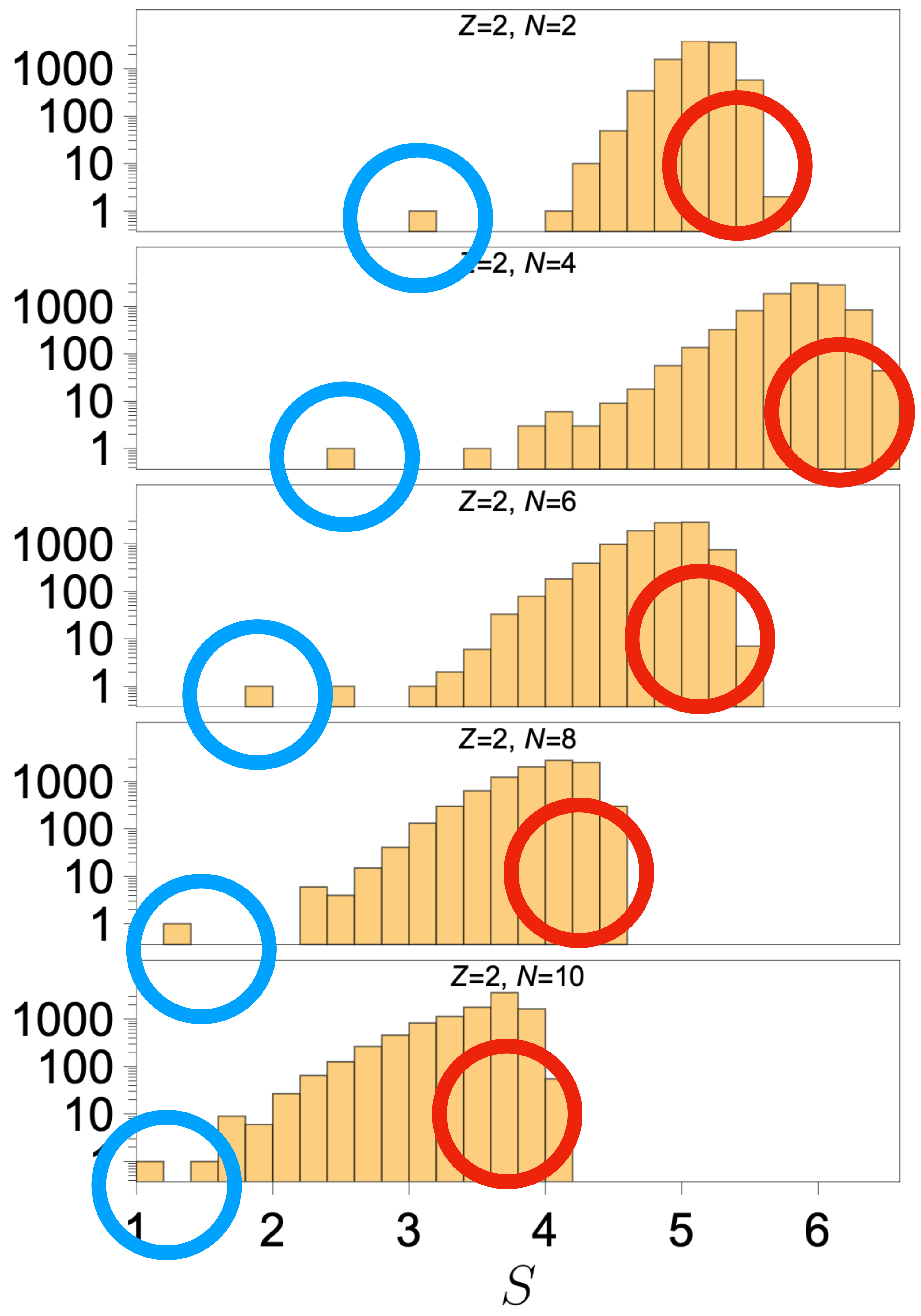
Equipartition entanglement

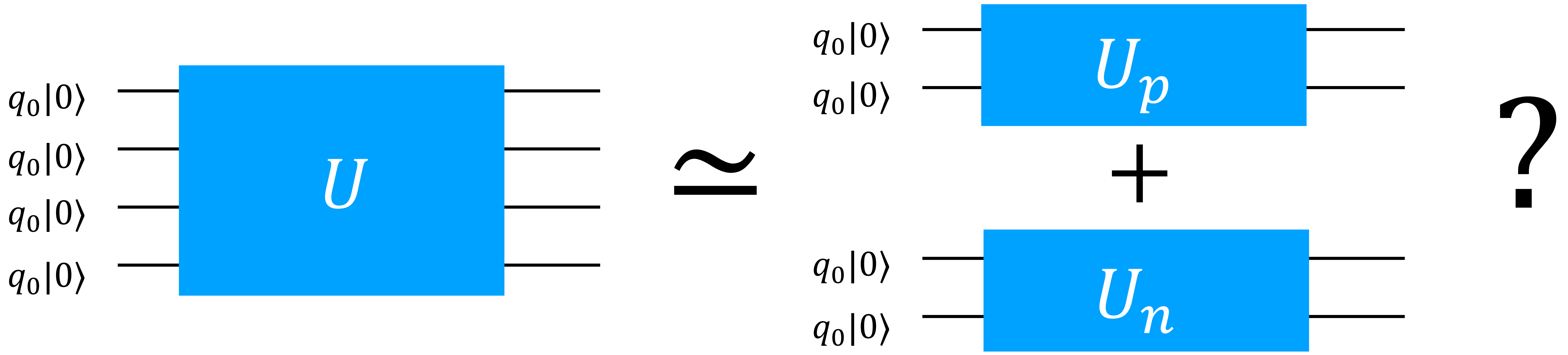
most natural partitions







Can we harness (low) entanglement?



Schmidt decomposition:

$$
\begin{aligned}
|\psi_{GS}\rangle = \lambda_1|\psi_p^{(1)}\rangle \otimes |\psi_n^{(1)}\rangle \\
+ \lambda_2|\psi_p^{(2)}\rangle \otimes |\psi_n^{(2)}\rangle \\
+ \lambda_3|\psi_p^{(3)}\rangle \otimes |\psi_n^{(3)}\rangle \\
+ \lambda_4|\psi_p^{(4)}\rangle \otimes |\psi_n^{(4)}\rangle \\
+ \lambda_5|\psi_p^{(5)}\rangle \otimes |\psi_n^{(5)}\rangle \\
+ \ \ldots
\end{aligned}
$$

Orthogonal:

$$\left\langle \psi_k^{(i)} \middle| \psi_k^{(j)} \right\rangle = \delta_{ij} \quad (k = n, p)$$

Normalized:

$$\sum_j \lambda_j^2 = 1$$

Can we harness (low) entanglement?

Non-degenerate
$\boldsymbol{\lambda = 0.83}$
$\boldsymbol{M = 0, 0}$

Schmidt decomposition:

$$
\begin{aligned}
|\psi_{GS}\rangle = &\ \lambda_1 |\psi_p^{(1)}\rangle \otimes |\psi_n^{(1)}\rangle \\
&+ \lambda_2 |\psi_p^{(2)}\rangle \otimes |\psi_n^{(2)}\rangle \\
&+ \lambda_3 |\psi_p^{(3)}\rangle \otimes |\psi_n^{(3)}\rangle \\
&+ \lambda_4 |\psi_p^{(4)}\rangle \otimes |\psi_n^{(4)}\rangle \\
&+ \lambda_5 |\psi_p^{(5)}\rangle \otimes |\psi_n^{(5)}\rangle \\
&+ \lambda_6 |\psi_p^{(6)}\rangle \otimes |\psi_n^{(6)}\rangle \\
&+ \ \ldots
\end{aligned}
$$

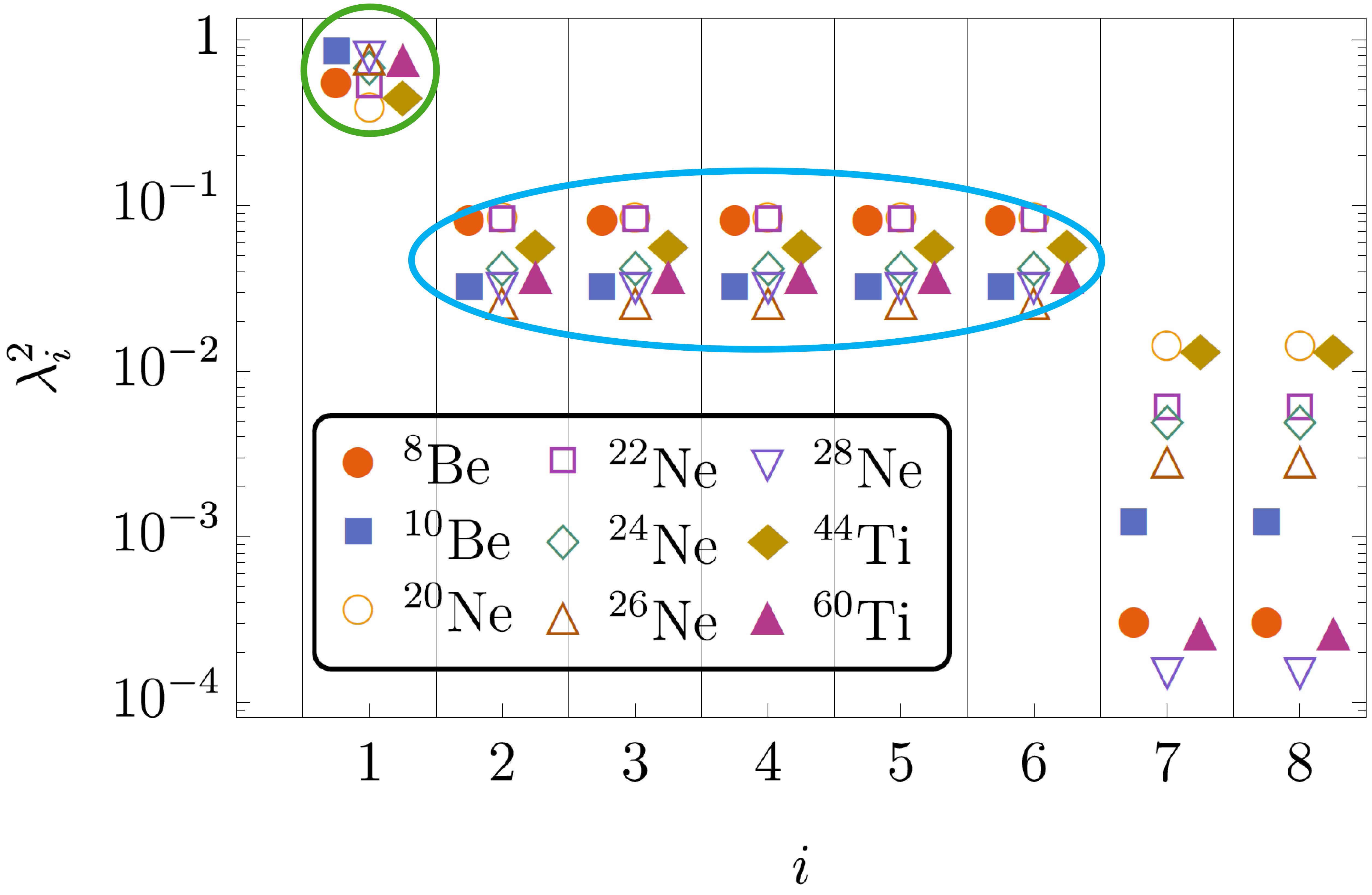
5-fold degeneracy
$\boldsymbol{M = -2, 2}$
$\boldsymbol{M = -1, 1}$
$\boldsymbol{M = 0, 0}$
$\boldsymbol{M = 1, -1}$
$\boldsymbol{M = 2, -2}$

Orthogonal:

$$\left\langle \psi_k^{(i)} \middle| \psi_k^{(j)} \right\rangle = \delta_{ij} \quad (k = n, p)$$

Normalized:

$$\sum_j \lambda_j^2 = 1$$



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Adapt VQE

1. Initial state: lowest energy basis state

$$|\Psi_0\rangle = \prod_i a_i^\dagger |\text{vac}\rangle, \text{ e.g. } |\psi_0\rangle = a_0^\dagger a_3^\dagger |0\rangle$$

2. Pool of operators for the ansatz

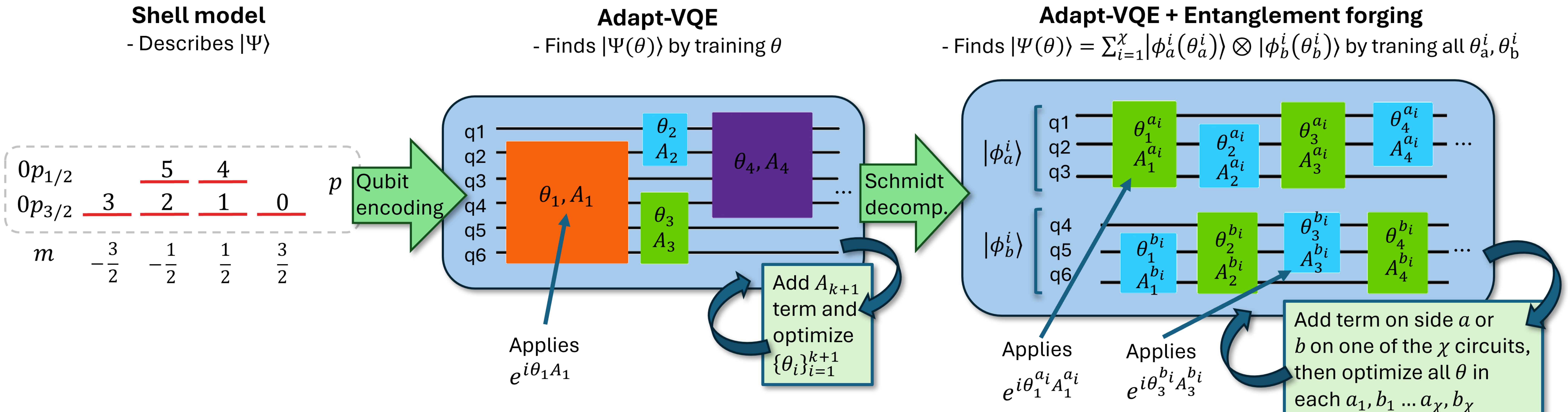
$$A_k = i(a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q)$$

3. Ansatz built adaptively: largest $\frac{\partial E^{(n)}}{\partial \theta_k}|_{\theta_k=0}$

After n steps: $|\psi(\vec{\theta})\rangle = \prod_{k=1}^{n} e^{i\theta_k A_k}|\psi_0\rangle$

Grimsley et al., *Nat. comm.* **10**, 1–9 (2019)

4. Minimize: $E = \min_{\theta_k} \langle \Psi(\theta_k)|H|\Psi(\theta_k)\rangle$



Can we harness (low) entanglement?

let's simulate 6 product states

$|\psi_p(\vec{\alpha})\rangle = e^{i\alpha_1 T_1} \dots e^{i\alpha_N T_N}|ref_p^{(1)}\rangle$ **M = 0**

$|\psi_n(\vec{\phi})\rangle = e^{i\alpha'_1 T'_1} \dots e^{i\alpha'_{N'} T'_{N'}}|ref_n^{(1)}\rangle$ **M = 0**

$+$

$|\psi_p(\vec{\beta})\rangle = e^{i\beta_1 T_1} \dots e^{i\beta_N T_N}|ref_p^{(2)}\rangle$ **M = -2**

$|\psi_n(\vec{\beta})\rangle = e^{i\beta'_1 T'_1} \dots e^{i\beta'_{N'} T'_{N'}}|ref_n^{(2)}\rangle$ **M = 2**

$+$

$(\dots)$

$|\psi_p(\vec{\alpha})\rangle = e^{i\alpha_1 T_1} \dots e^{i\alpha_N T_N}|ref_p^{(6)}\rangle$ **M = 0**

$|\psi_n(\vec{\phi})\rangle = e^{i\alpha'_1 T'_1} \dots e^{i\alpha'_{N'} T'_{N'}}|ref_n^{(6)}\rangle$ **M = 0**

Minimize energy with adapt-vqe

$$\lambda\langle \psi_p(\vec{\alpha}), \psi_n(\vec{\alpha})|H|\psi_p(\vec{\alpha}), \psi_n(\vec{\alpha})\rangle + \sqrt{\frac{1-\lambda^2}{5}}\langle \psi_p(\vec{\beta}), \psi_n(\vec{\beta})|H|\psi_p(\vec{\beta}), \psi_n(\vec{\beta})\rangle + \cdots$$

Need to optimize $\lambda \in (0.5, 1)$

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$$+$$

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$$+$$

$$(\dots)$$

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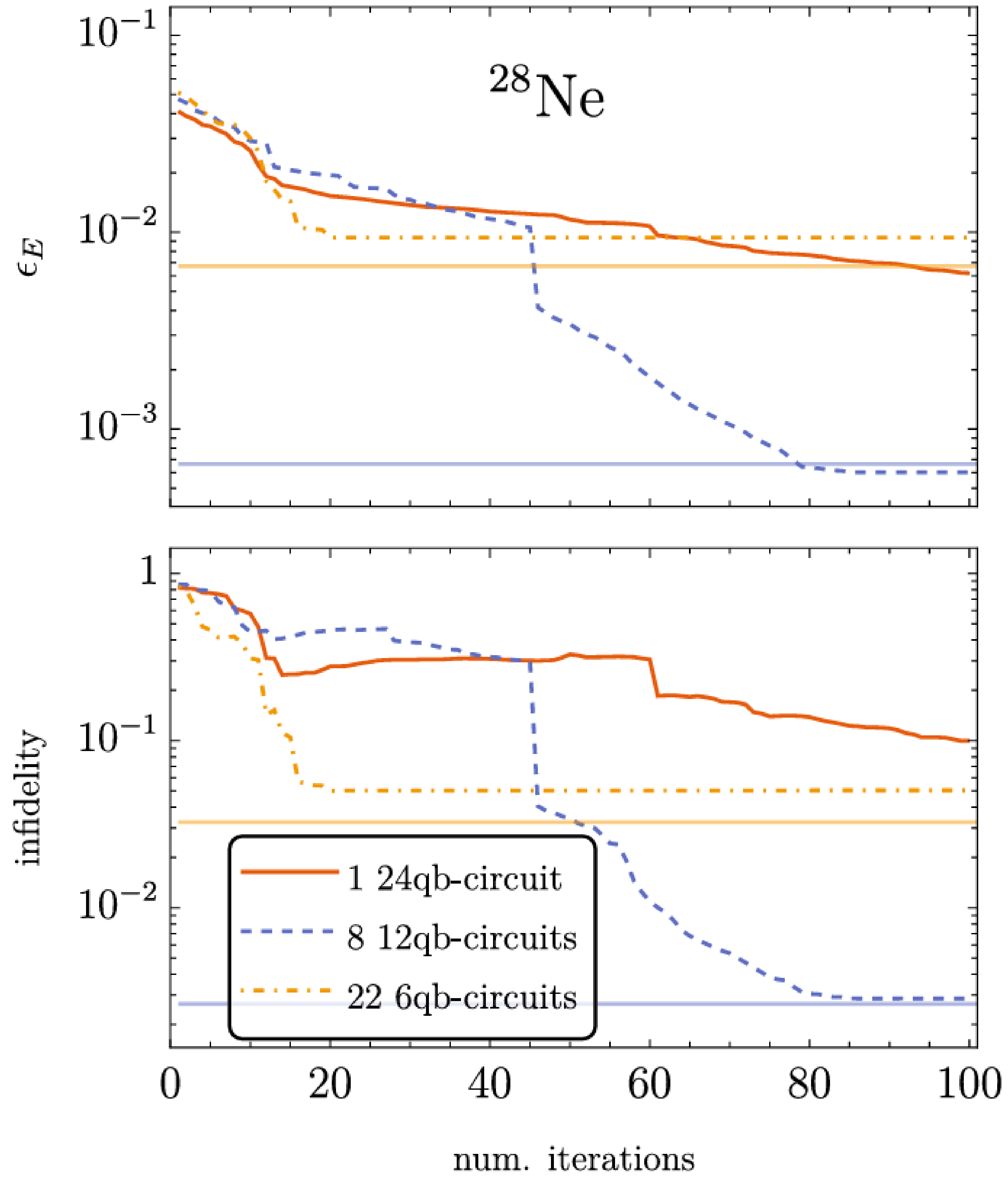
$$|\psi_n(\vec{\phi})\rangle = e^{i\alpha'_1 T'_1} \dots e^{i\alpha'_{N'} T'_{N'}} |ref_n^{(6)}\rangle$$ **M = 0**



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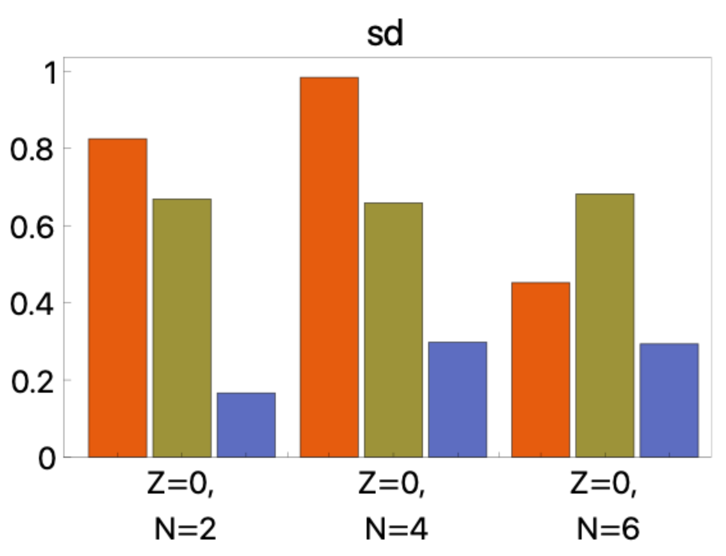
Conclusions

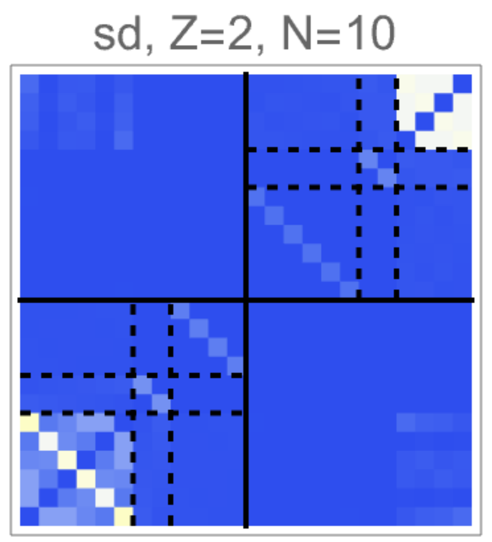
1. Entanglement in nuclei: fundamental & practical interests

2. Entanglement is low (lowest) between protons & neutrons and large (~largest) between M < 0 & M > 0

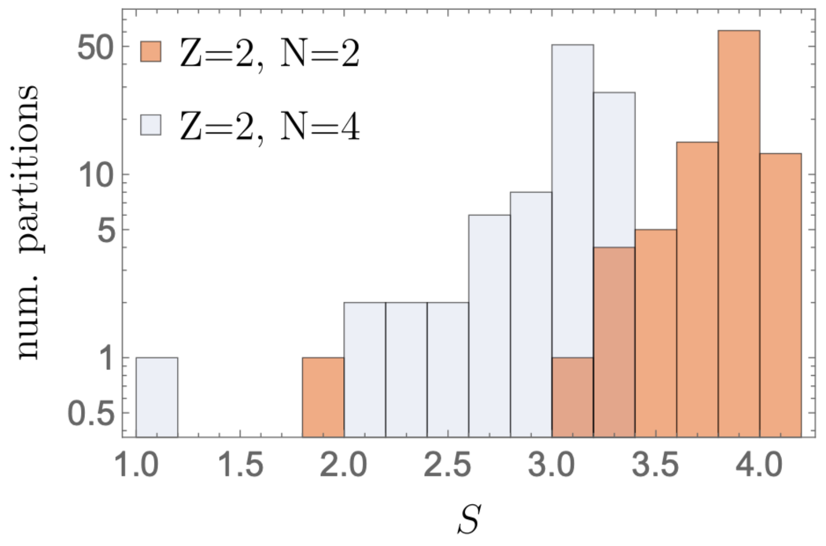
3. Circuit cutting + degeneracy of SV improves adapt VQE (smaller circuits, faster convergence)



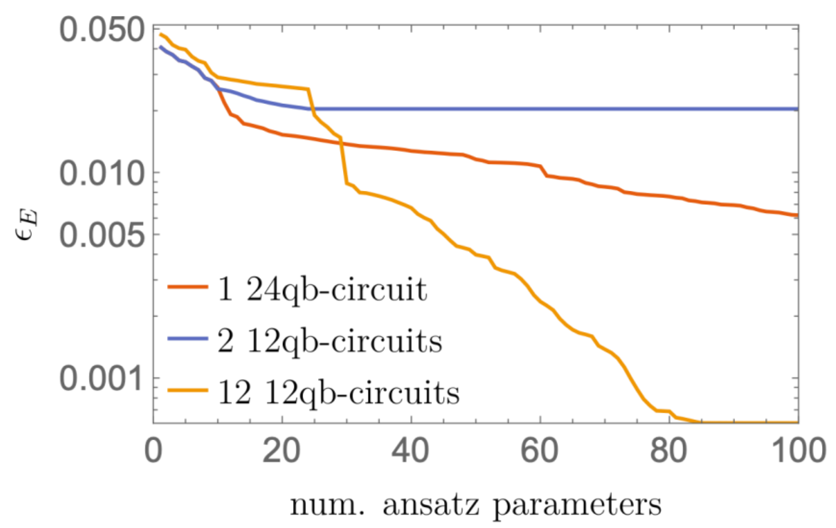
1. single-orbital / filling of subshells



2. general picture of entanglement



3. min. vs max. entanglement



4. circuit cutting improves VQE

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