Entanglement in nuclear shells

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Nuclear & particle physics in a QC, where do we stand now?

ECT*, Trento, June 8th 2023

Gobierno de España
Vicepresidencia Primera del Gobierno
Ministerio de Asuntos Económicos y Transformación Digital
Secretaría de Estado de Digitalización e Inteligencia Artificial
Financiado por la Unión Europea NextGenerationEU
Quantum Spain
Plan de Recuperación, Transformación y Resiliencia
RES Red Española de Supercomputación

Outline

1. Short nuclear entanglement intro

2. Quantifying entanglements in the nuclear shell model

3. Harnessing (low) entanglement with circuit cutting

Entanglement in many-body physics

Measures unseparability of quantum states:

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

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1st quantization

"entangled"

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2nd quantization

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$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \quad \rightarrow \quad a^\dagger_\uparrow a^\dagger_\downarrow |0\rangle \quad \rightarrow \quad |11\rangle$$

1st quantization "entangled"

2nd quantization

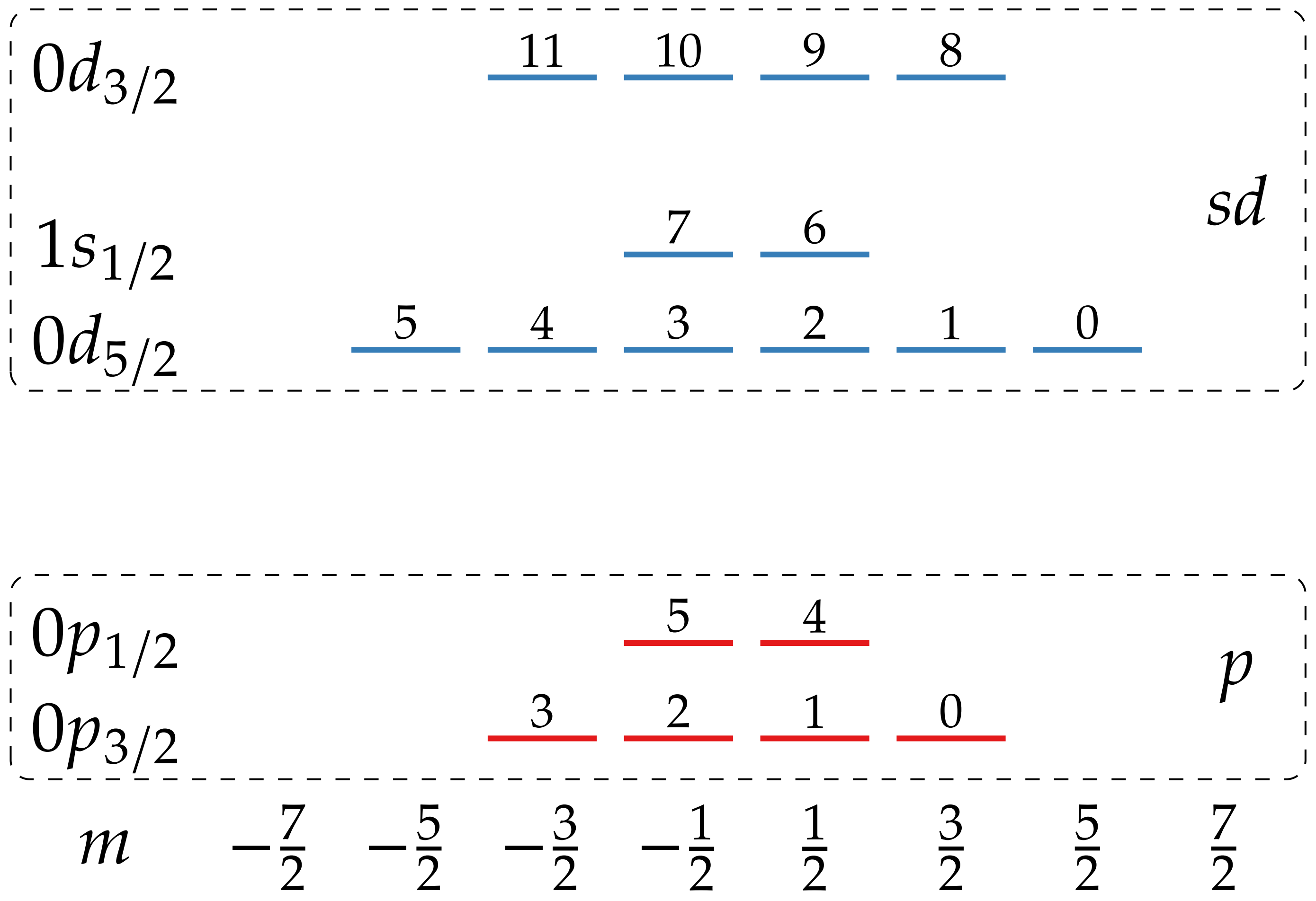
Jordan-Wigner (not entangled)

Entanglement in nuclear physics

1. C. Robin, M. Savage et al: basis rearrangement PRC **103**, 034325 (2021)
2. C. Johnson, O. Gorton: low proton-neutron entanglement in sd, pf shells J. Phys. G: NPP 50, 045110 (2023) see also, Papenbrock & Dean PRC 67, 051303(R) (2003)
3. I. Stetcu et al: orbital-orbital mutual information in Be (VQE) PRC **105**, 064308 (2022)
4. C. Gu et al: volume law in nuclear matter? arXiv:2303.04799
5. Entanglement from the fundamental point of view A. Cervera et al., SciPost Phys. 3, 036 (2017) Beane et al PRL122,102001 (2019) Beane et al JMP. A 36, 2150205 (2021)
6. Talks, M. Hjorth; N. Mueller; etc
7. A. P-O, Antoñito et al: ADAPT-VQE continuation arXiv:2302.03641

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:
     $$\mathscr{H} = \sum_{ij} K_{ij}\, a_i^\dagger a_j + \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l$$
   - ➡ Diagonalization problem

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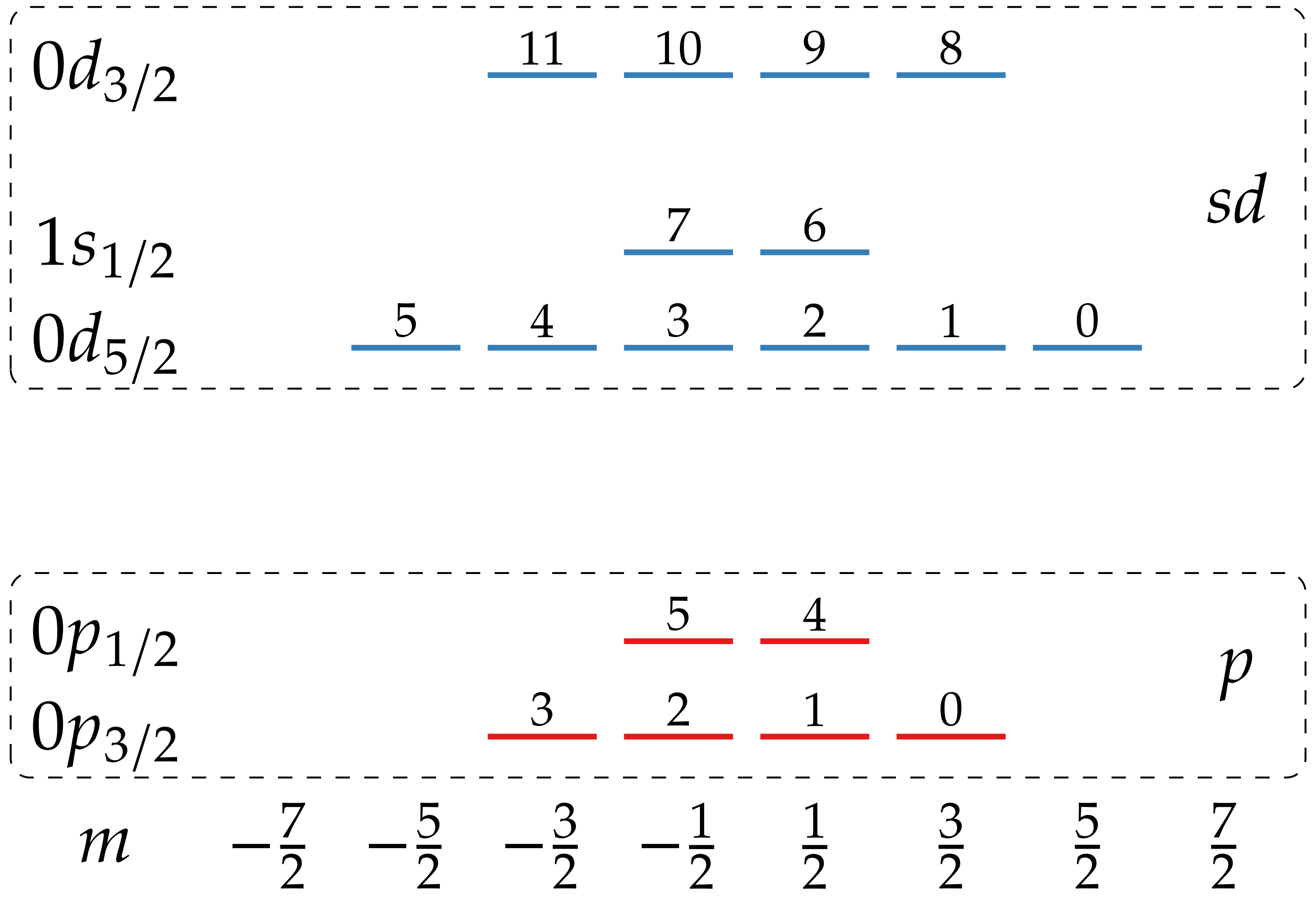

Jordan-Wigner mapping:

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

+ adapt-VQE

arXiv:2302.03641

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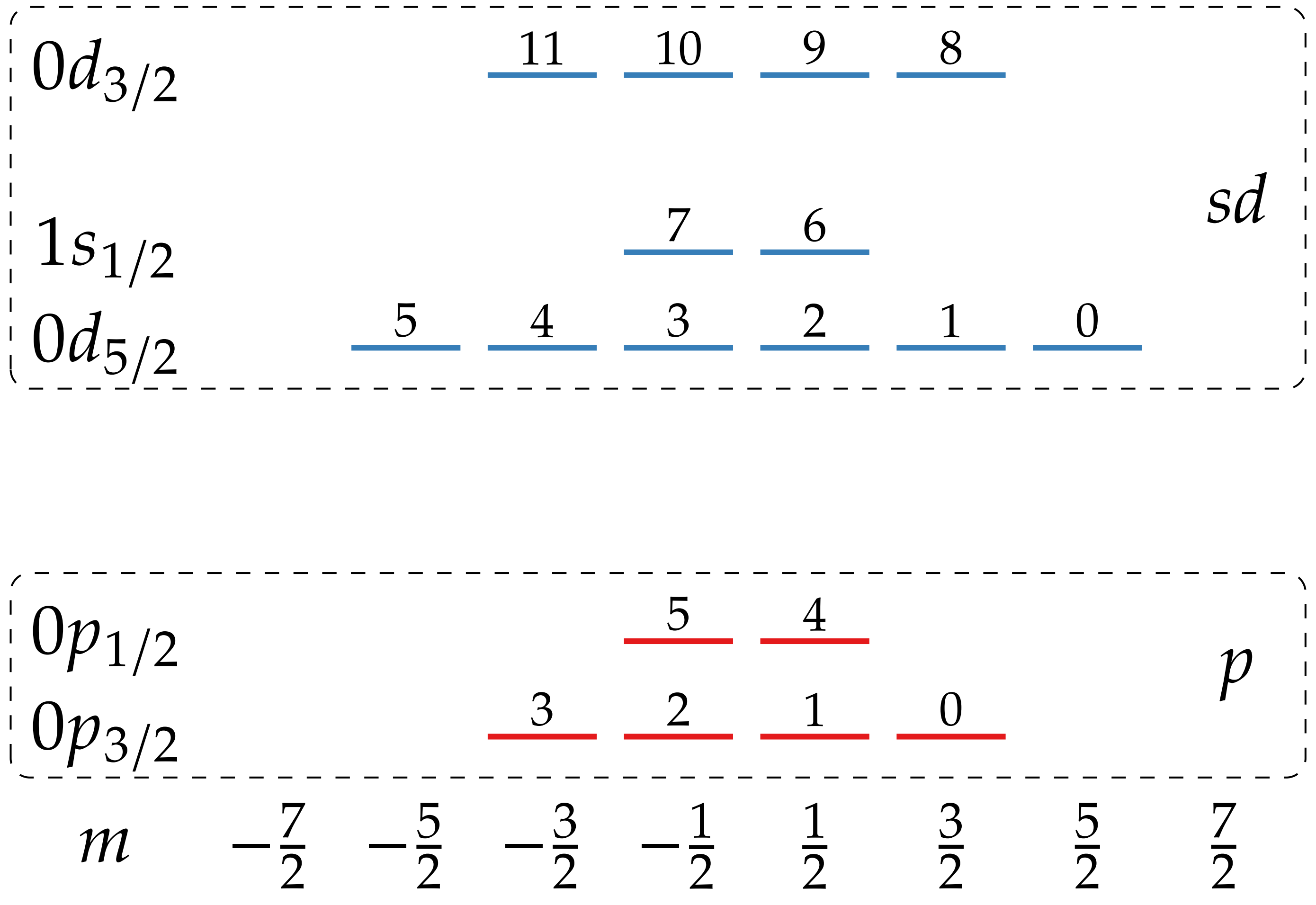

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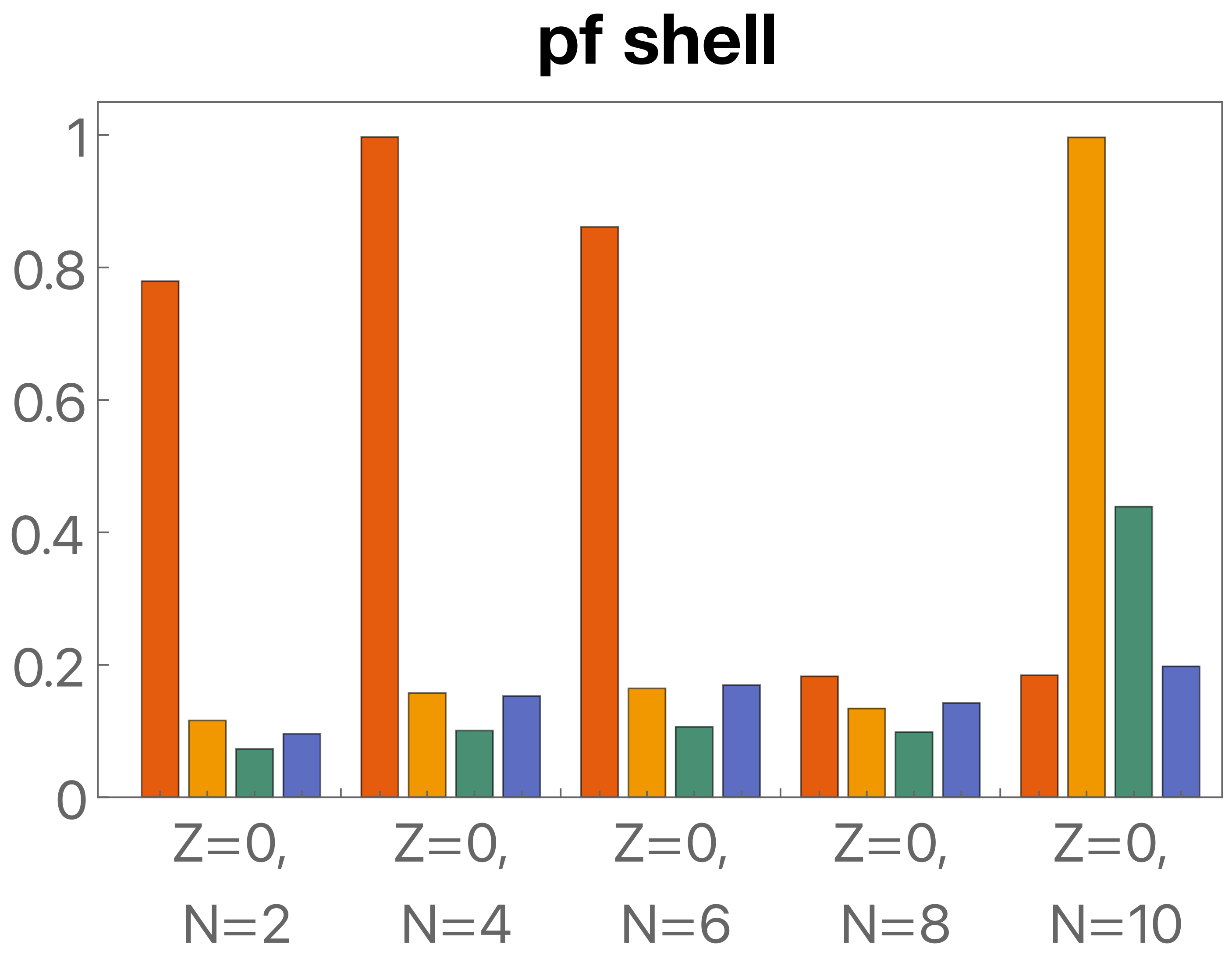
3. Entanglement depends on:

   ➡ Basis chosen (M-scheme, J-scheme)

   ➡ fermion-qubit mappings (JW, BK, VC)

   ➡ Partition (1 orbital, 2 orbital, equipartition)

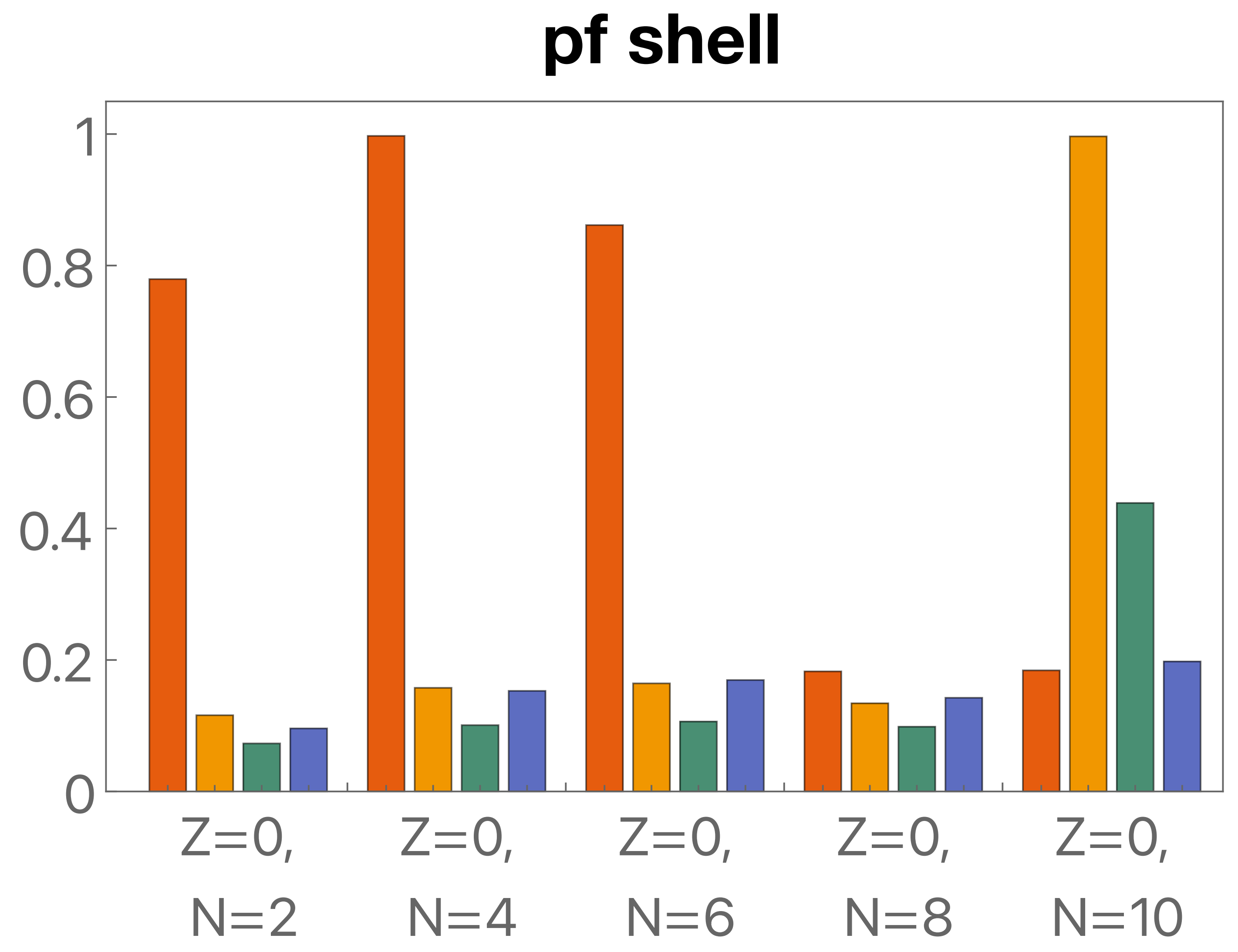
single orbital & orbital-orbital entanglement



$$S_i = -Tr(\rho_i \log(\rho_i))$$

↔ **“naive” filling of the shells**

single orbital & orbital-orbital entanglement



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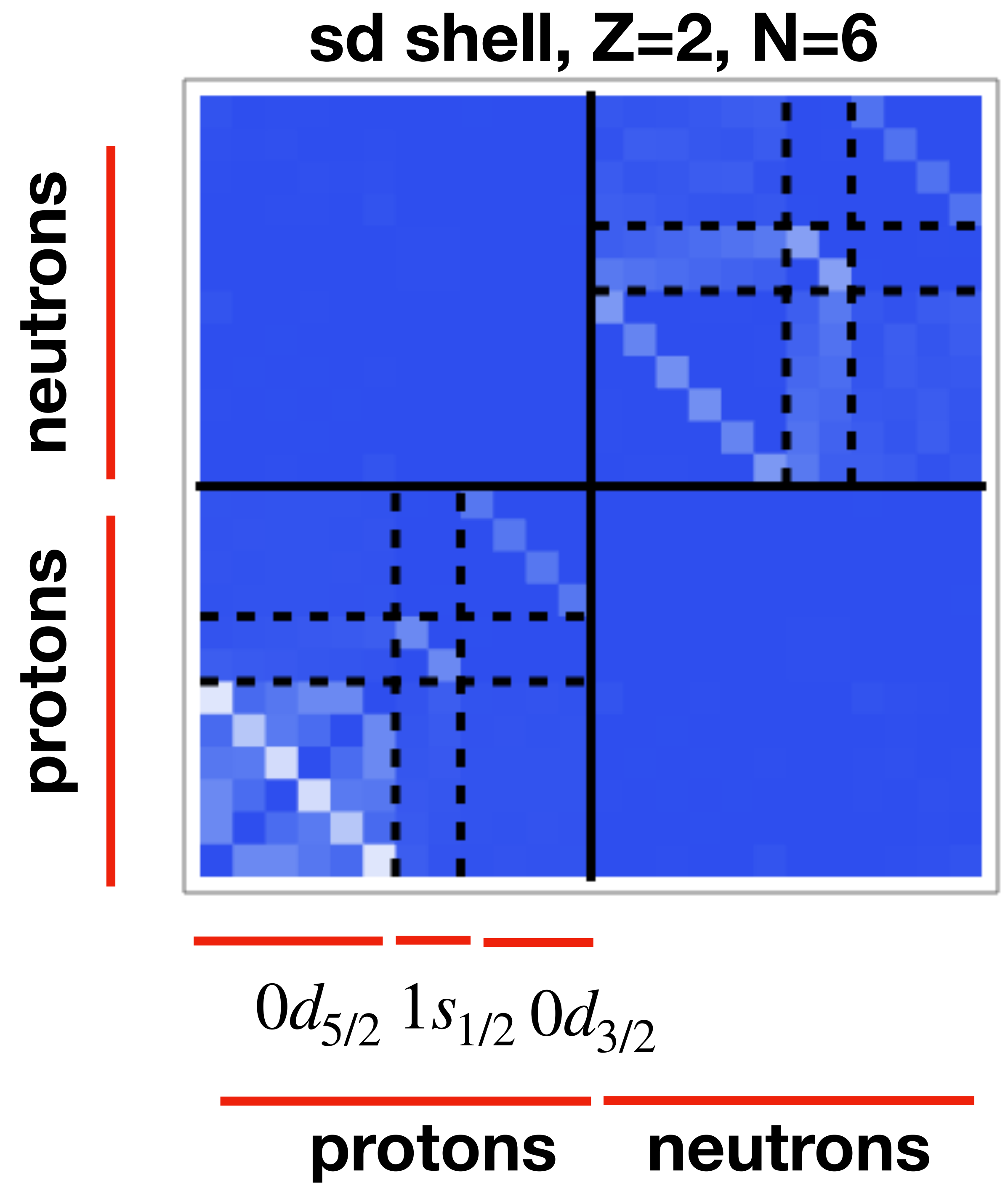
"naive" filling of the shells

mutual information

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

gives a better overall picture:



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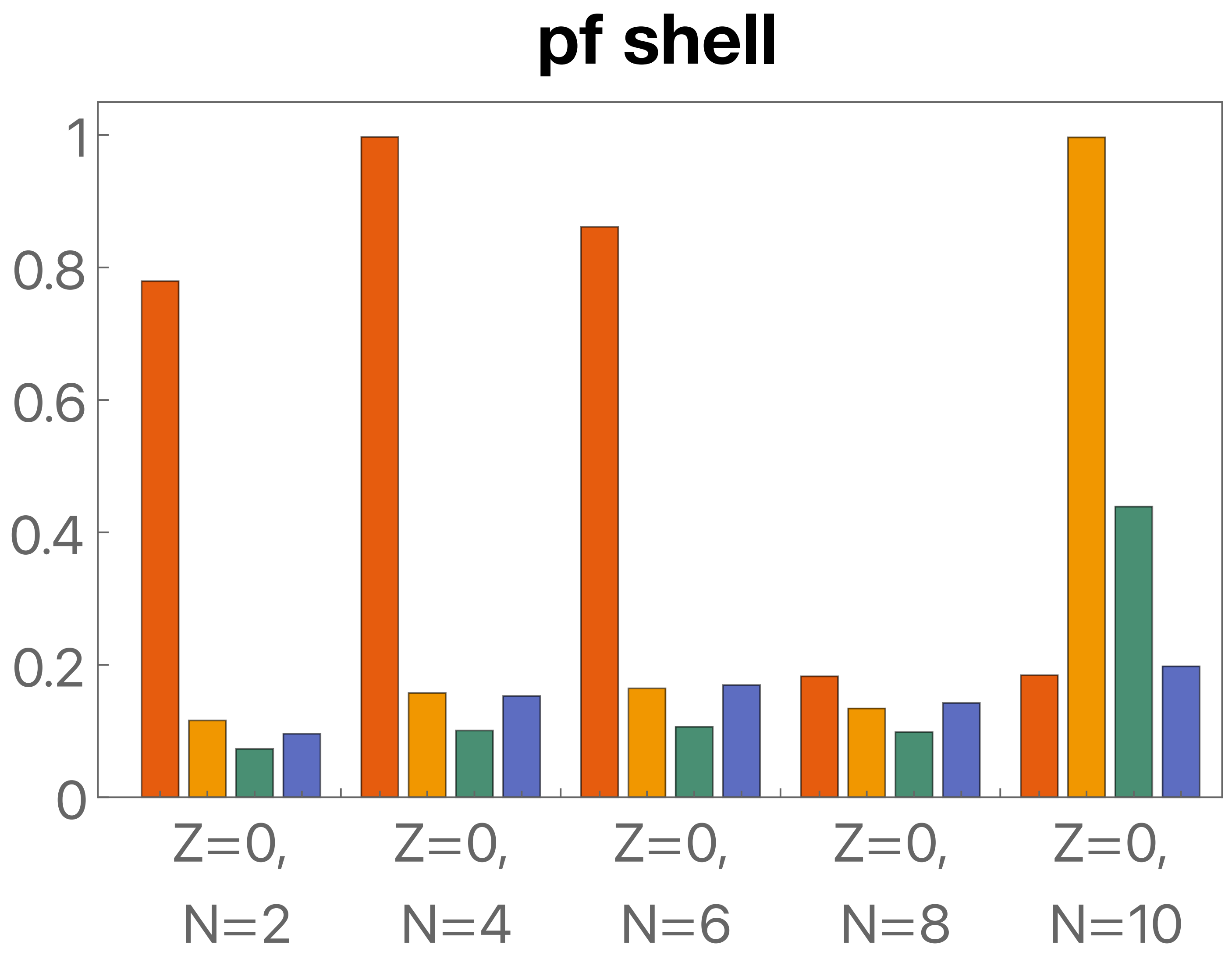

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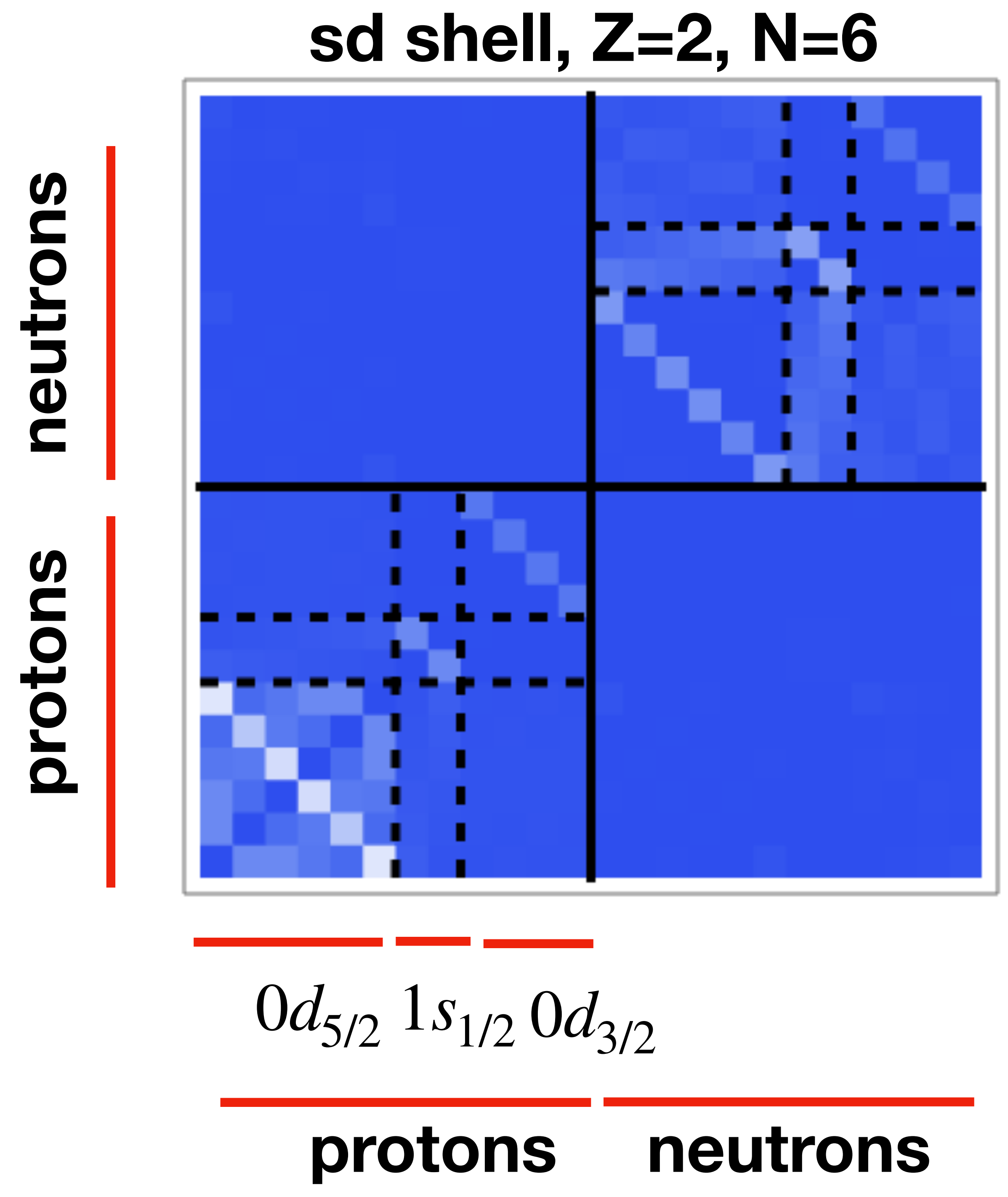
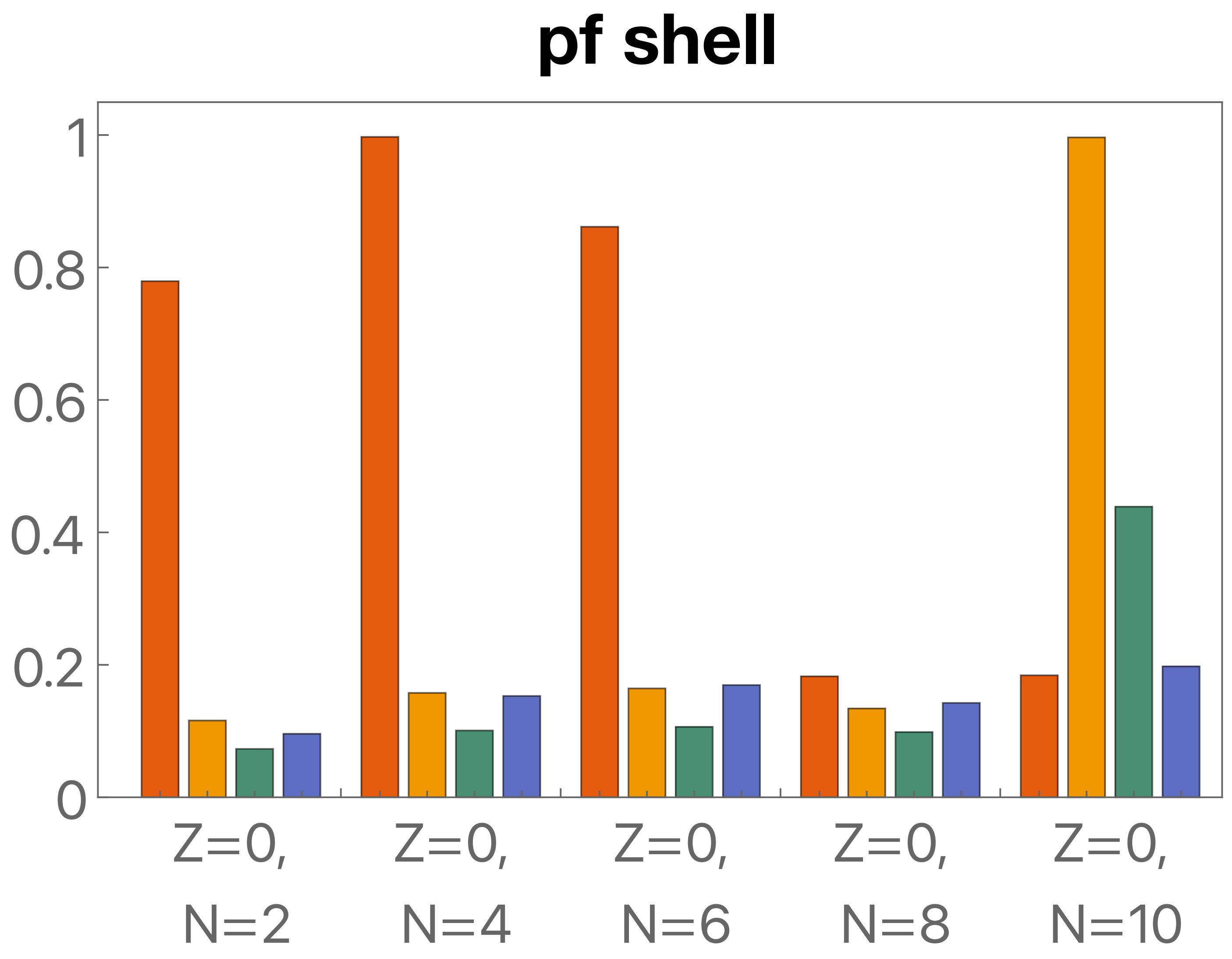


Is entanglement correlated with complexity of the VQE ansatz?

single orbital & orbital-orbital entanglement



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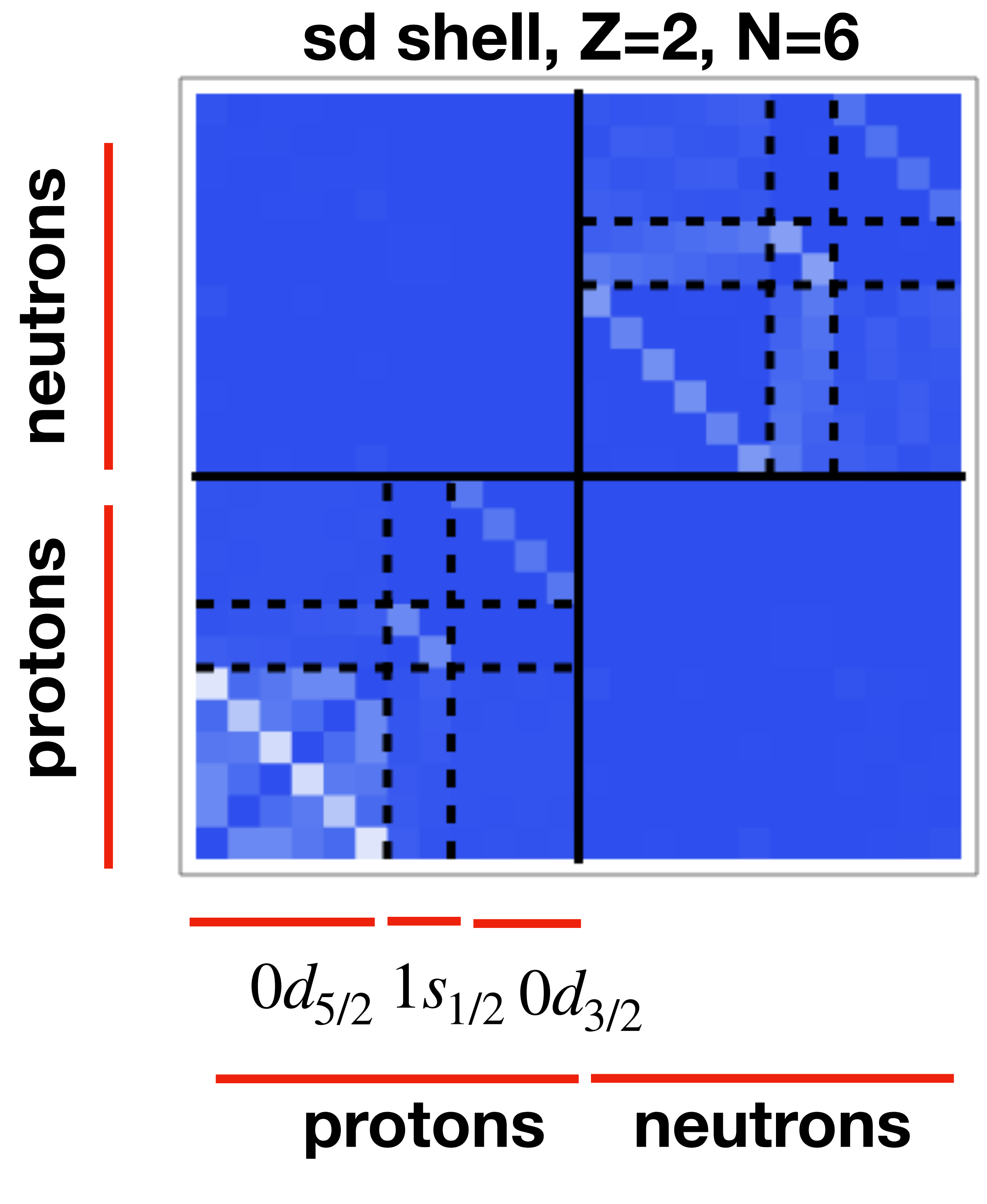

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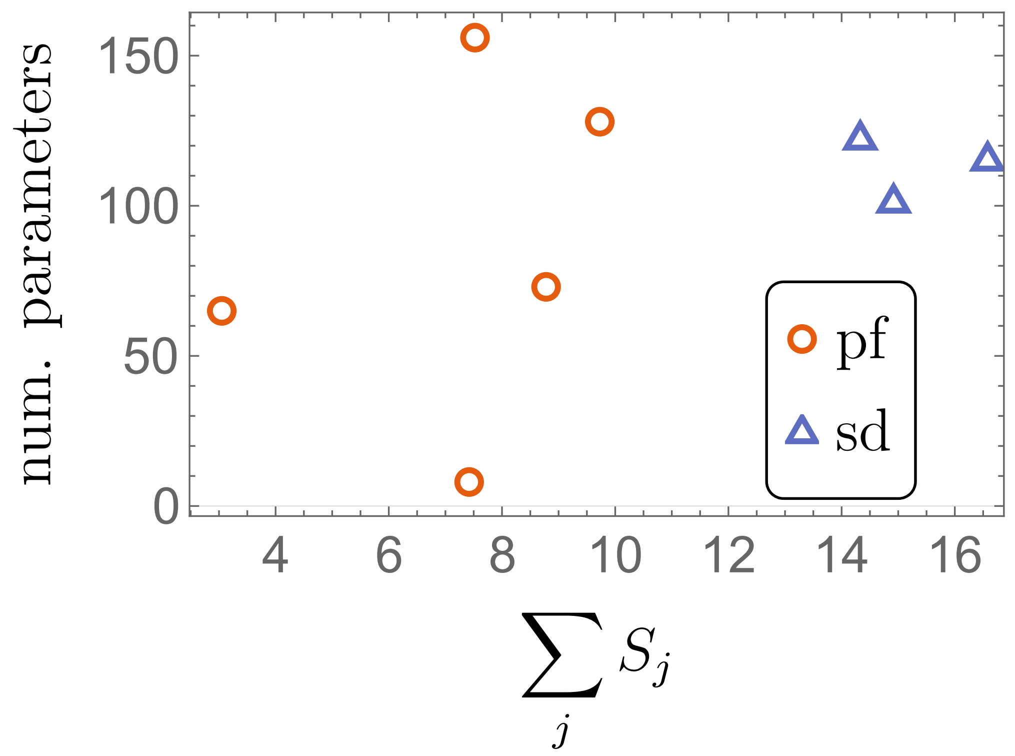
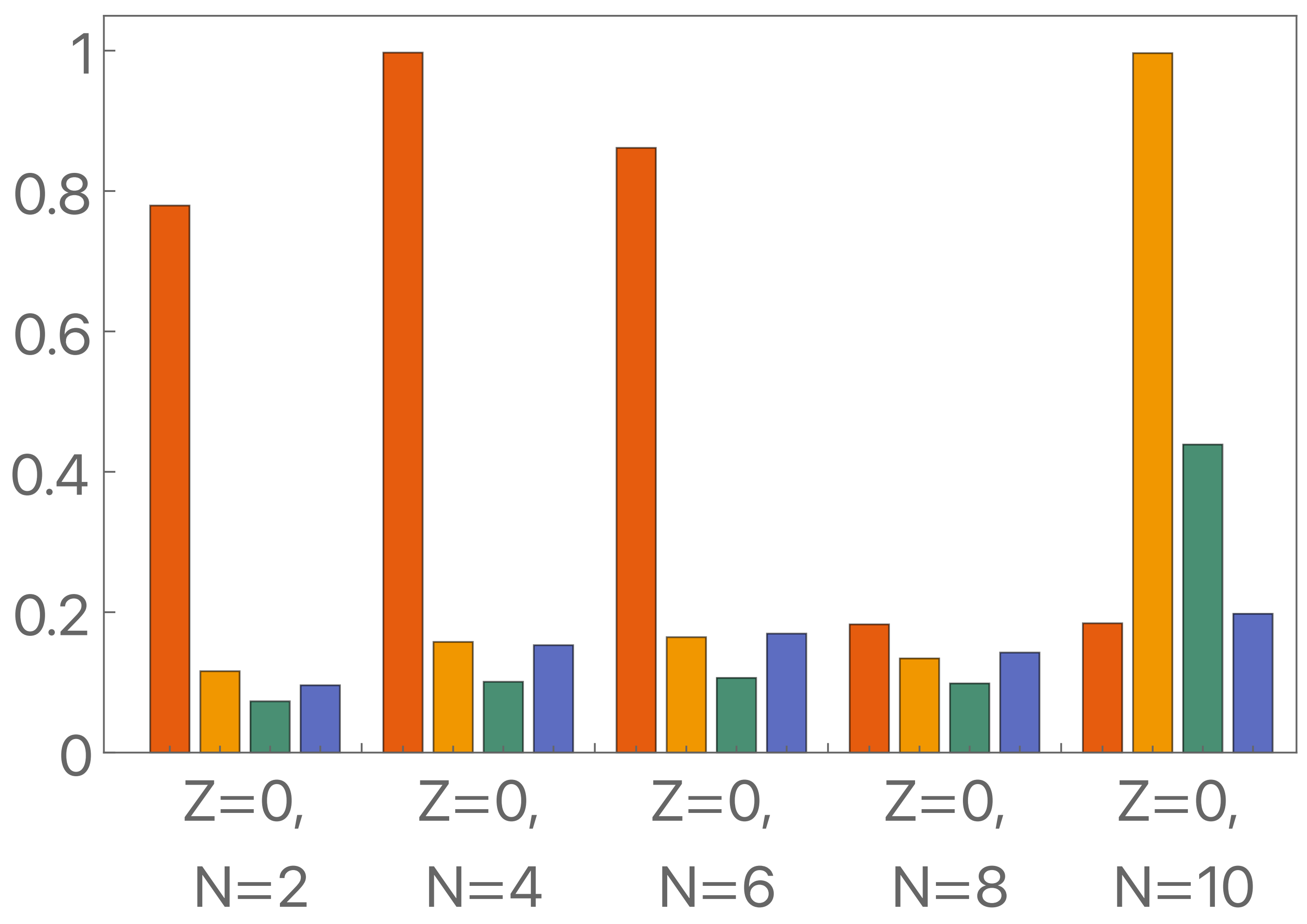


(no)

single orbital & orbital-orbital entanglement

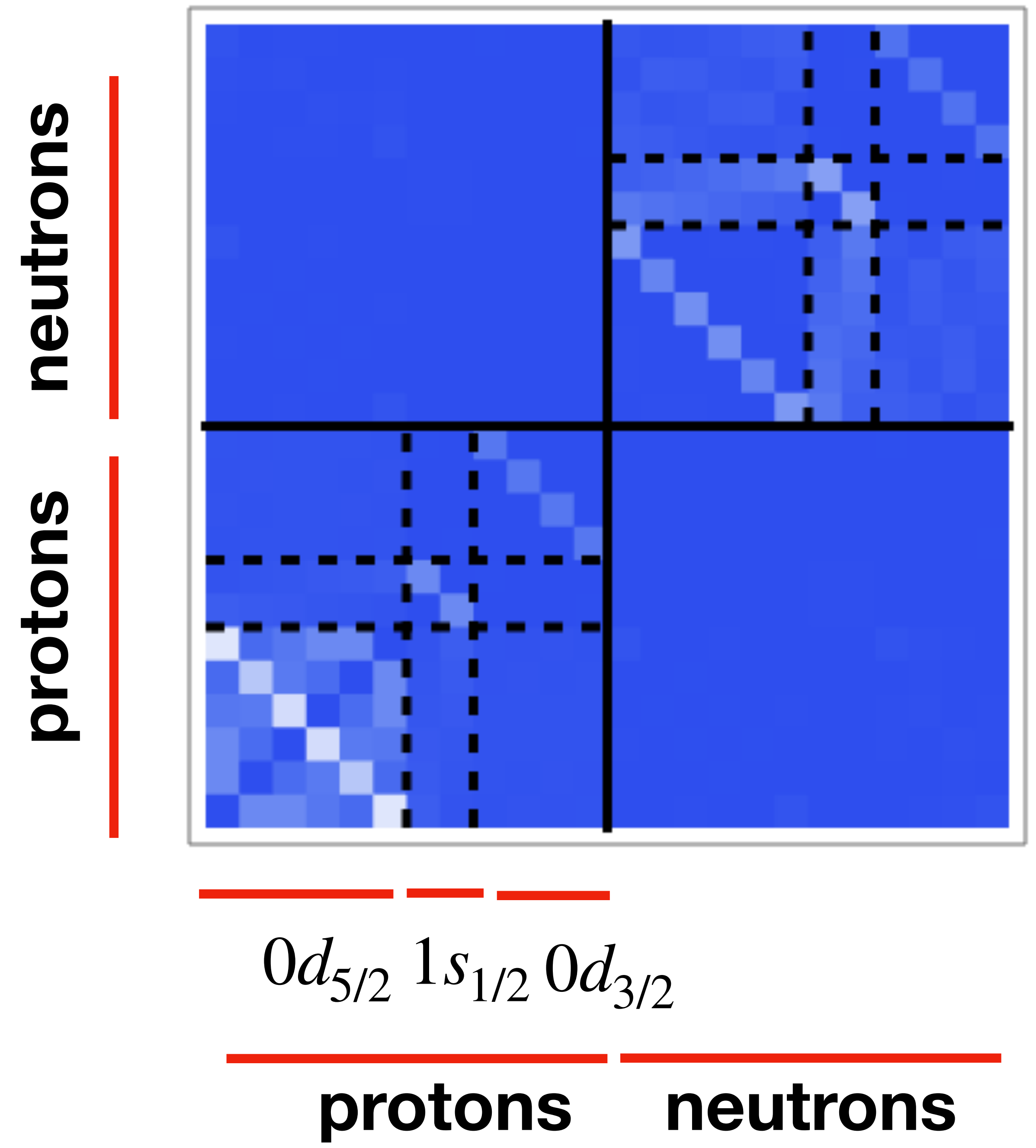
pf shell



$S_i = -Tr(\rho_i \log(\rho_i))$ ⟷ **"naive" filling of the shells**

sd shell, Z=2, N=6

mutual information $S_i + S_j - S_{ij}$ gives a better overall picture:



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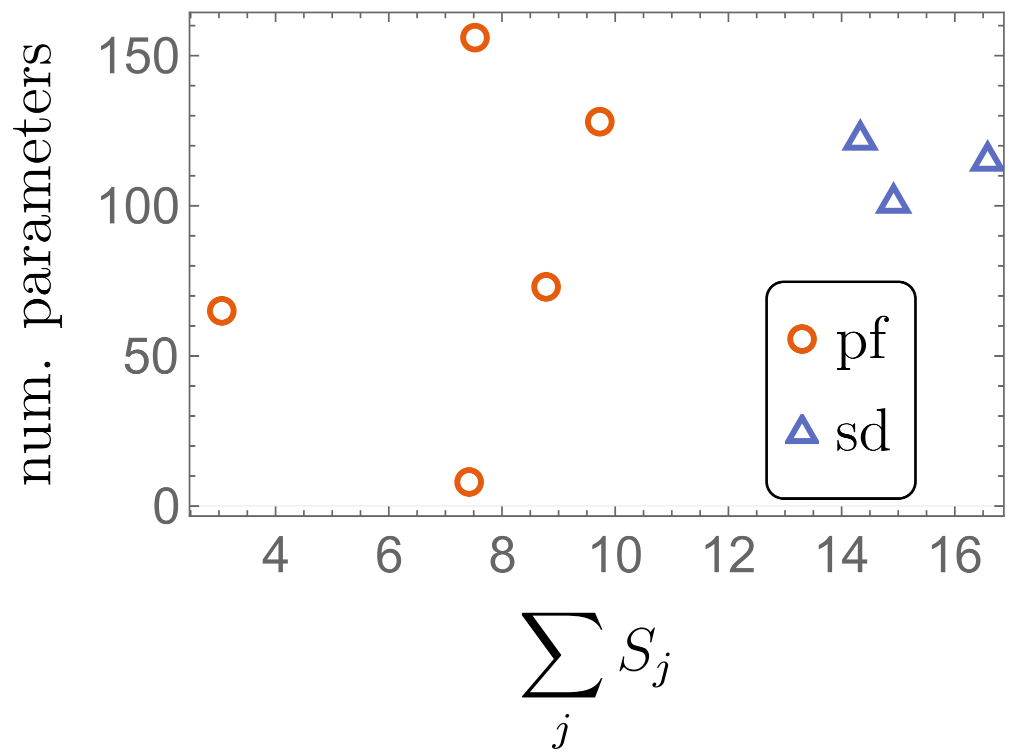

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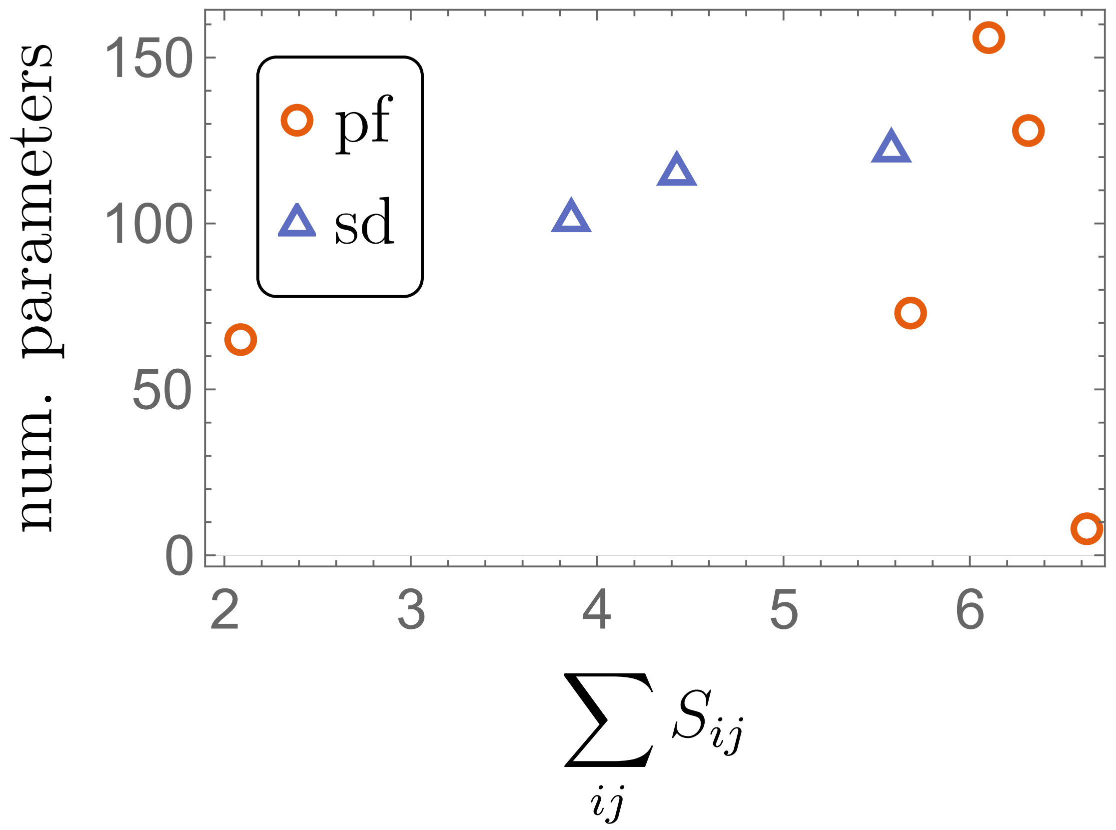
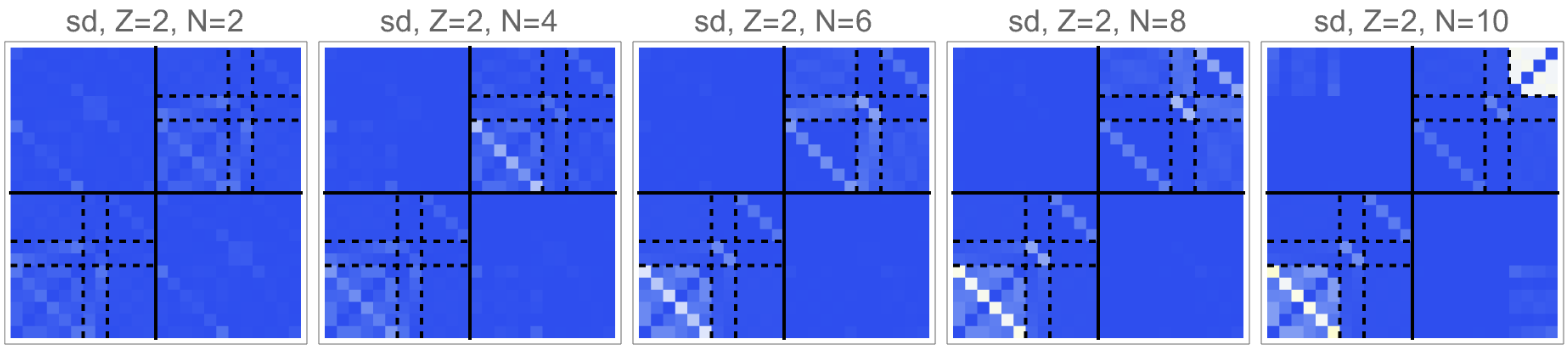


(a little?)

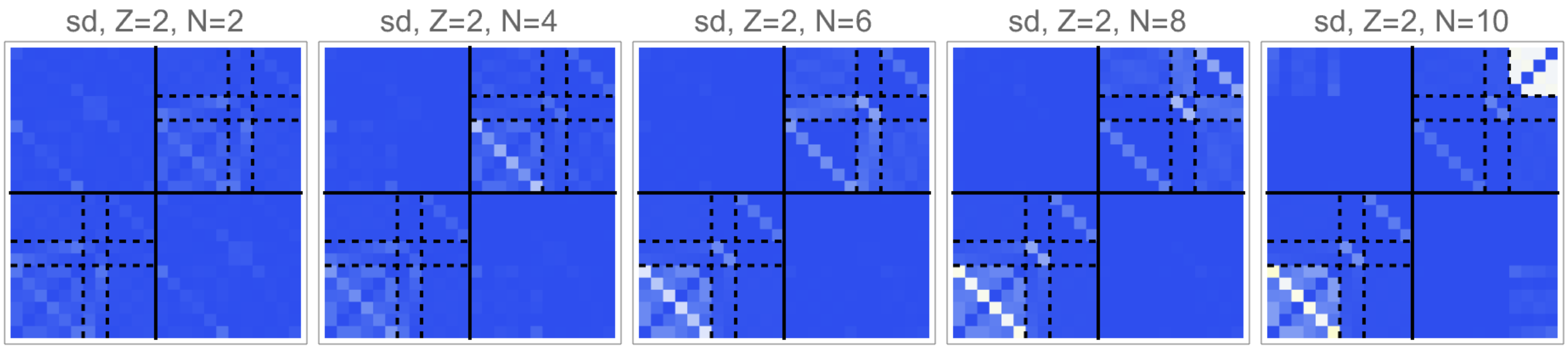
-only localized entanglement

-VQE might not entangle efficiently

mutual information across the sd shell

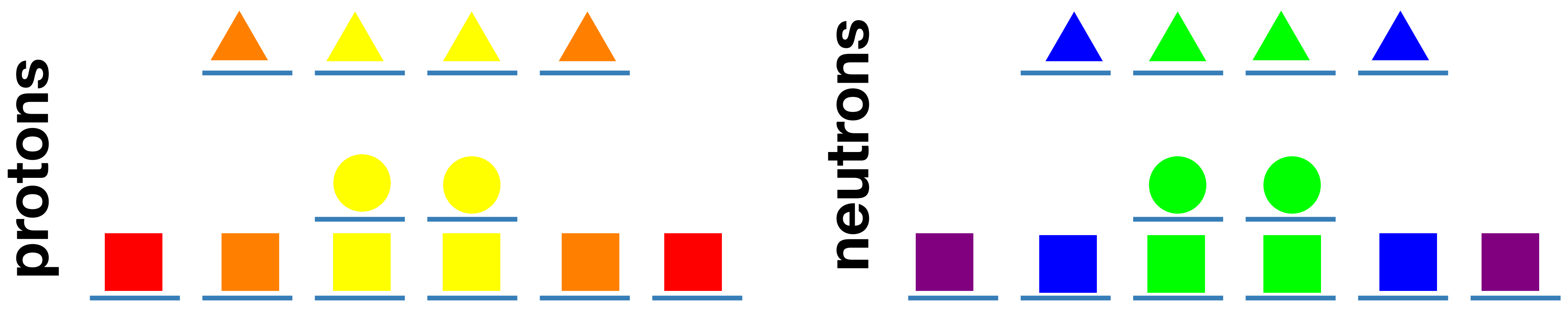


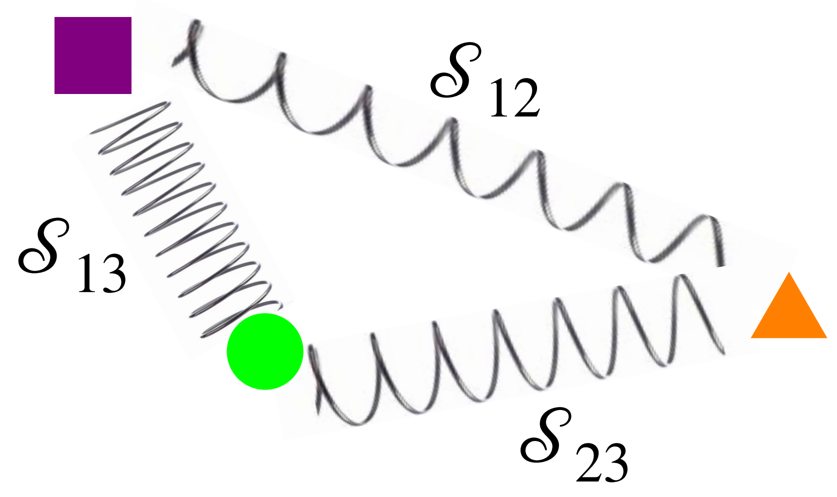
mutual information across the sd shell



color ↔ |M|

shape ↔ subshell





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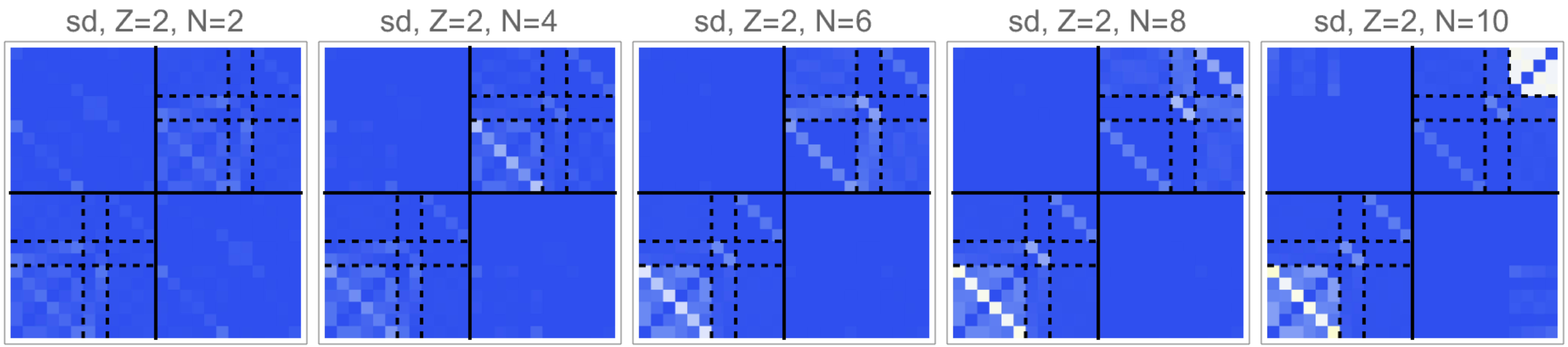

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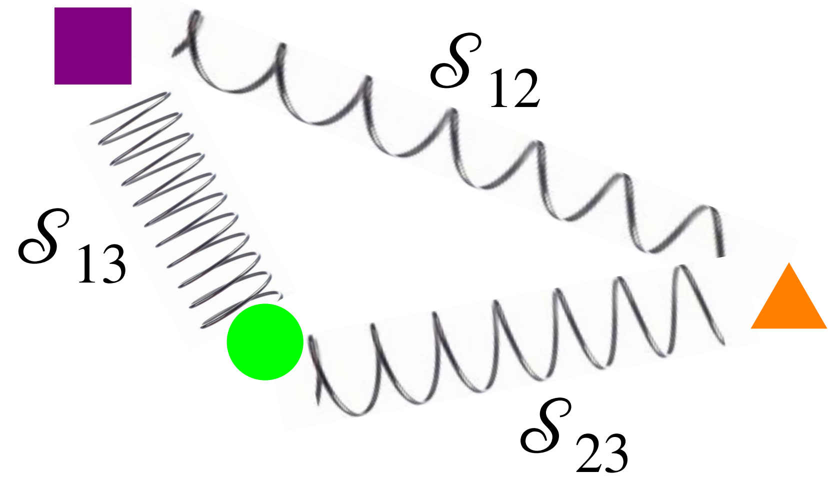

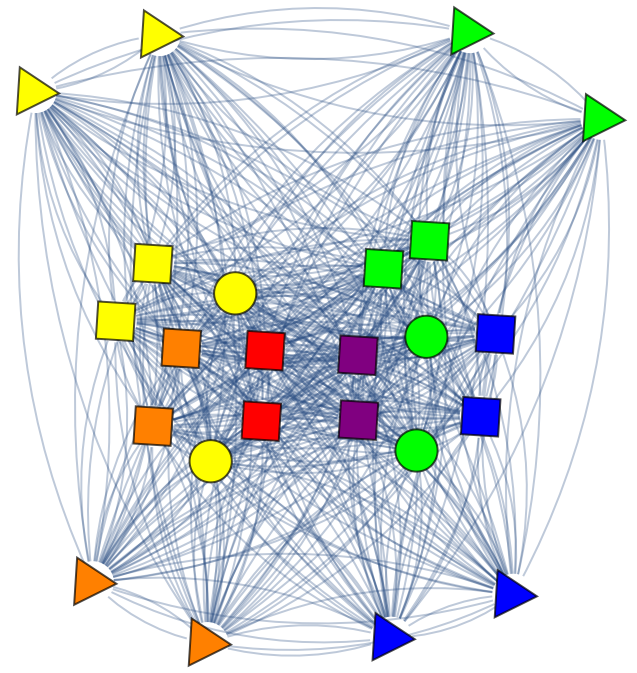

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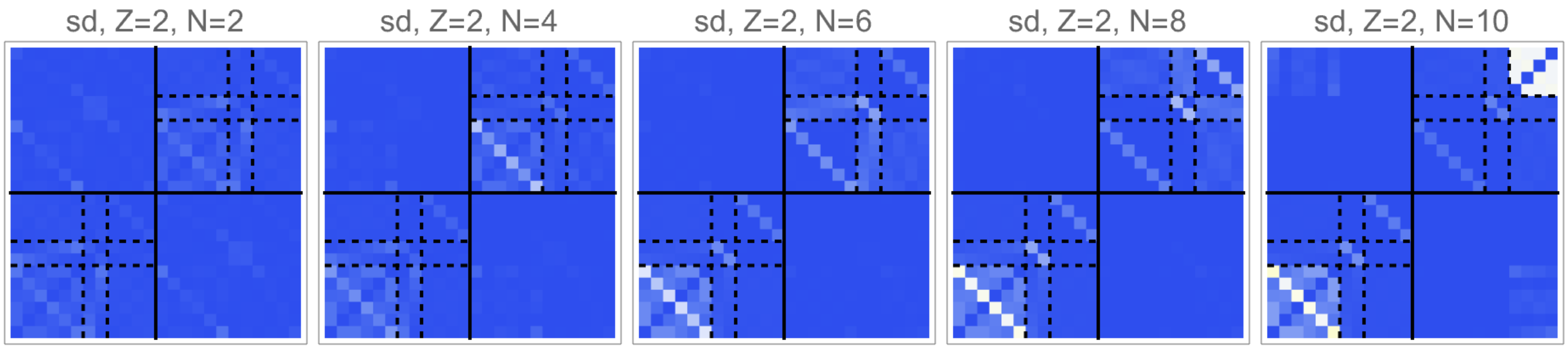

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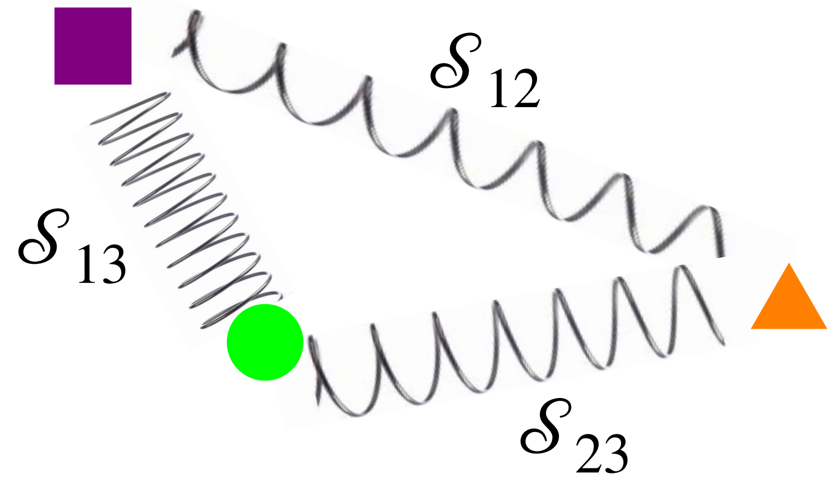
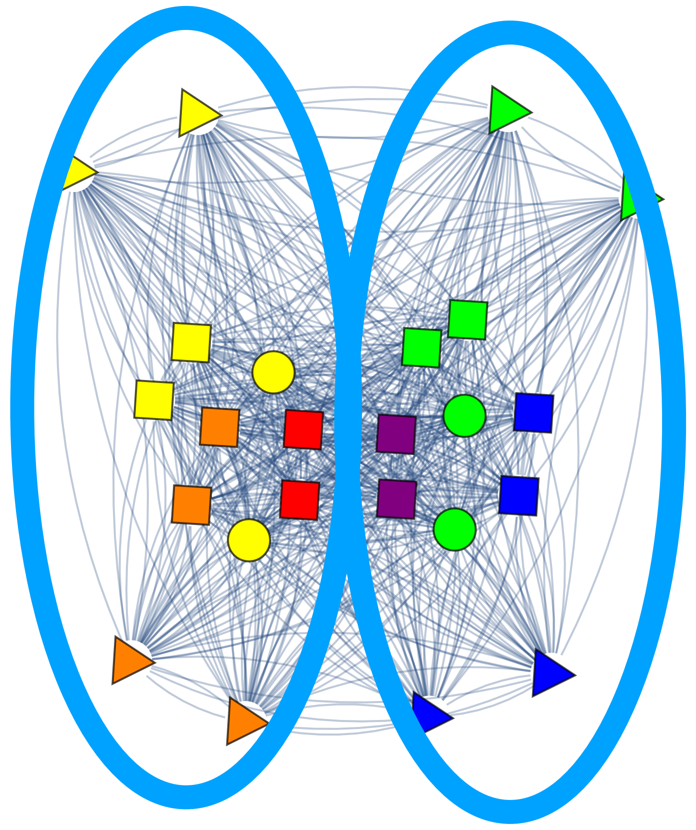
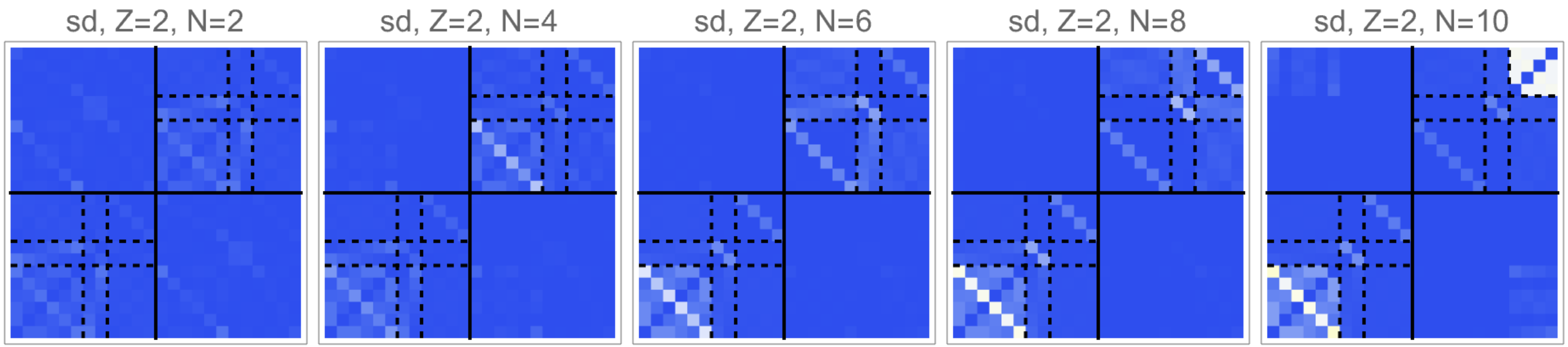




-minimizing "energy" clusters protons and neutrons

mutual information across the sd shell



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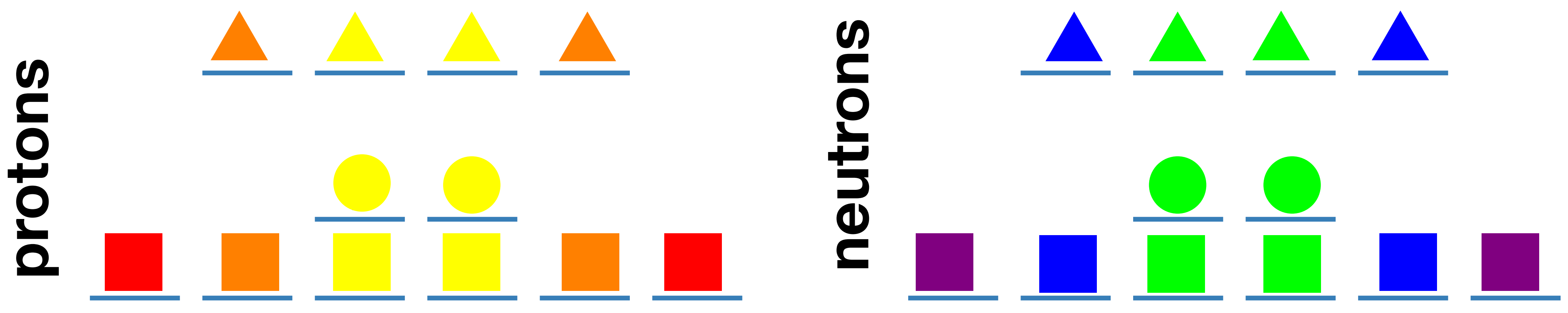
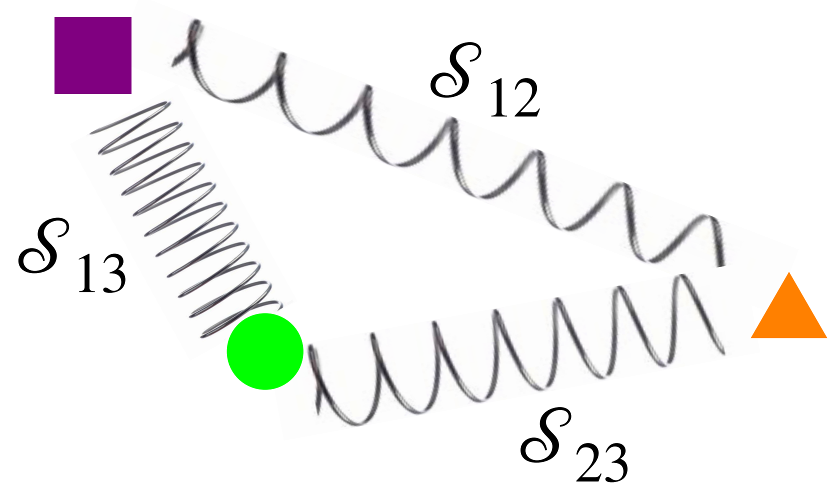
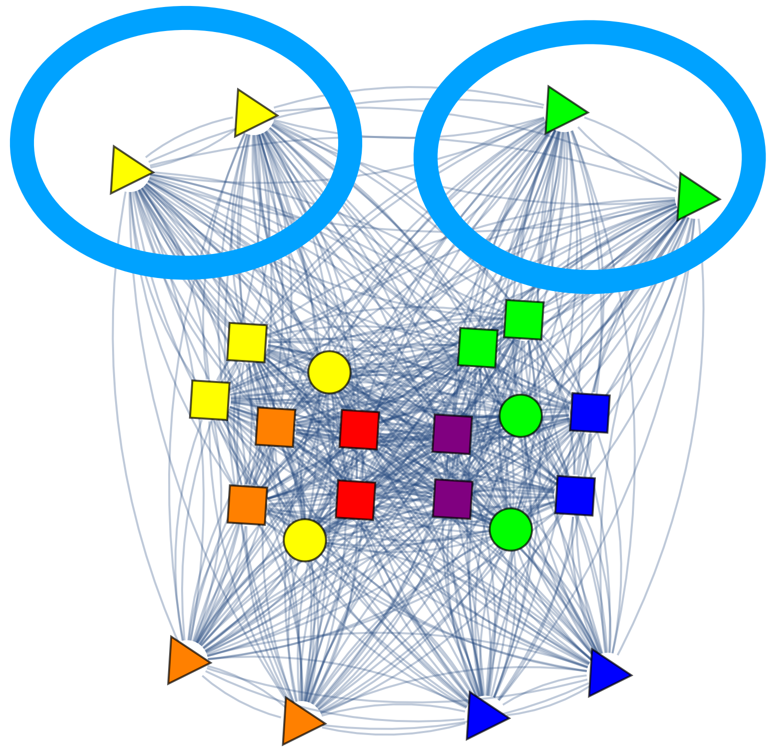
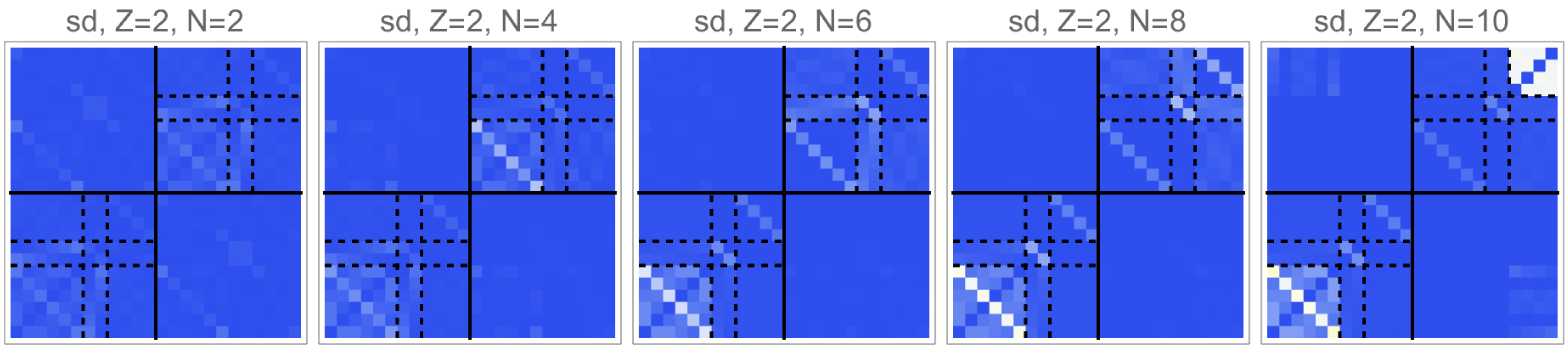






-empty / not entangled orbitals in the periphery

mutual information across the sd shell



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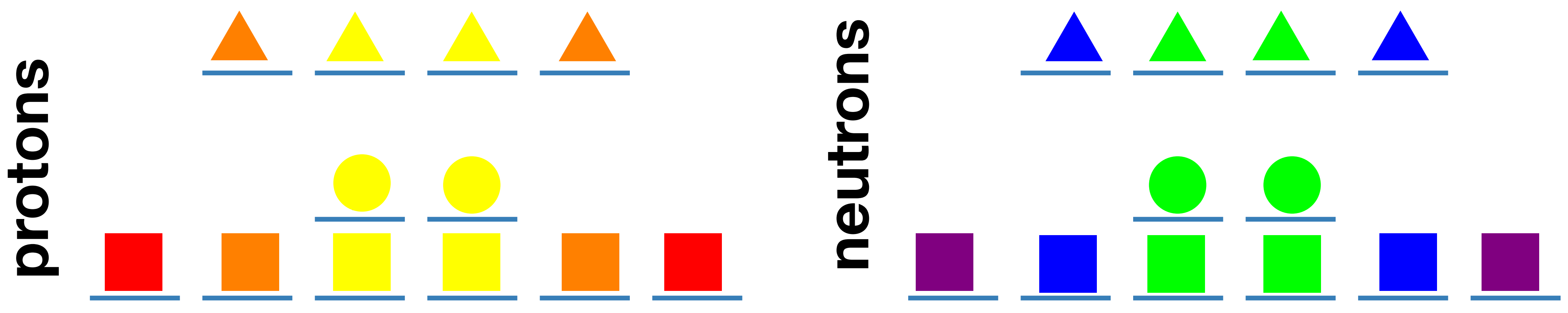
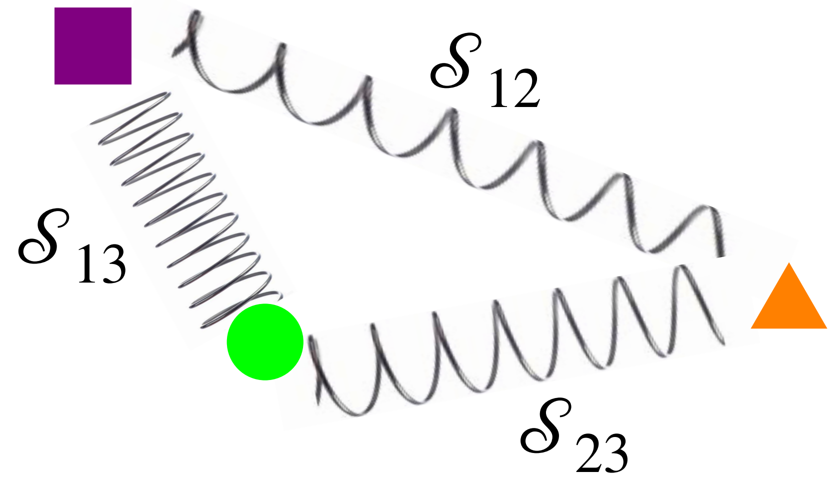
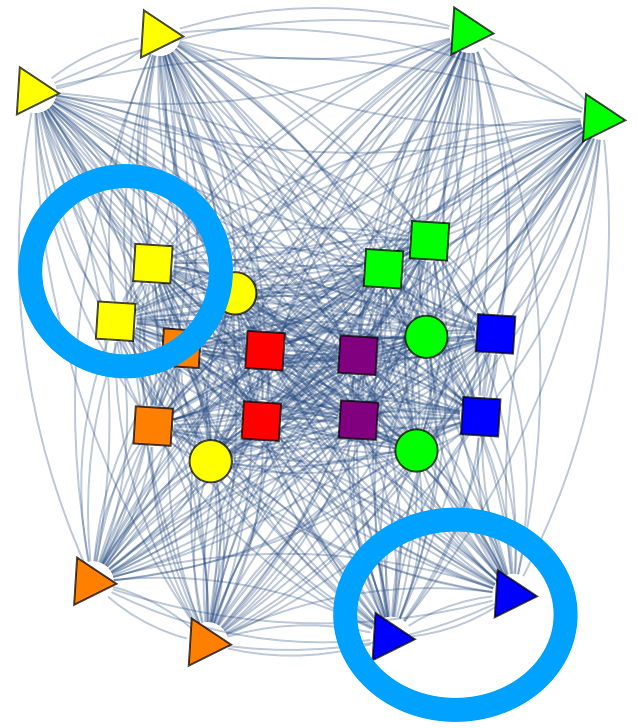
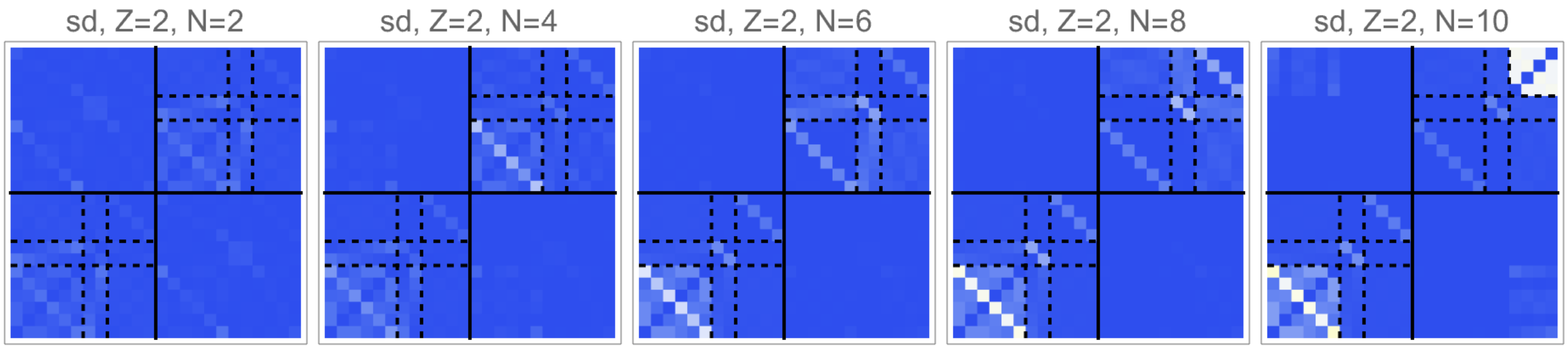






-automatic pairing
M<0 & M>0

mutual information across the sd shell



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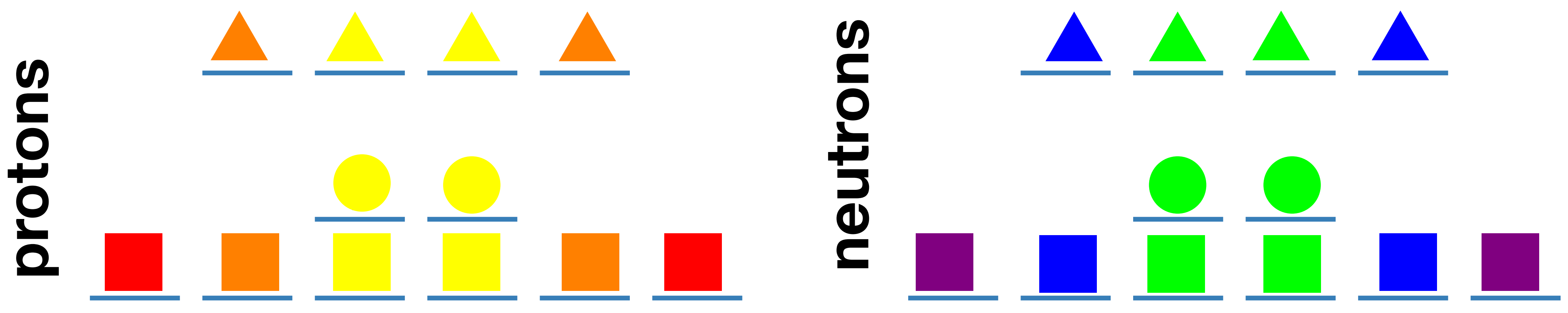
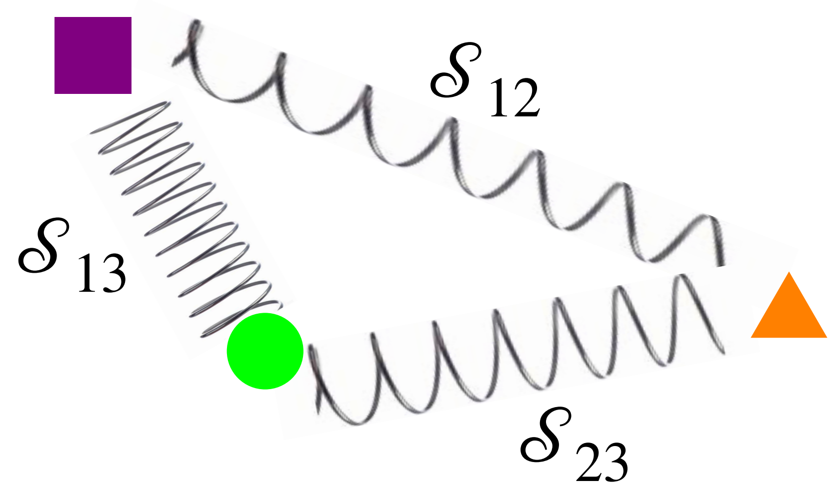
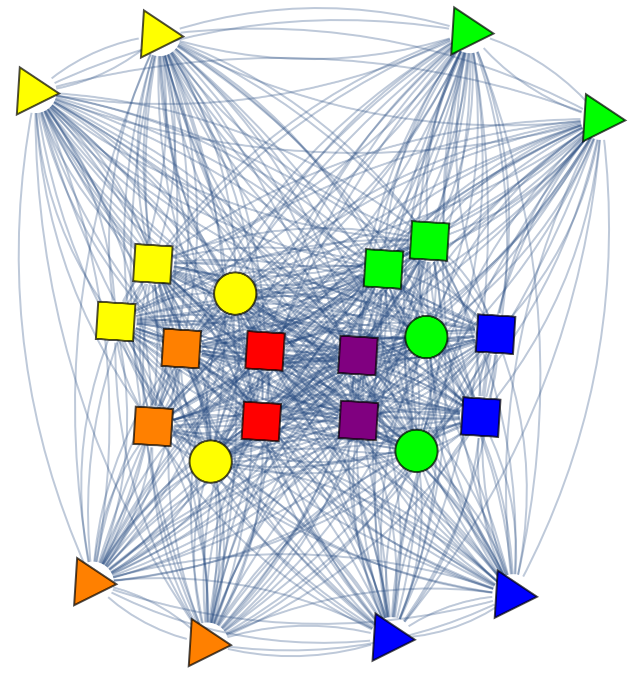
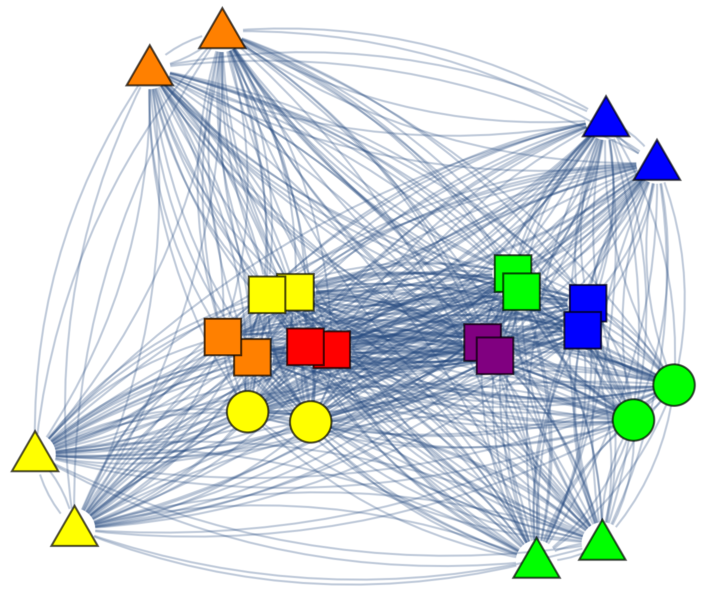
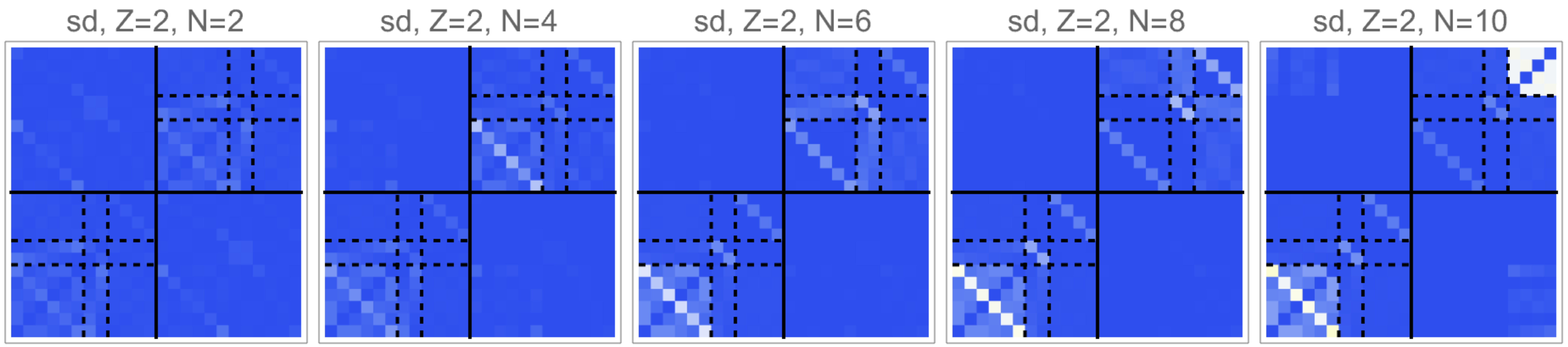








mutual information across the sd shell



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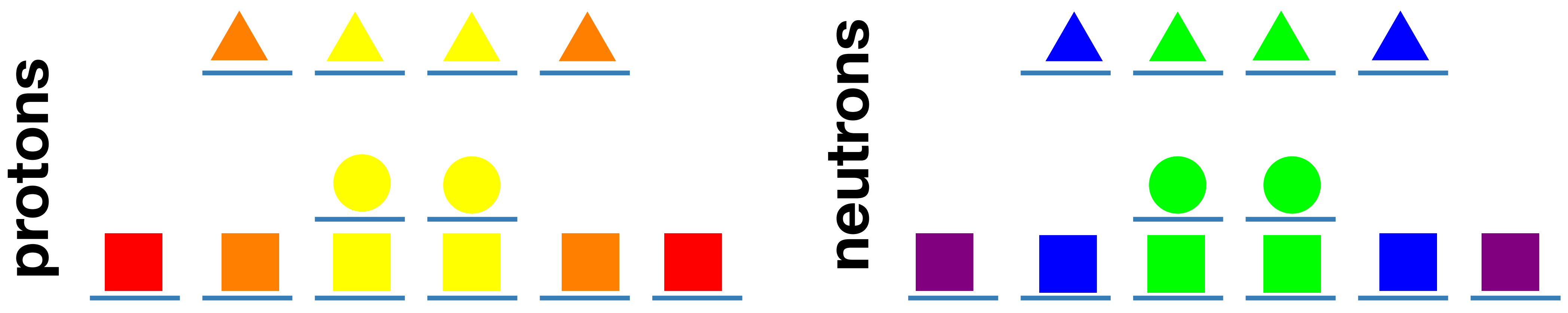

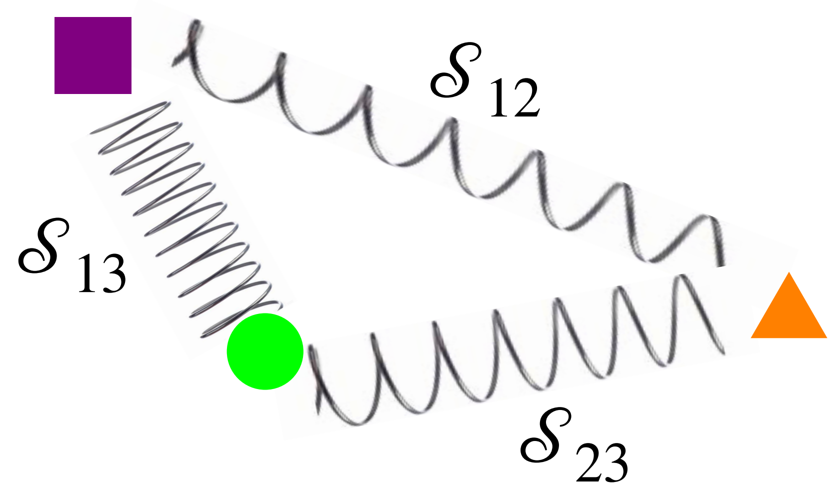

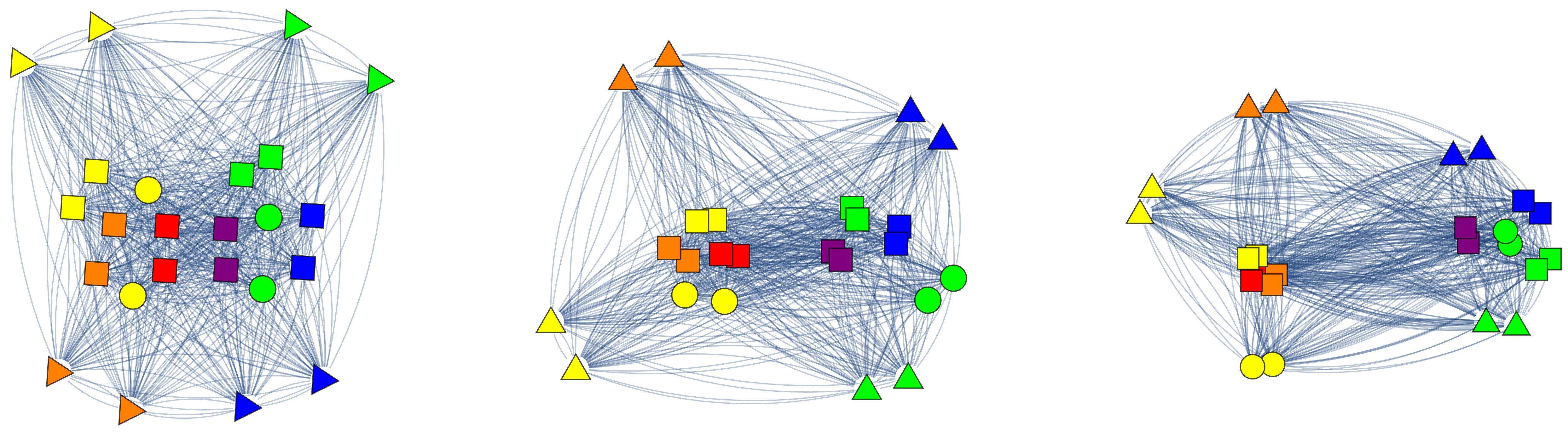

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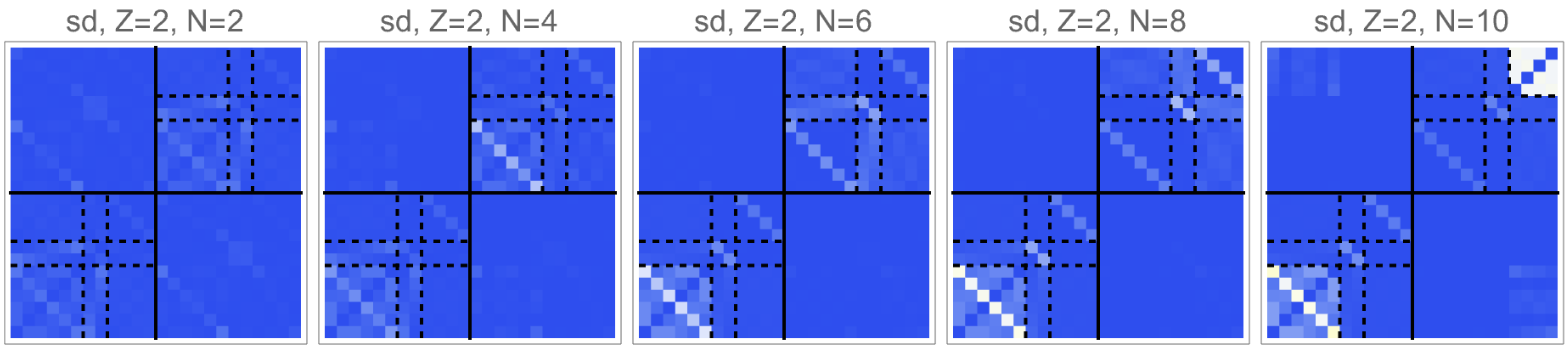

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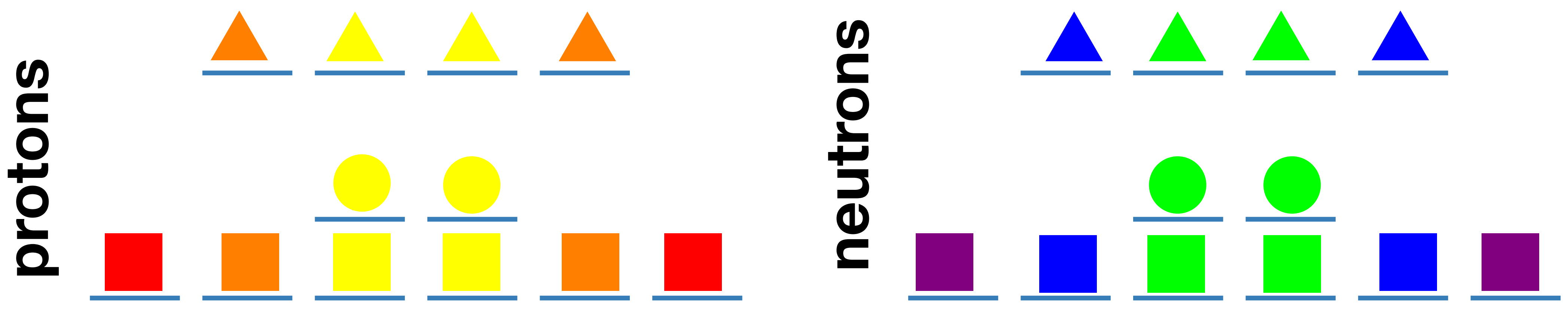

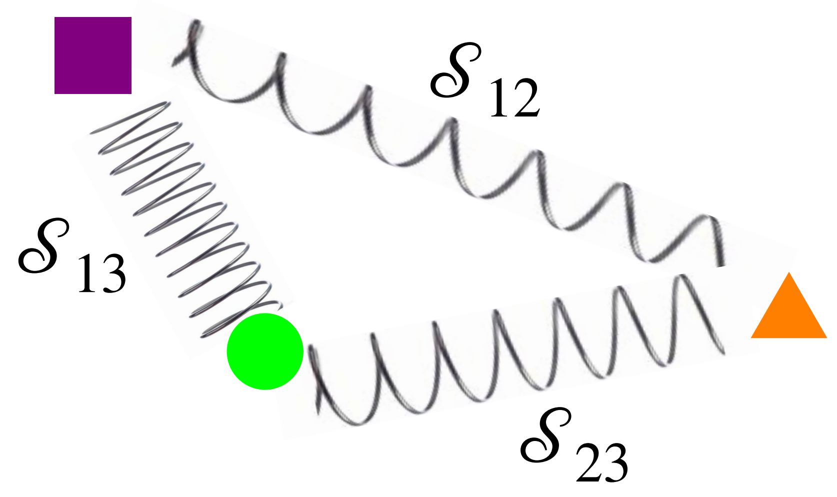

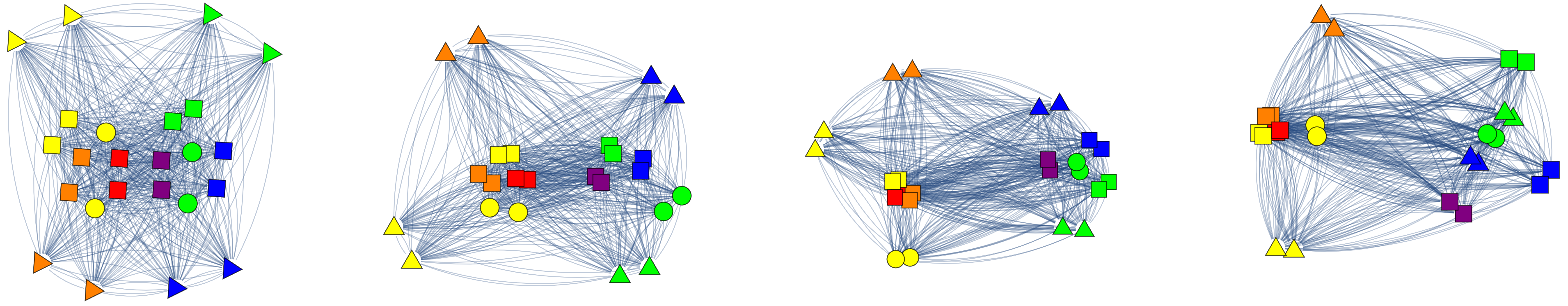

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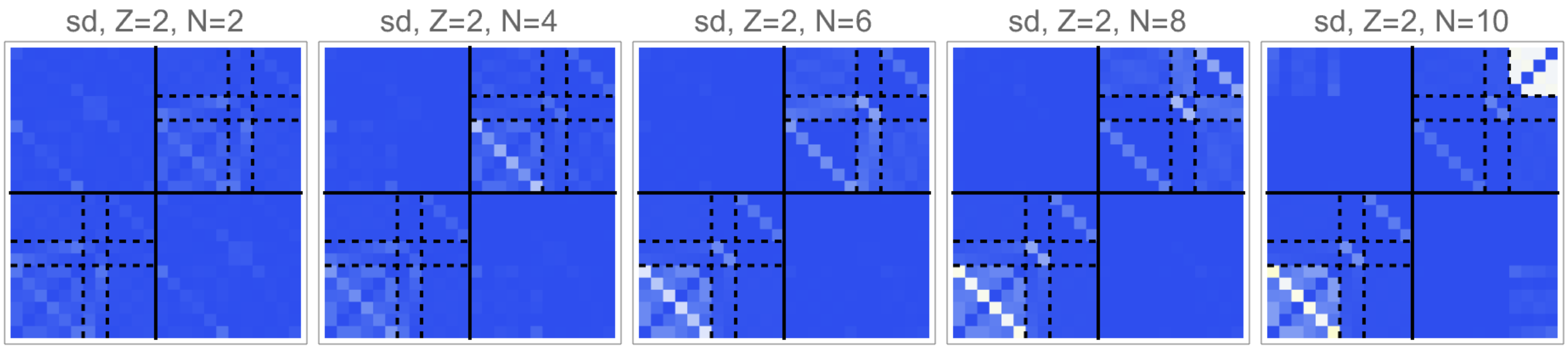
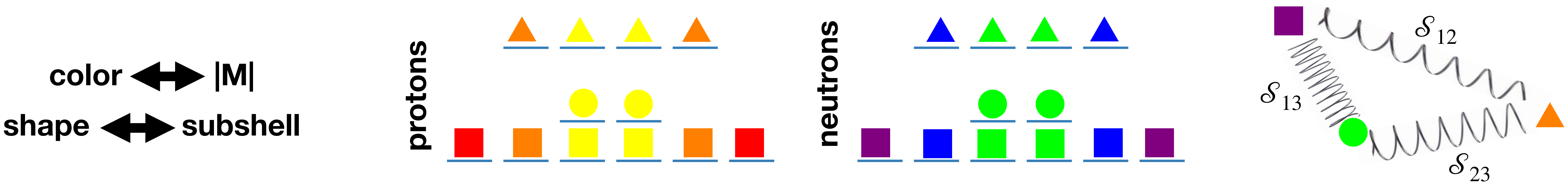
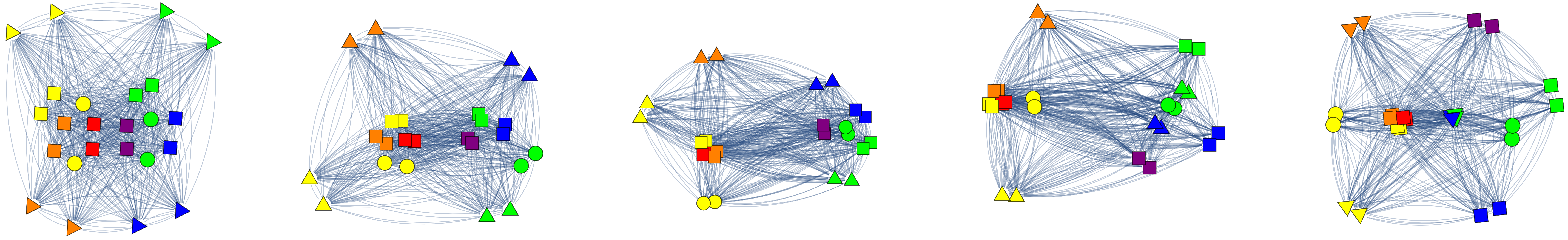
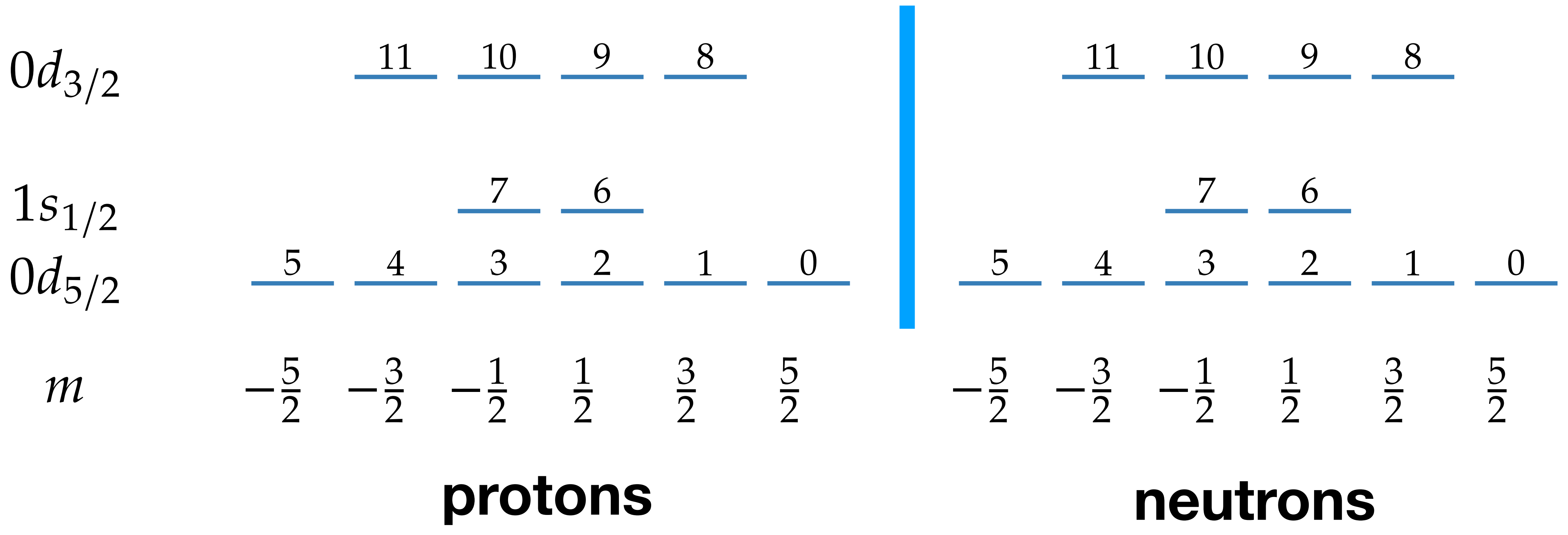


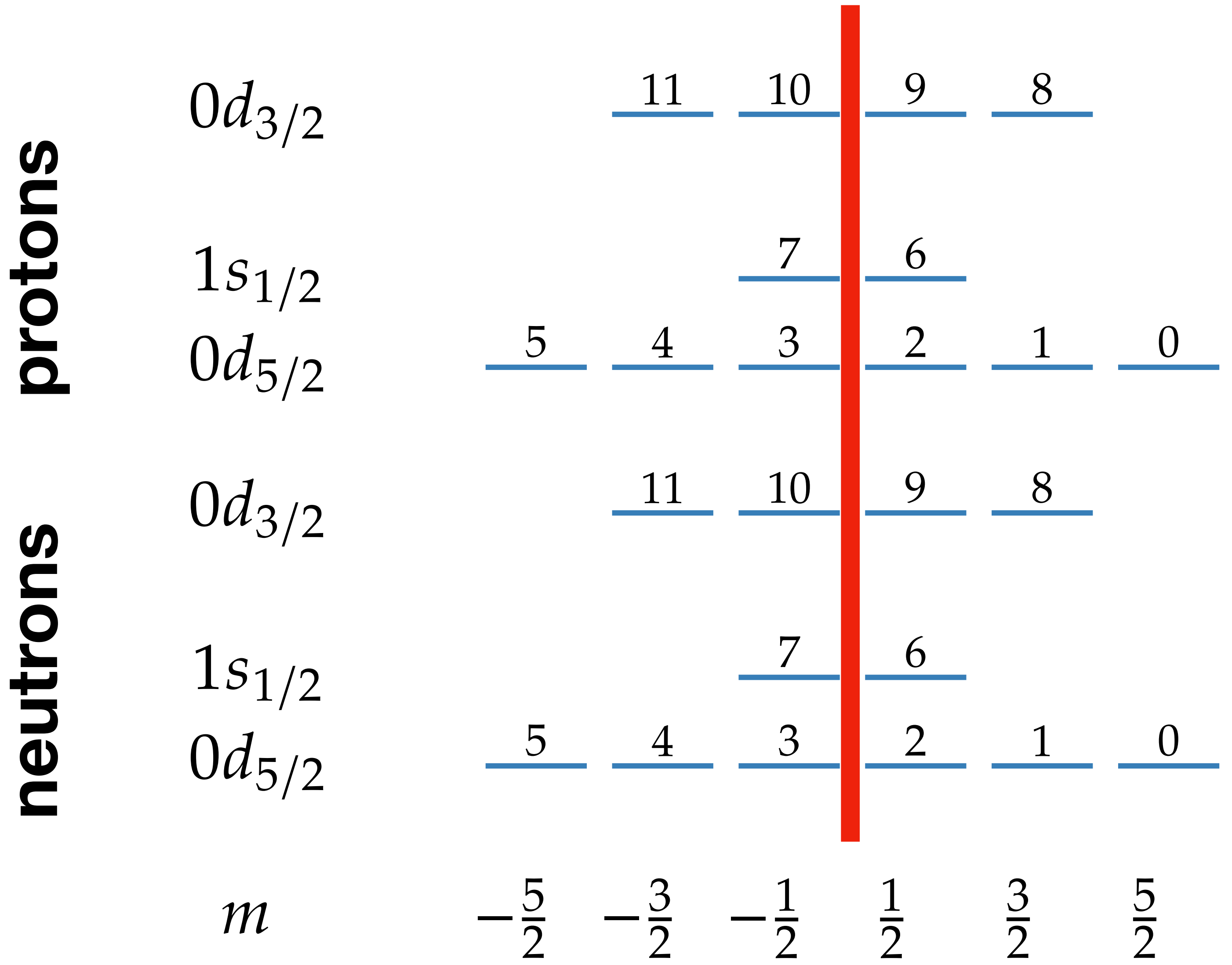




equipartition entanglement

most natural partitions





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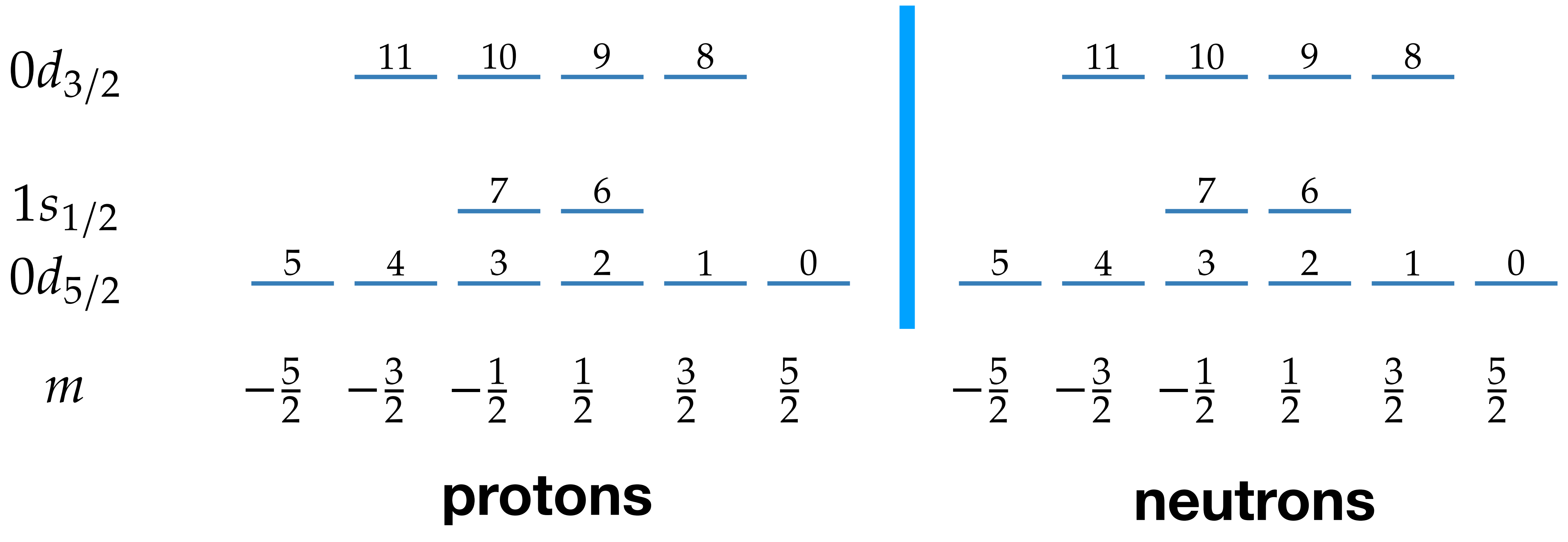
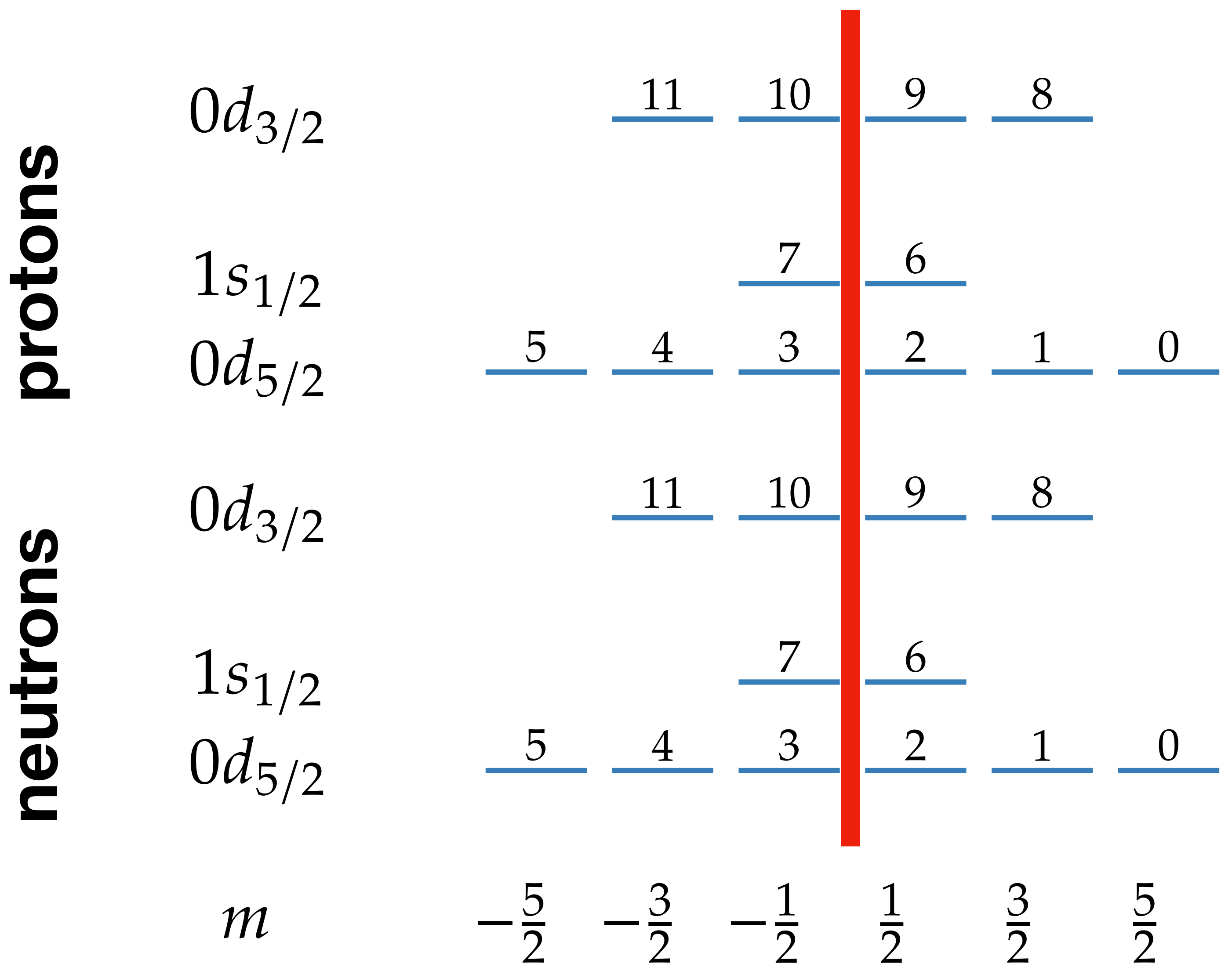
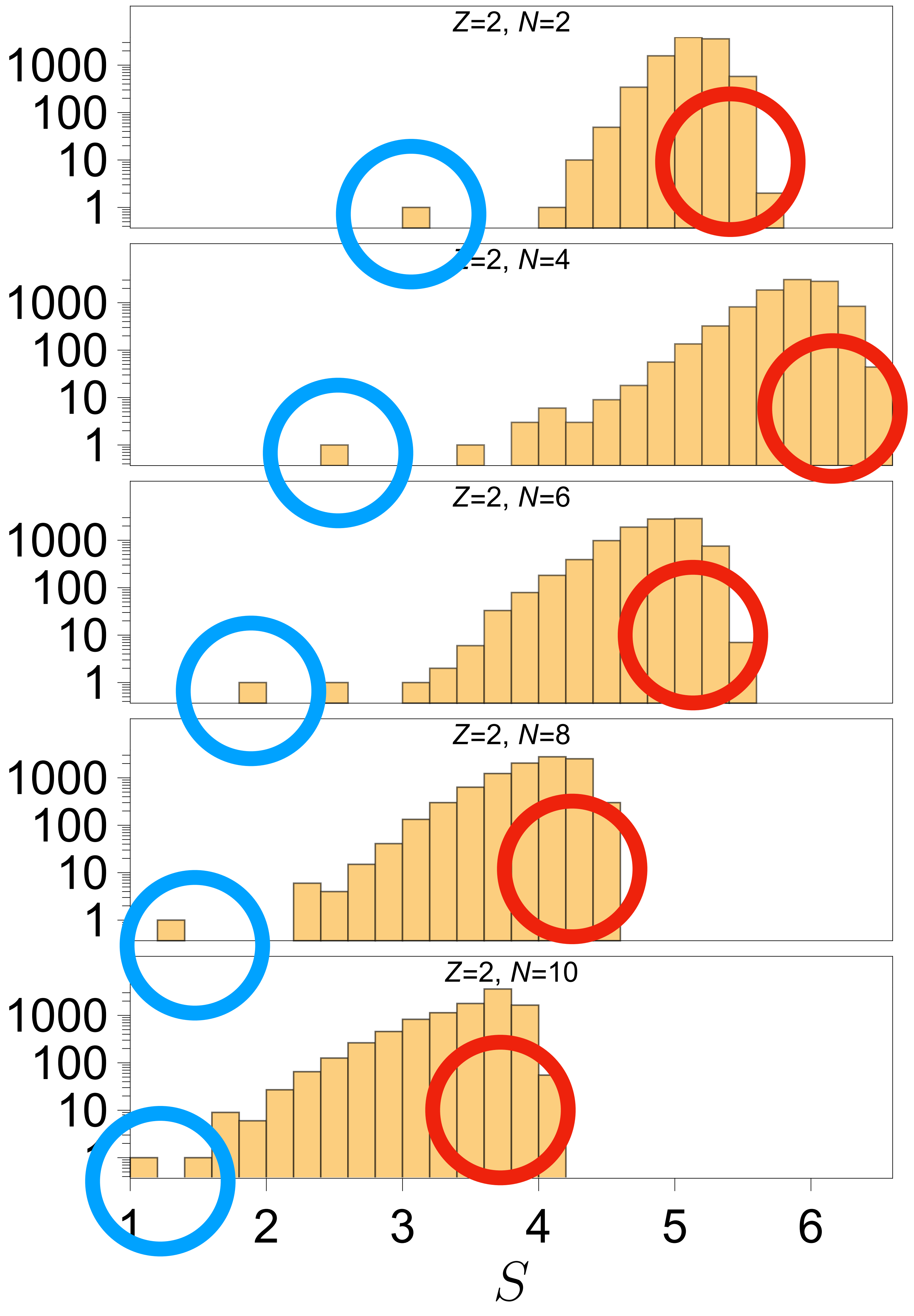
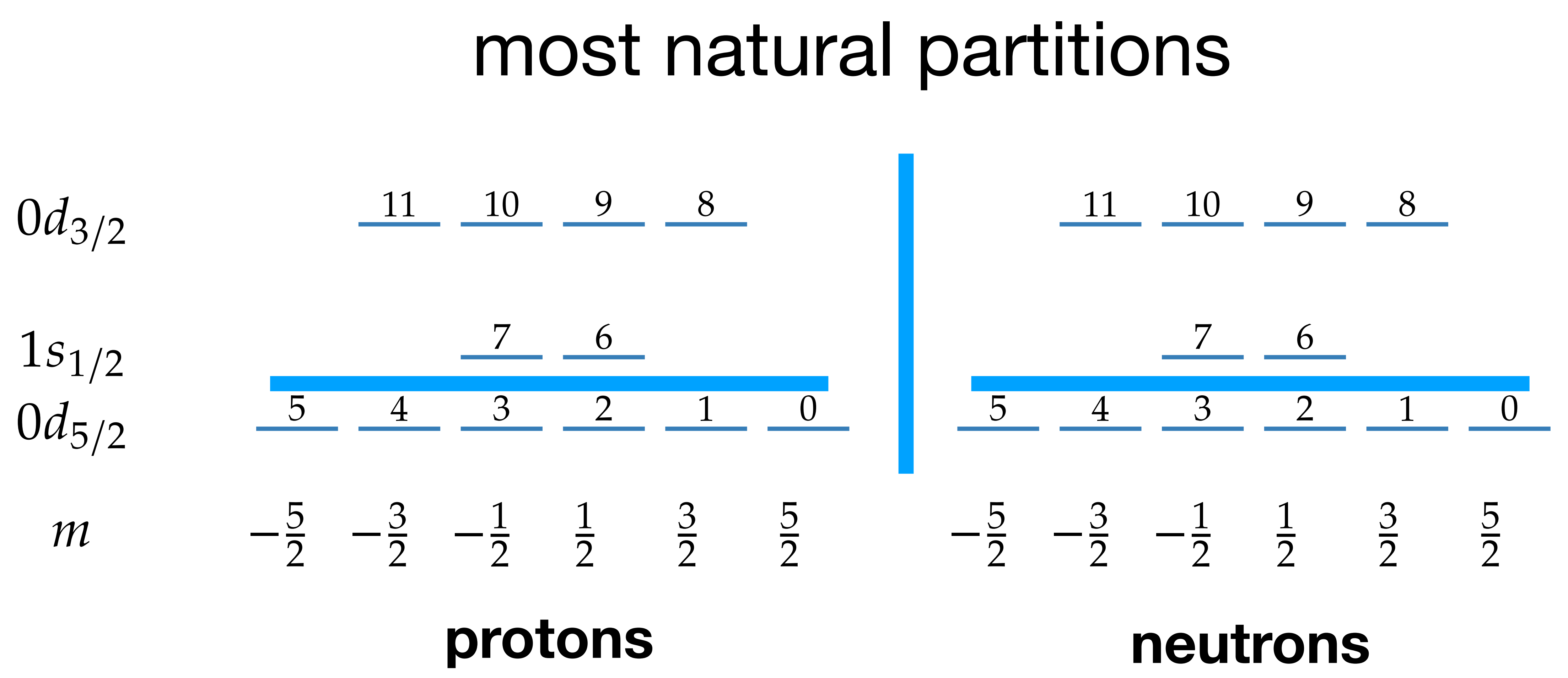
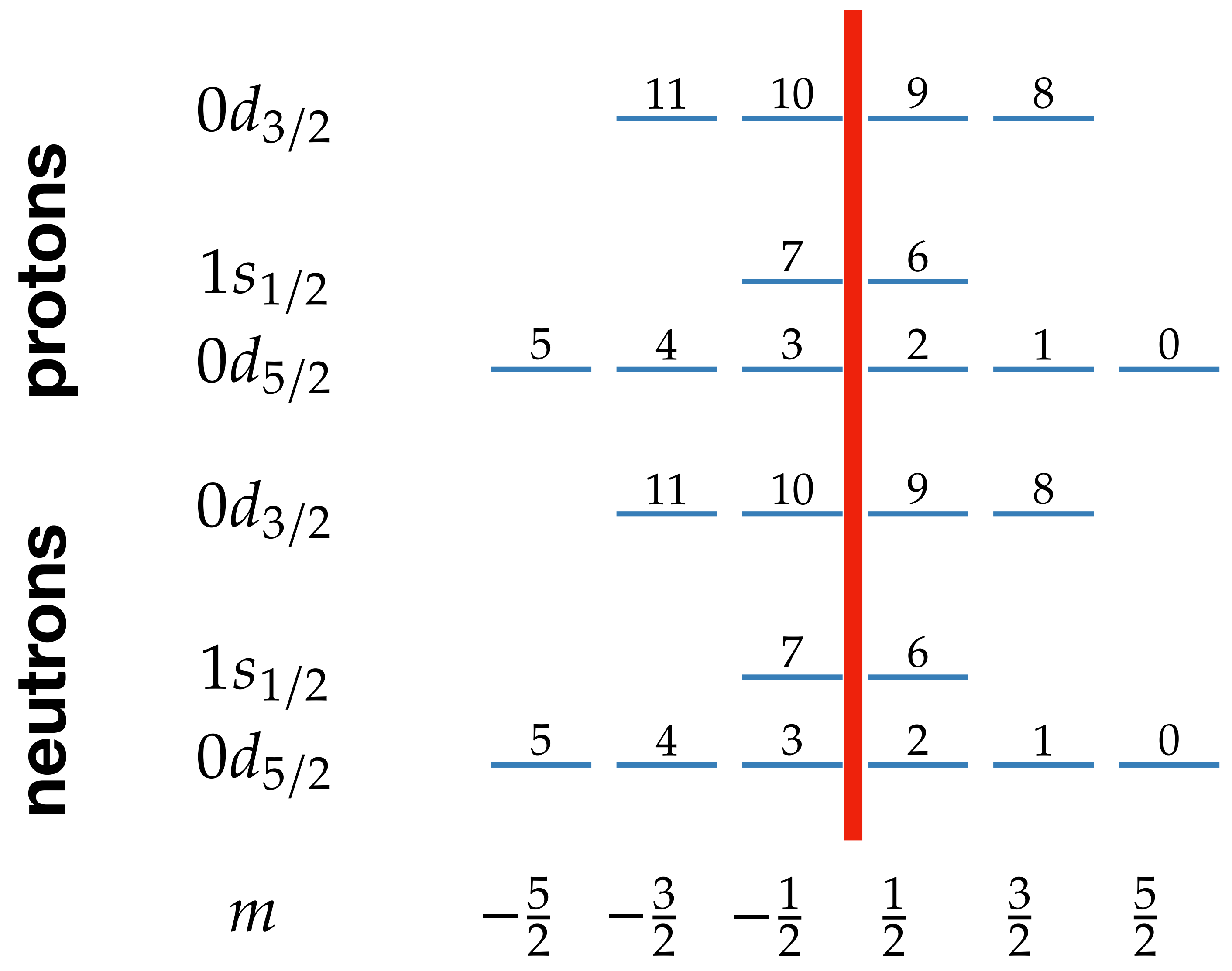


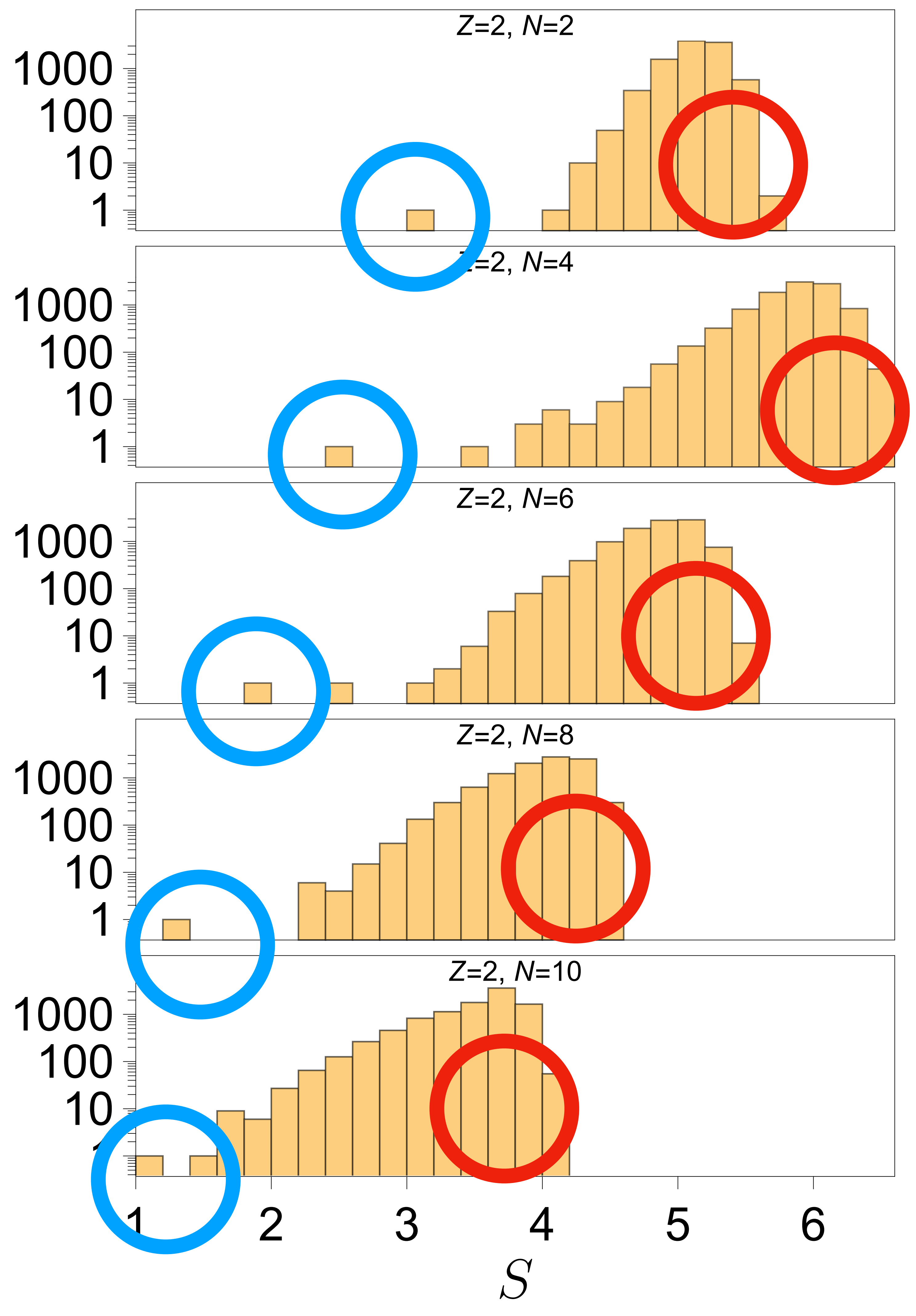




equipartition entanglement







Can we harness (low) entanglement?

1. Tensor networks
2. Basis rearrangement (C. Robin, M. Savage)
3. Lanczos (C. Johnson) ?
4. Circuit cutting $|\psi\rangle \simeq |\psi_1\rangle \otimes |\psi_2\rangle$?

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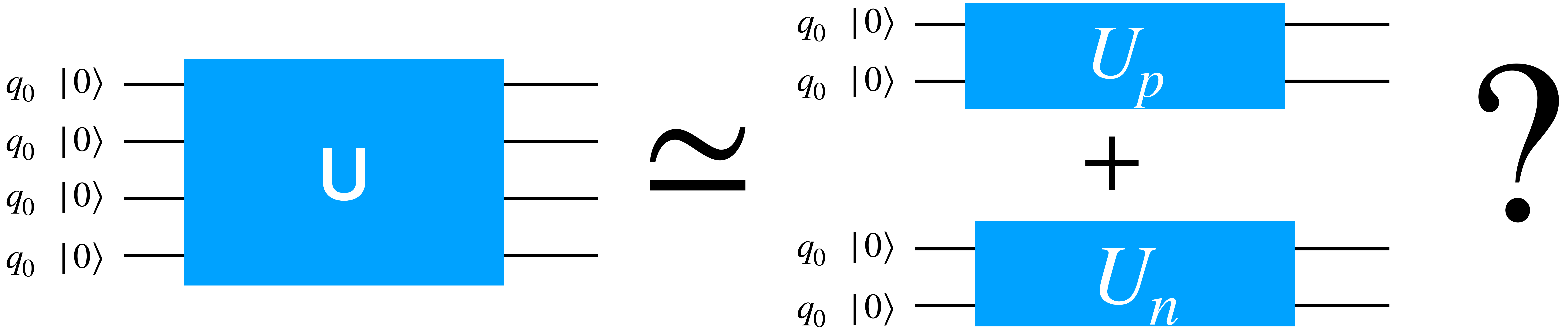

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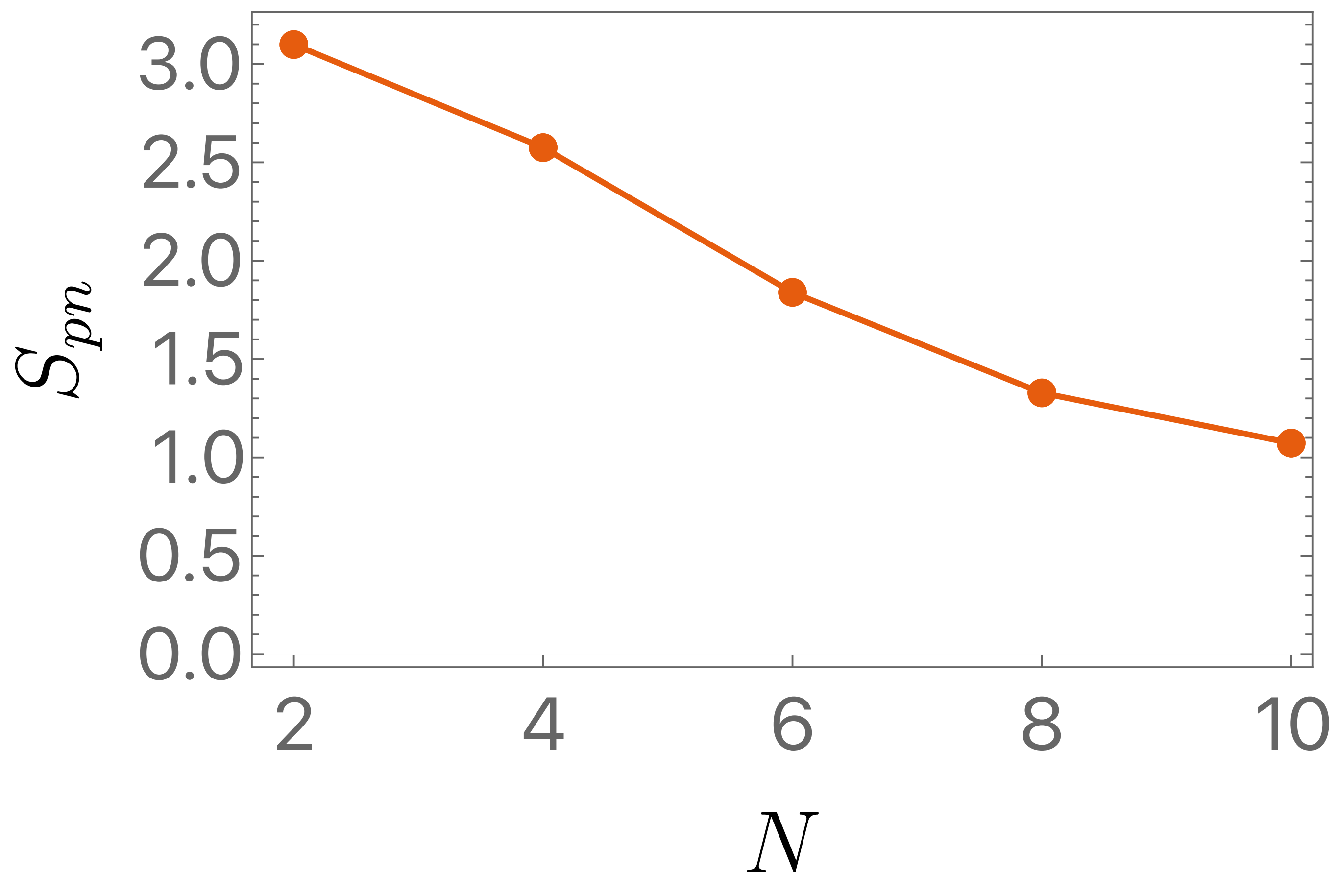
Reminder:

1. low p-n entanglement
2. specially low for nuclei with large N excess

sd shell with Z=2 ($S_{max} = 6.04$)



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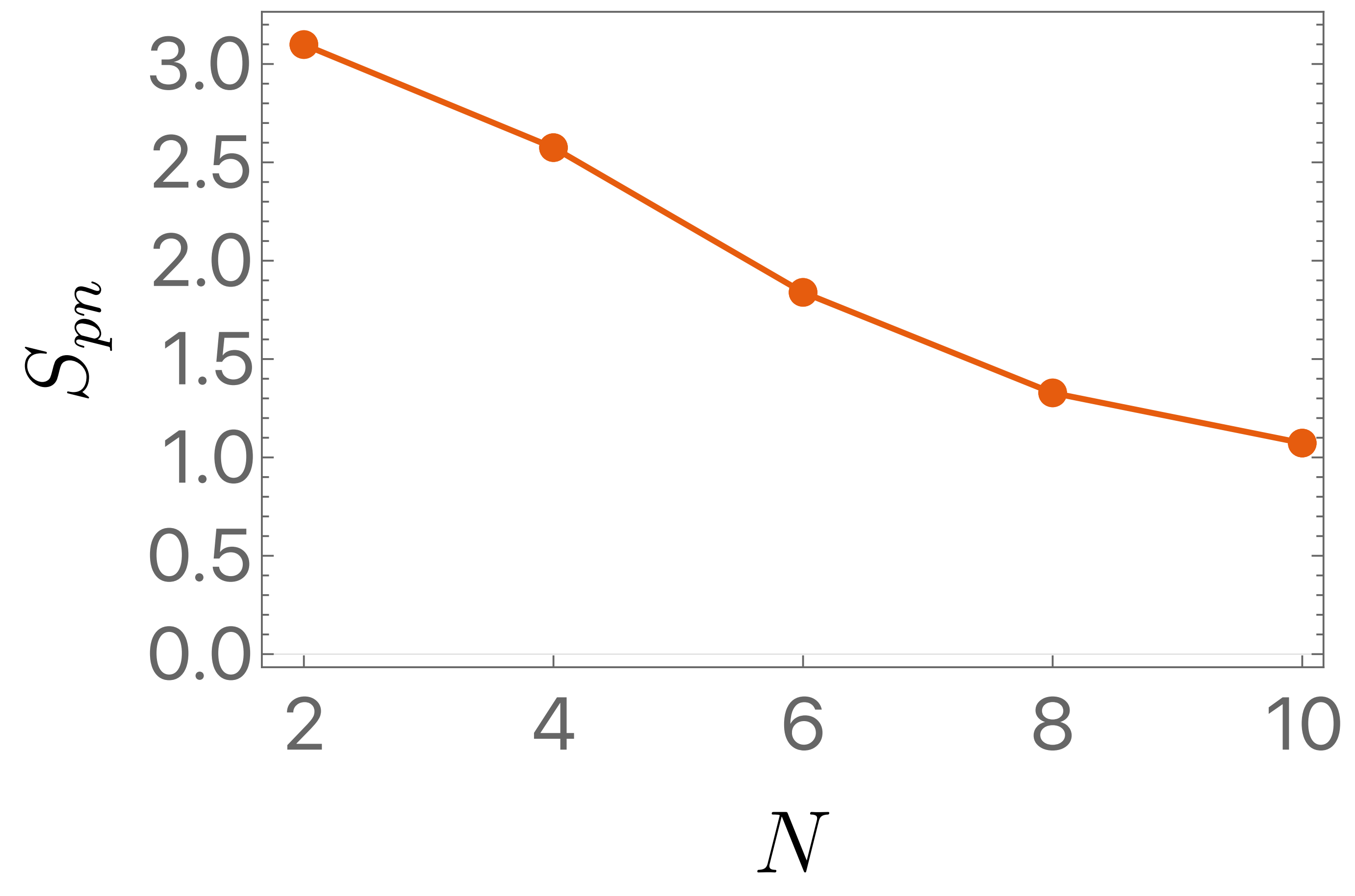

Use ADAPT-VQE with two separate ansatz (circuits) for protons/neutrons

1. $|\psi_p(\overrightarrow{\theta})\rangle = e^{i\theta_1 T_1} \ldots e^{i\theta_N T_N} | ref_p\rangle$
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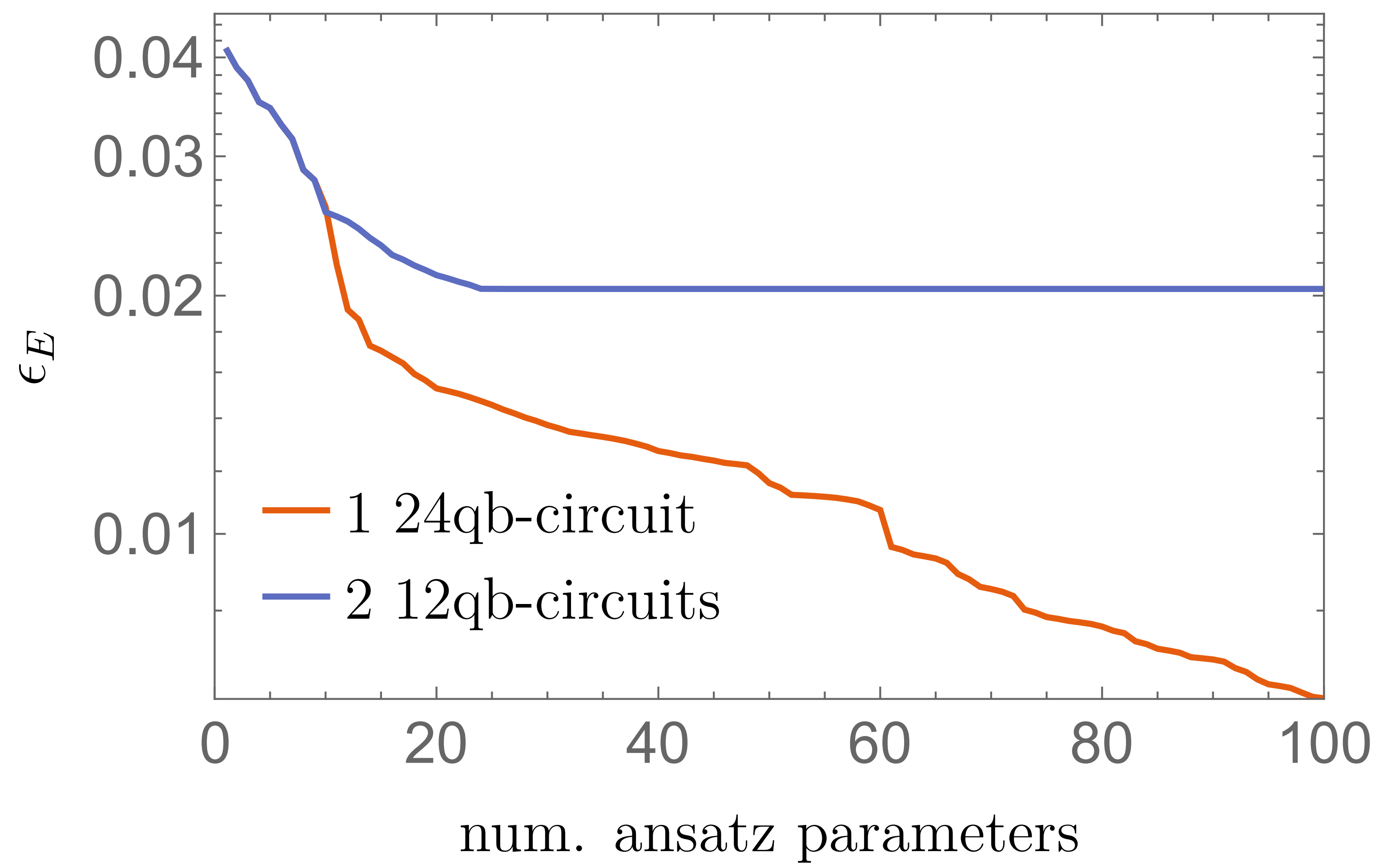

Can we harness (low) entanglement?

Maybe that was too naive/optimistic

➡ Let's be systematic (Schmidt decomposition)

$$
\begin{aligned}
|\psi_{GS}\rangle = \lambda_1 |\psi_p^{(1)}\rangle \otimes |\psi_n^{(1)}\rangle \\
+\lambda_2 |\psi_p^{(2)}\rangle \otimes |\psi_n^{(2)}\rangle \\
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+\dots
\end{aligned}
$$

orthogonality

$$\langle \psi_p^{(j)}, \psi_n^{(j)} | \psi_p^{(k)}, \psi_n^{(k)} \rangle = \delta_{jk}$$

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

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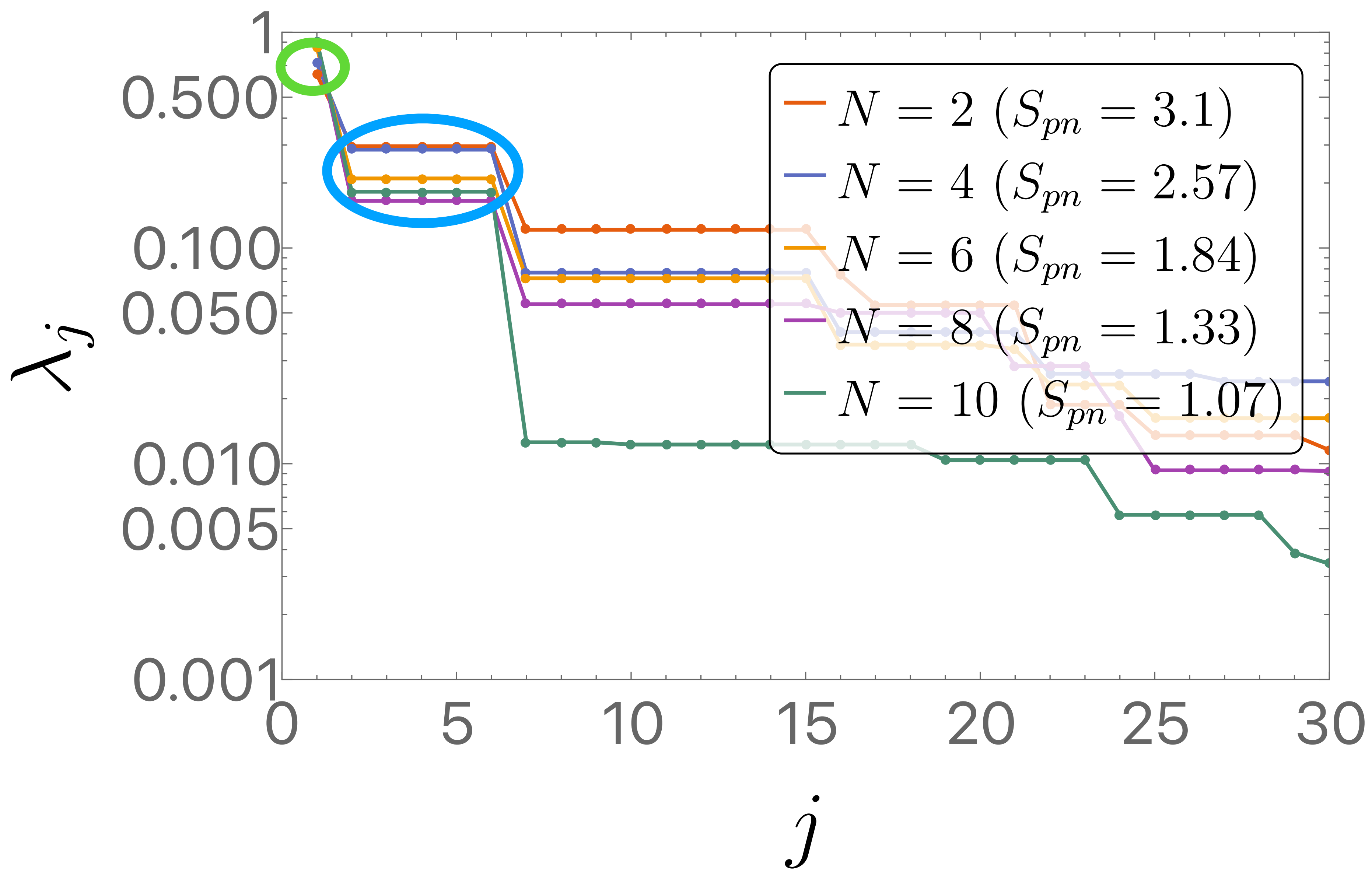

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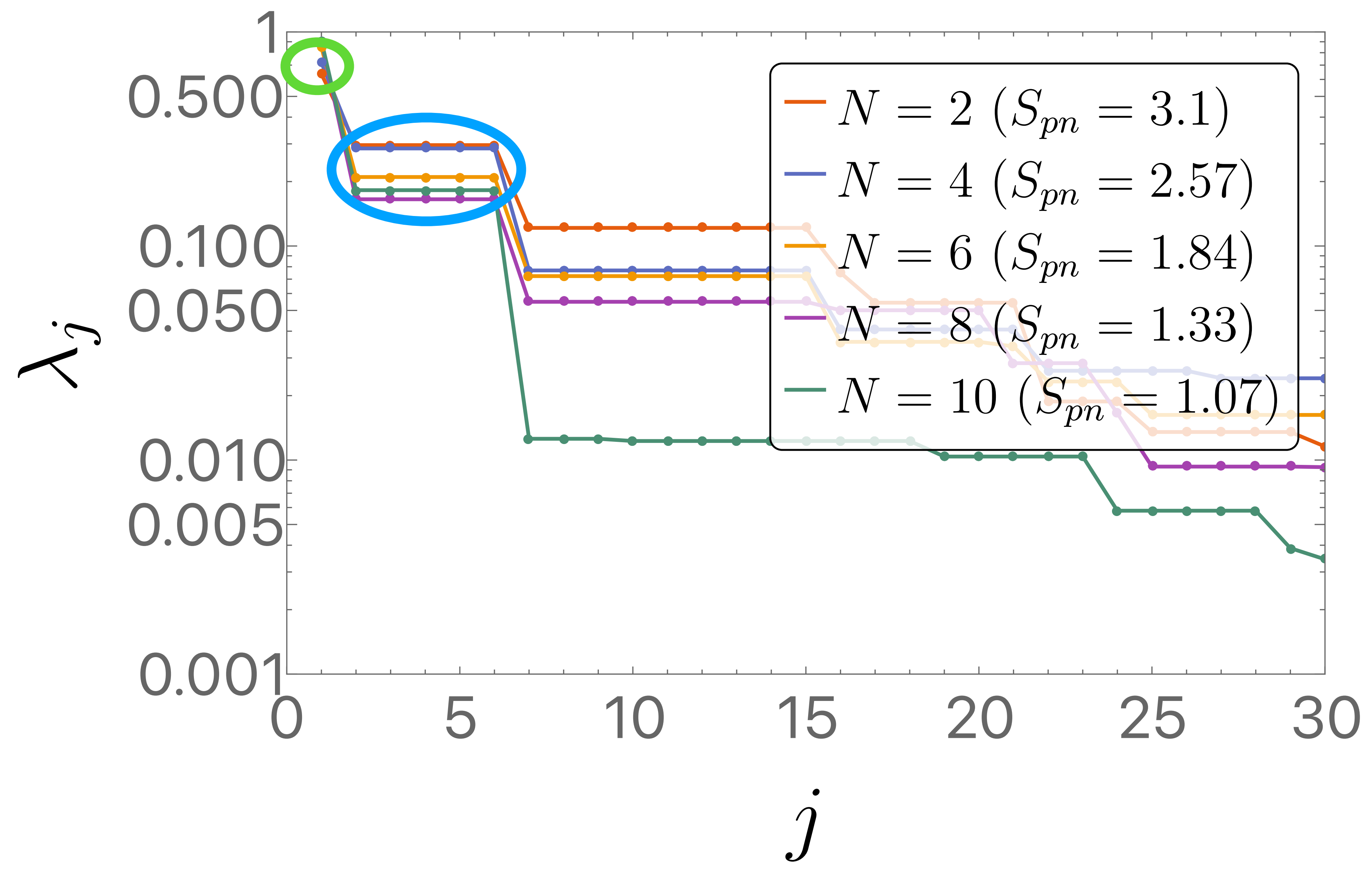

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5-fold degeneracy:

M=-2, 2
M=-1, 1
M= 0, 0
M=1,-1
M=2, -2

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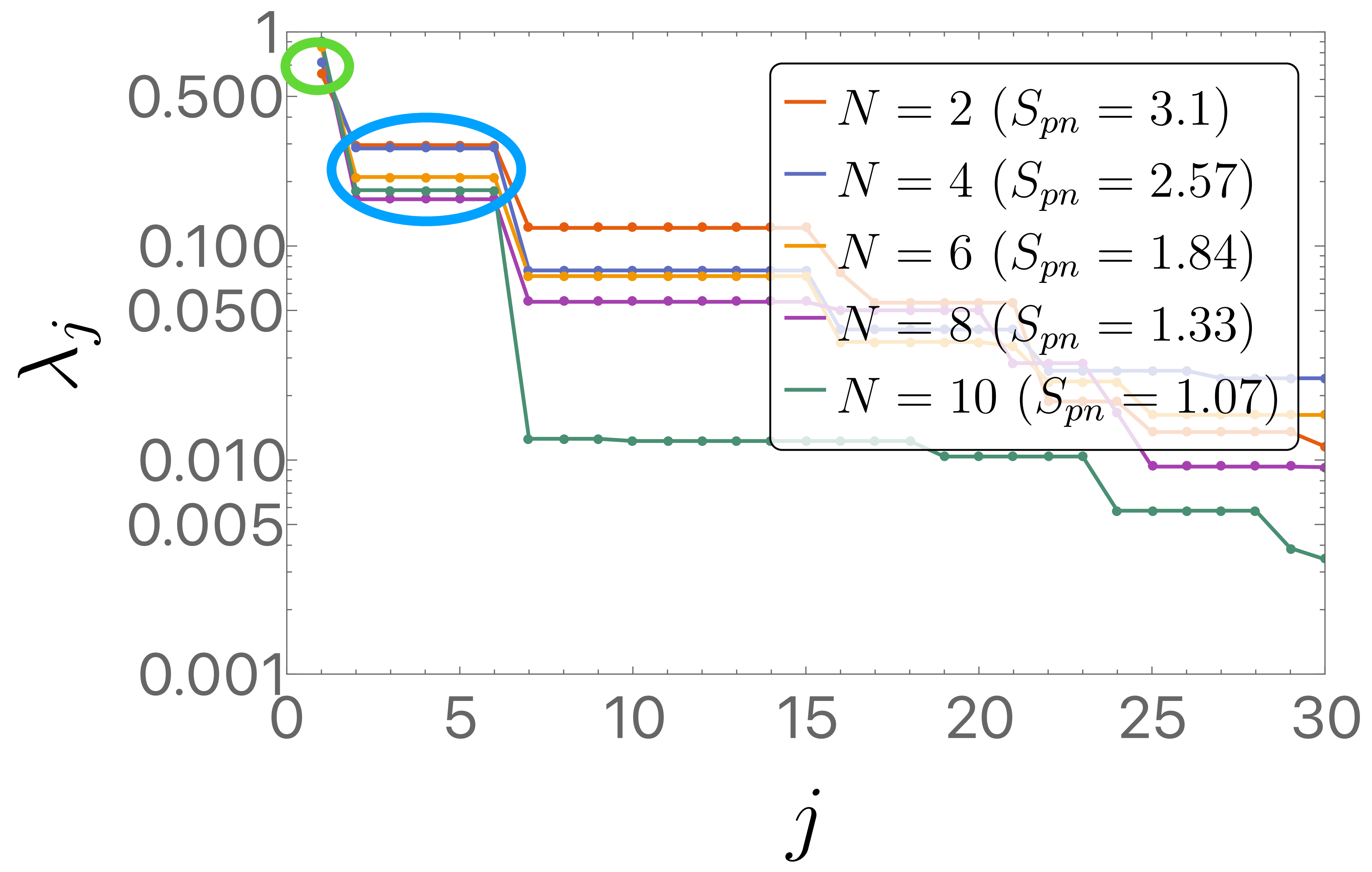

Can we harness (low) entanglement?

let's simulate 6 product states

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

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$$+$$

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Minimize energy with adapt-vqe

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

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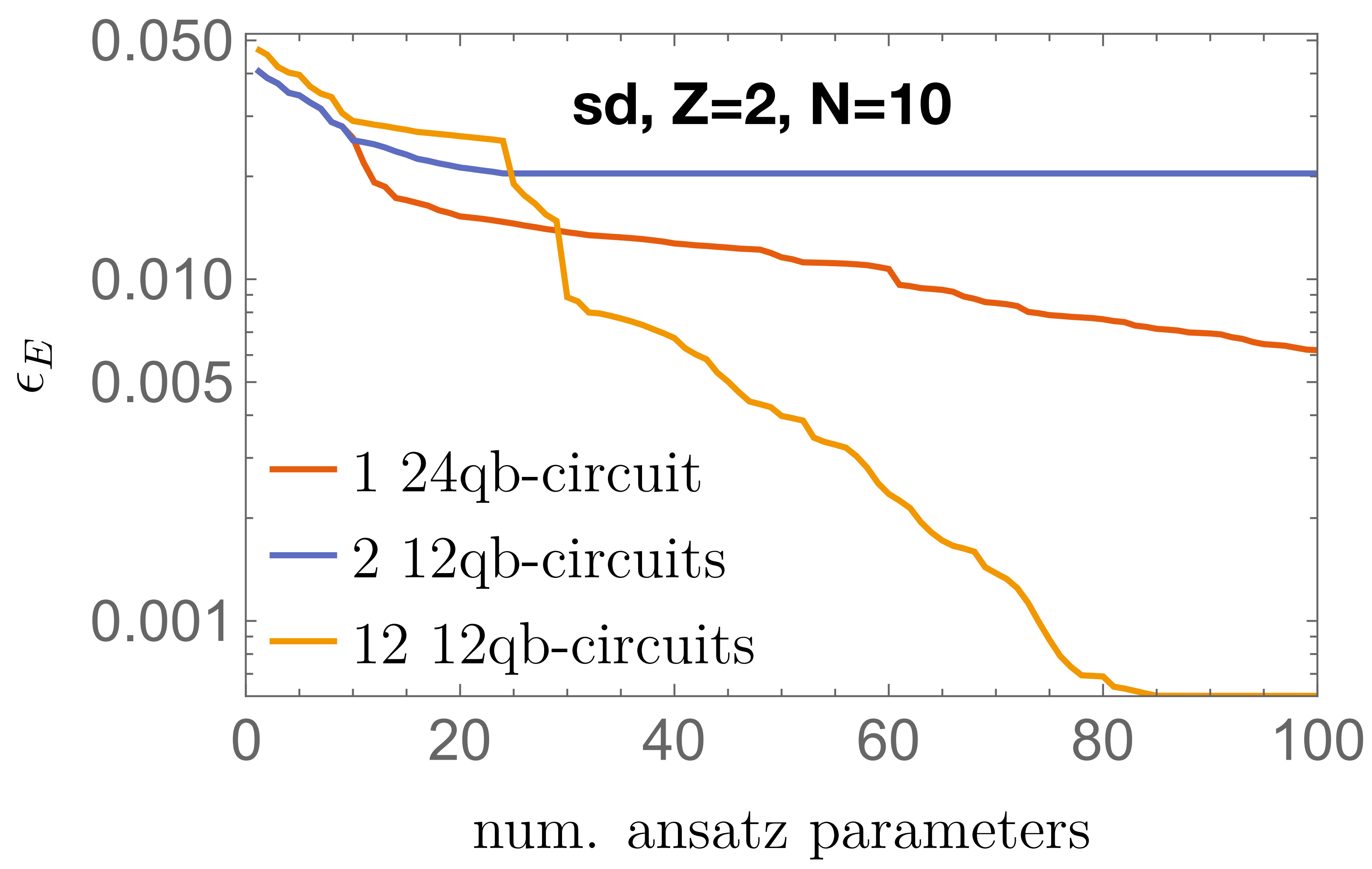

works well!

Conclusions

1. Entanglement in nuclei: fundamental & practical interests

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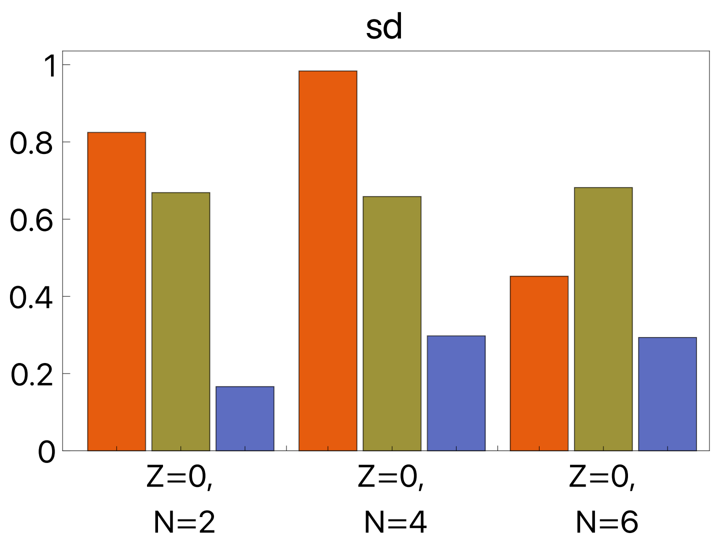
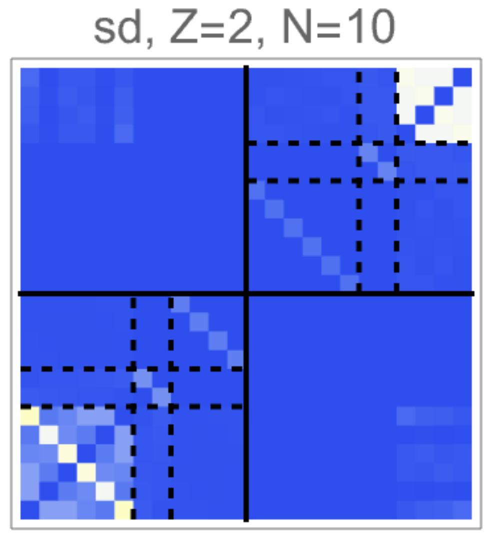
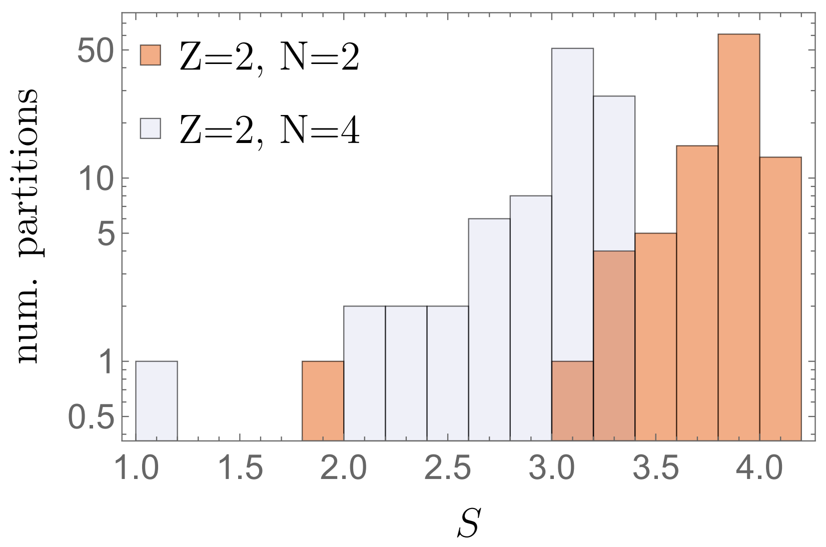


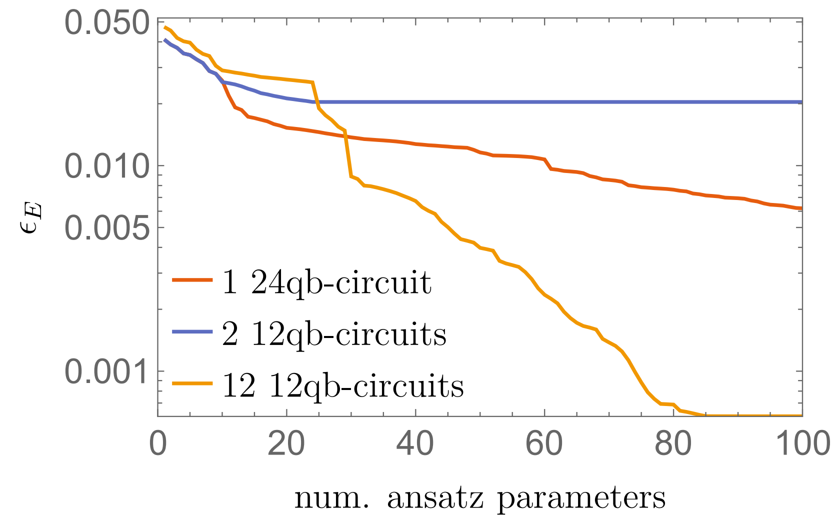
1. single-orbital / filling of subshells



2. general picture of entanglement



3. min. vs max. entanglement



4. circuit cutting improves VQE