ECT* workshop "Nuclear and particle physics on a quantum computer: where do we stand now?"

June 8, 2023

Entanglement and quantum simulations of nuclear systems in effective model spaces

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In collaboration with:
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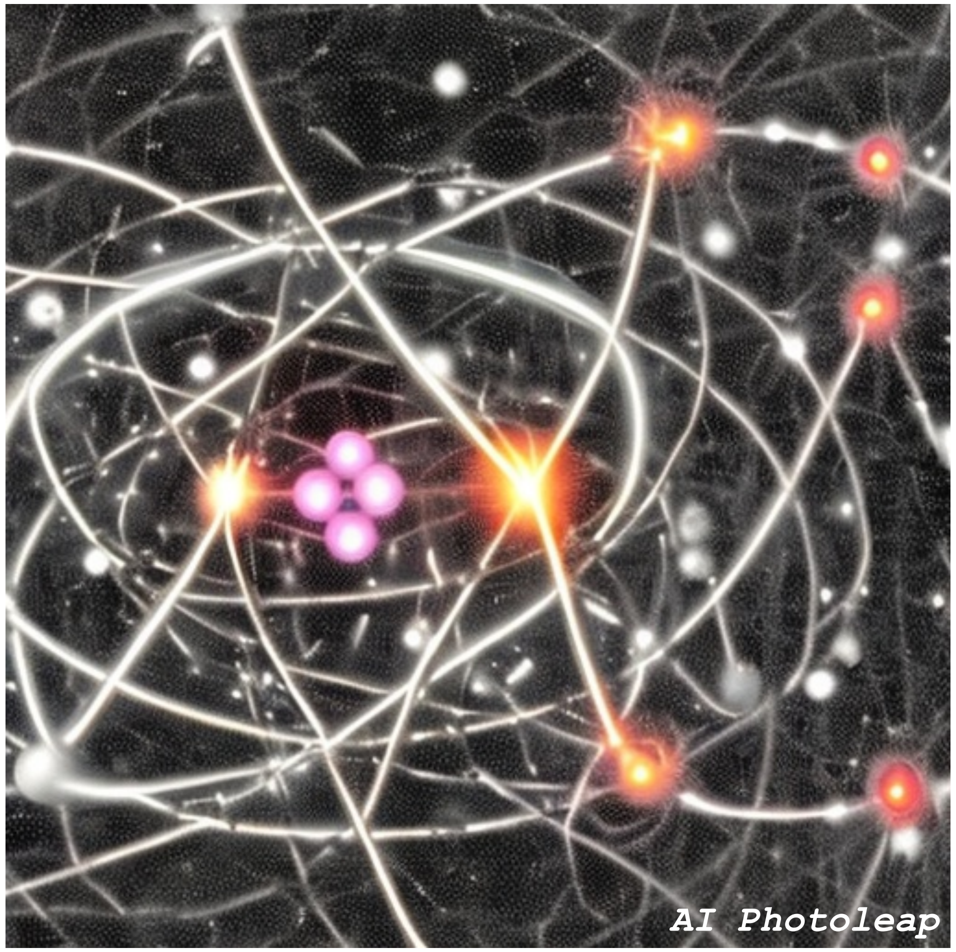
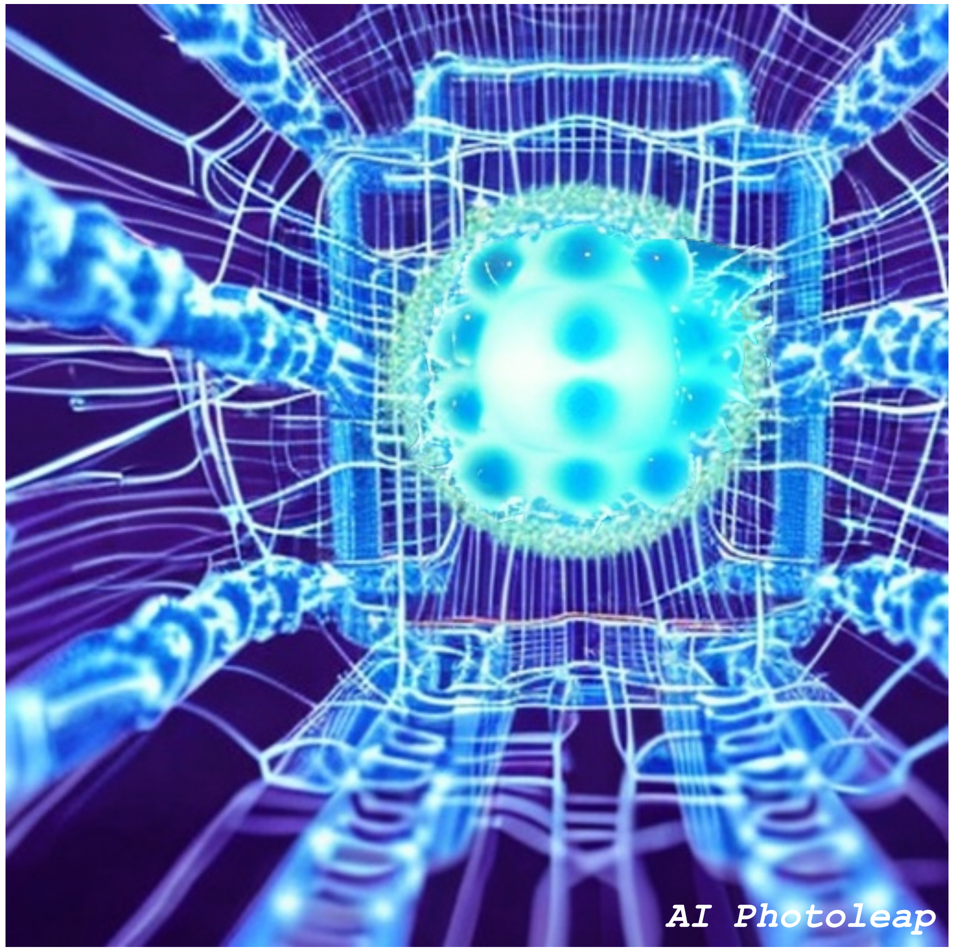
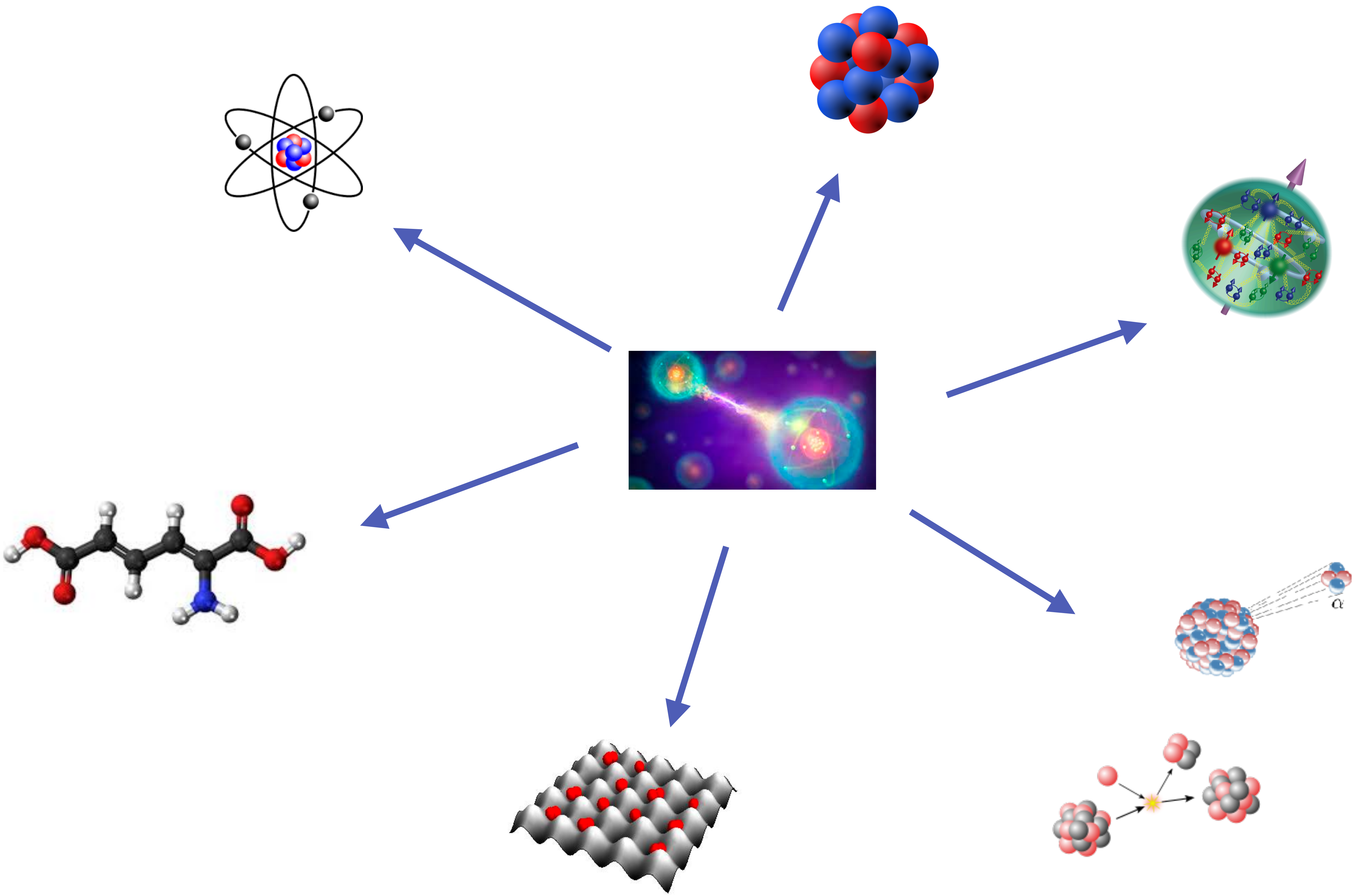
Marc Illa (IQuS Seattle), Martin J. Savage (IQuS Seattle)



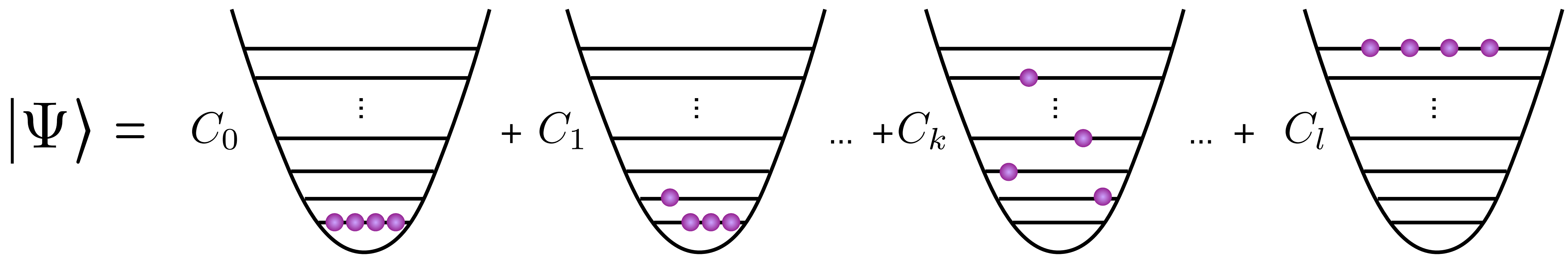


Entanglement in quantum many-body systems

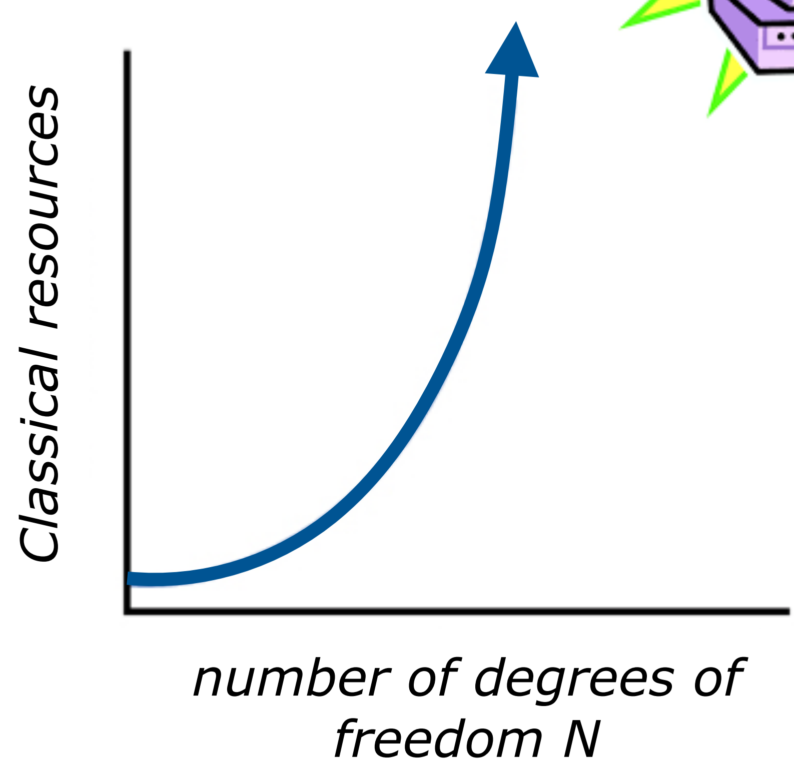


etc...

Entanglement in quantum many-body systems



$$= \sum_{n}^{\sim 2^N} C_n |\Phi_n\rangle$$

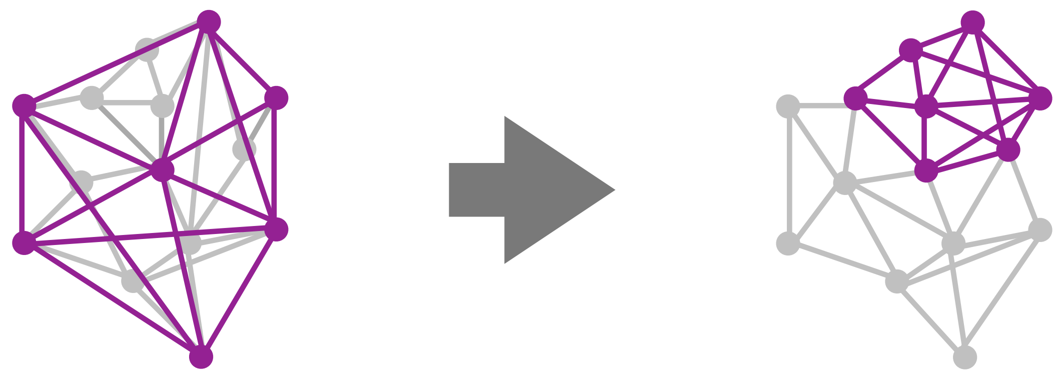


Entanglement in quantum many-body systems

☞ **Understanding and manipulating entanglement can advance:**

- The formulation of more efficient many-body schemes amenable to classical computers

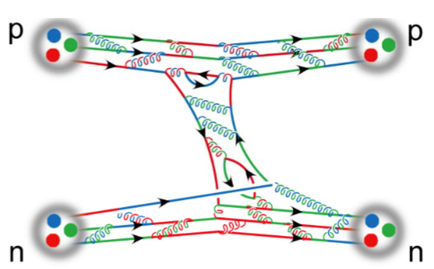
density matrix renormalization group (DMRG), tensor networks…



- The development of efficient quantum simulations of physical systems

in particular on current noisy intermediate scale quantum (NISQ) devices

- Our fundamental understanding of nature



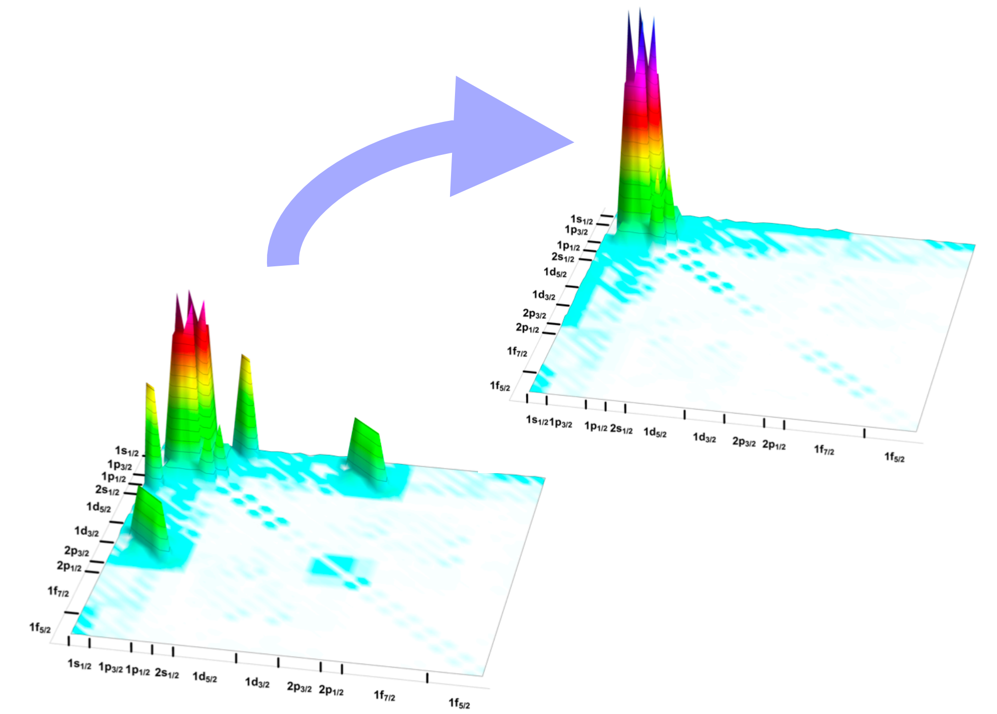
e.g. *"Entanglement Suppression and Emergent Symmetries of Strong Interactions"*
Beane, Kaplan, Klco, Savage, PRL122,102001 (2019).

"Entanglement minimization in hadronic scattering with pions"
Beane, Farrell, Varma. Int. J. Mod. Phys. A 36,2150205 (2021).

…

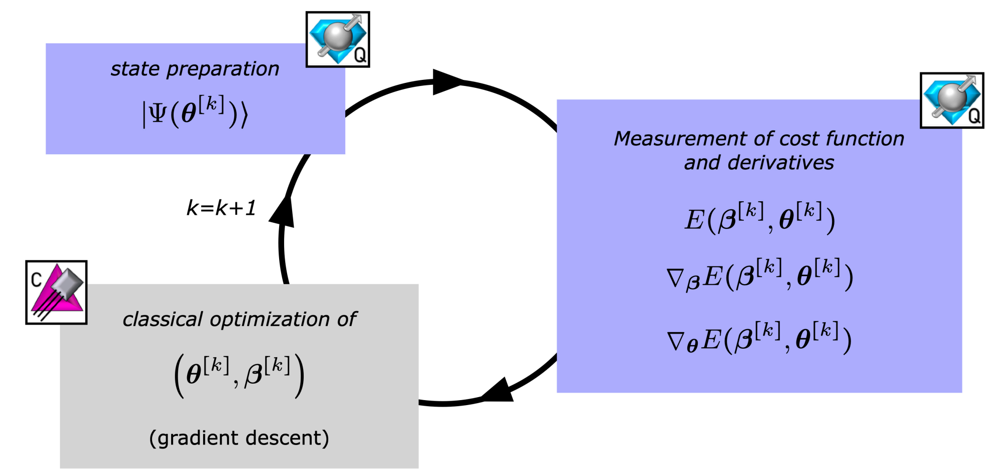
Outline

★ **Entanglement rearrangement in effective model-space calculations of light nuclei**



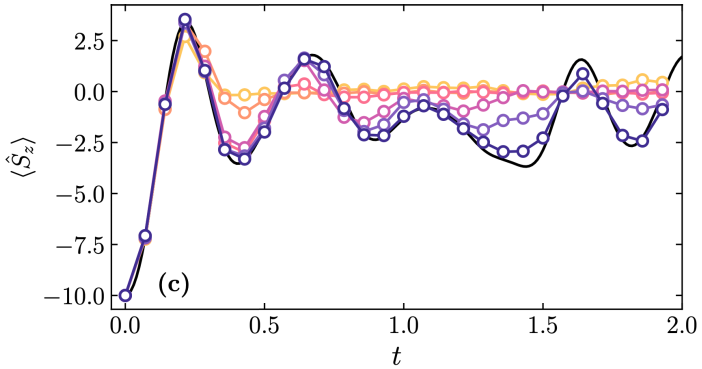
★ **Using entanglement rearrangement to efficiently leverage quantum resources?**

→ Hamiltonian-Learning-VQE algorithm applied to the Lipkin model



★ **Symmetry-guided mapping of quantum systems onto qudits**

→ Application to the Agassi model and SO(5) symmetry



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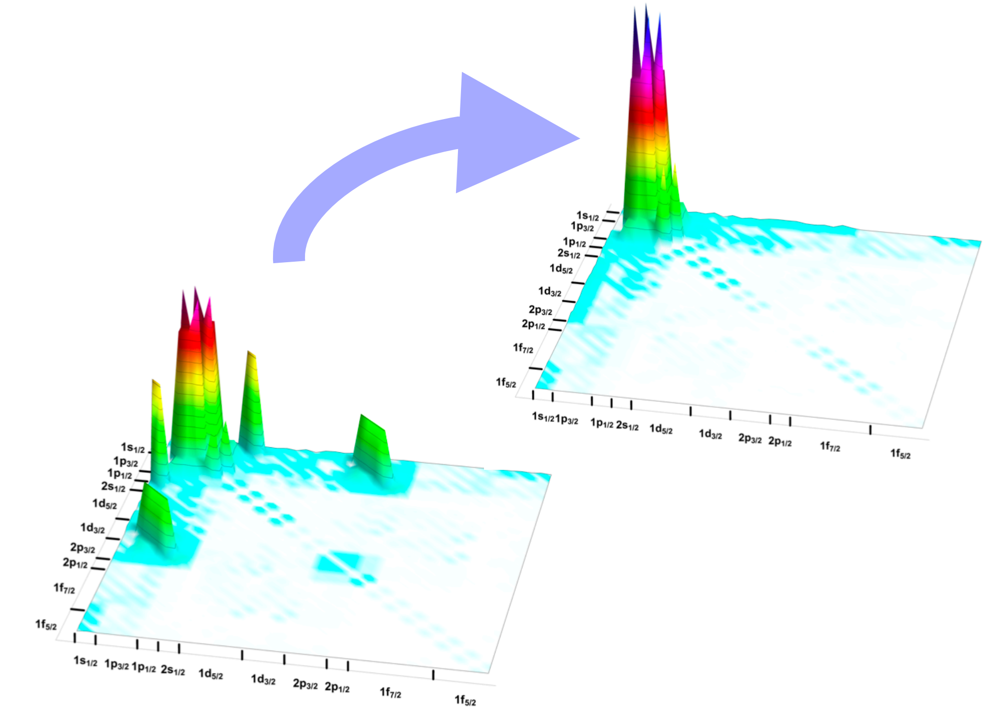

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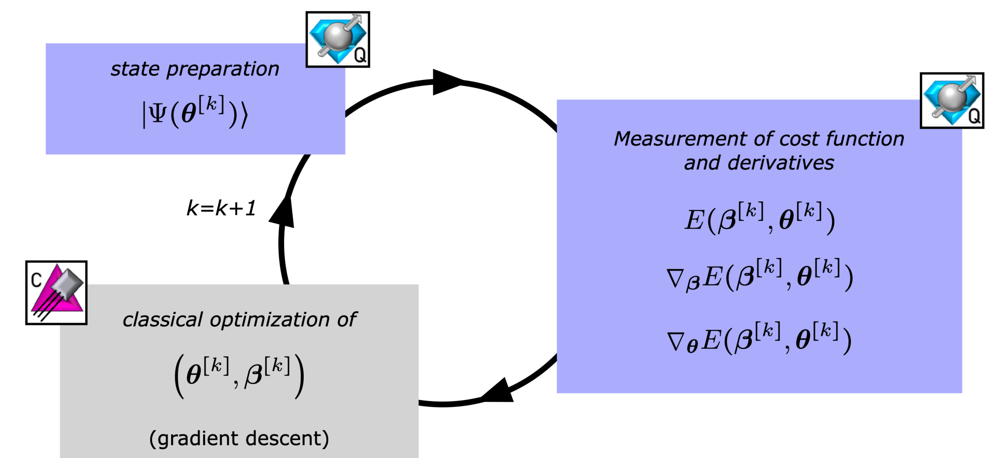

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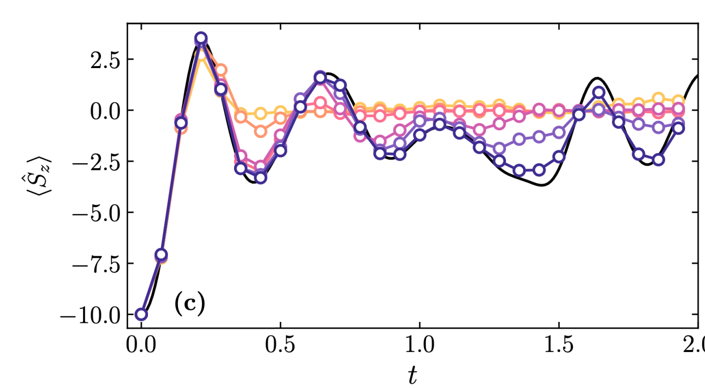
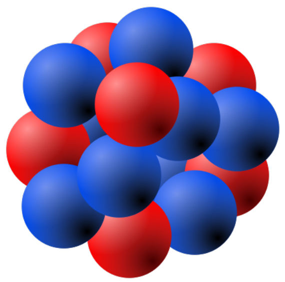
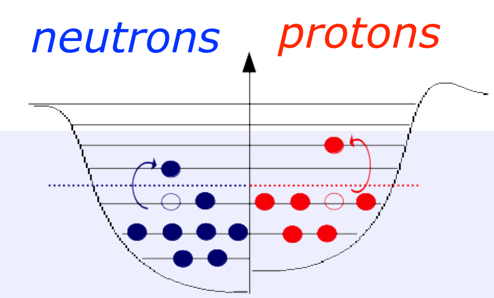


Characterization of Entanglement in Atomic Nuclei



= Z protons + N neutrons



$$|\Psi\rangle = \sum_{\pi\nu} C_{\pi\nu} |\phi_\pi\rangle \otimes |\phi_\nu\rangle$$

$$= \sum_{n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots} C_{n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots} |n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots\rangle$$

occupation numbers $n_i = 0 \text{ or } 1$

✳ Entanglement between proton and neutron subsystems

see e.g. Papenbrock & Dean PRC 67, 051303(R) (2003), DMRG and wave function factorisation for nuclei; Johnson & Gorton J. Phys. G: Nucl. Part. Phys. 50, 045110 (2023) + Gorton MSc thesis (2018), proton-neutron entanglement in the nuclear Shell Model.

✳ Entanglement of modes (single-nucleon orbitals)

see e.g.: Legeza et al. PRC 92, 051303(R) (2015) in the framework of DMRG using Shell Model interactions
Kruppa et al. J. Phys. G: Nucl. Part. Phys. 48 025107 (2021) two-nucleon systems in the Shell Model
CR, Savage, Pillet, PRC 103, 034325 (2021) He nuclei in effective no-core calculations with chiral interactions
Faba, Martín, Robledo, PRA 104 032428 (2021), Quantum correlations in the Lipkin Model
Kovács et al. PRC 106, 024303 (2022) Entanglement and seniority
Pazy arXiv:2206.10702 (2022) entanglement of SRC pairs
Tichai et al. arXiv:2207.01438 (2022) sd-shell nuclei with ab-initio valence-space DMRG
Bulgac et al. arXiv:2203.12079 (2022), arXiv:2203.04843 (2022) entanglement and SRC
A. Pérez-Obiol et al. arXiv:2302.03641 (2023) entanglement entropies of sd-shell nuclei with ADAPT-VQE
Gu et al. arXiv:2303.04799 (2023) entanglement entropies of nuclear systems and models

Nuclear structure calculations in effective model spaces

full space Hamiltonian and wave function

$$\hat{H}, \ |\Psi\rangle = \sum_n C_n |\Phi_n\rangle$$

$$\mathcal{H} = \mathcal{P} + \mathcal{Q}$$

effective model space and Hamiltonian

$$|\Psi\rangle^{\mathcal{P}} = \sum_{n \in \mathcal{P}} C_n \ |\Phi_n\rangle$$

$$H_{eff} = U^\dagger H U$$

$$\begin{pmatrix} H_{eff}^{(\mathcal{P}\mathcal{P})} & H_{eff}^{(\mathcal{P}\mathcal{Q})} \\ H_{eff}^{(\mathcal{Q}\mathcal{P})} & H_{eff}^{(\mathcal{Q}\mathcal{Q})} \end{pmatrix}$$

Determine U so that $\langle \Psi^{\mathcal{P}} | H_{eff} | \Psi^{\mathcal{P}} \rangle \simeq \langle \Psi | H | \Psi \rangle$

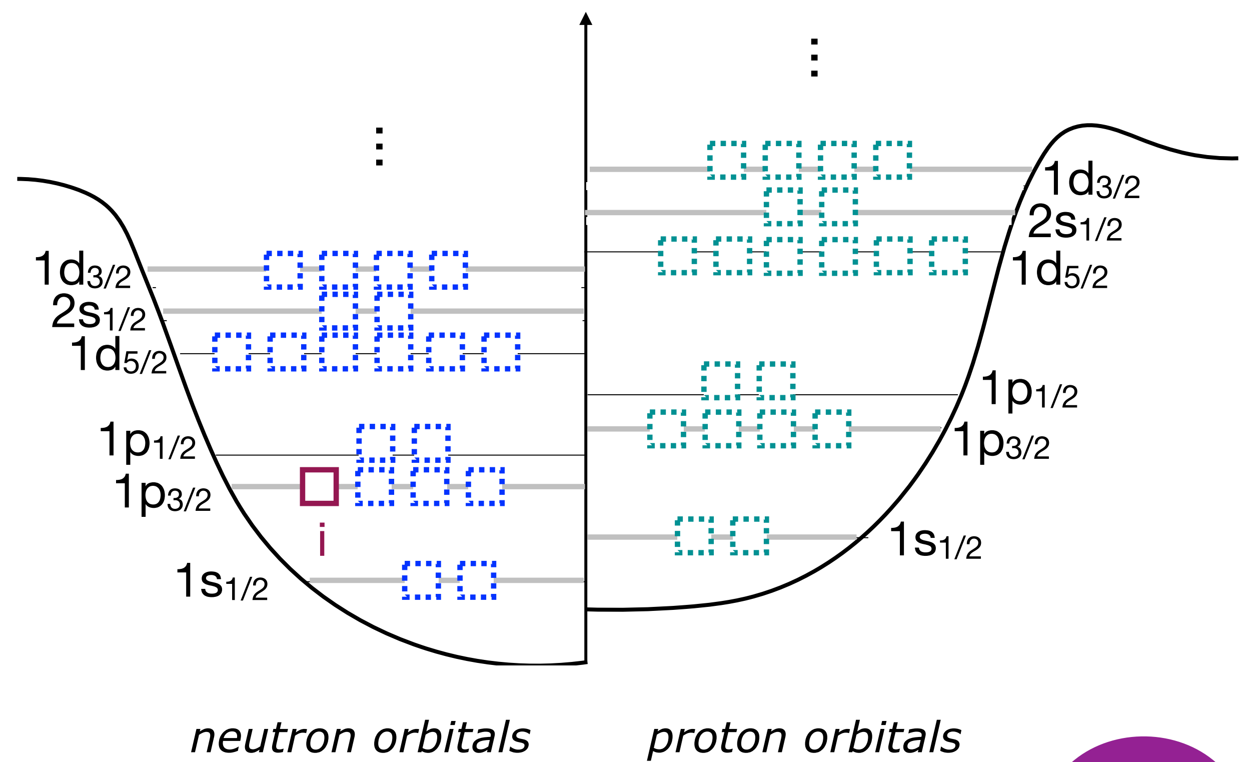
Entanglement rearrangement in light nuclei

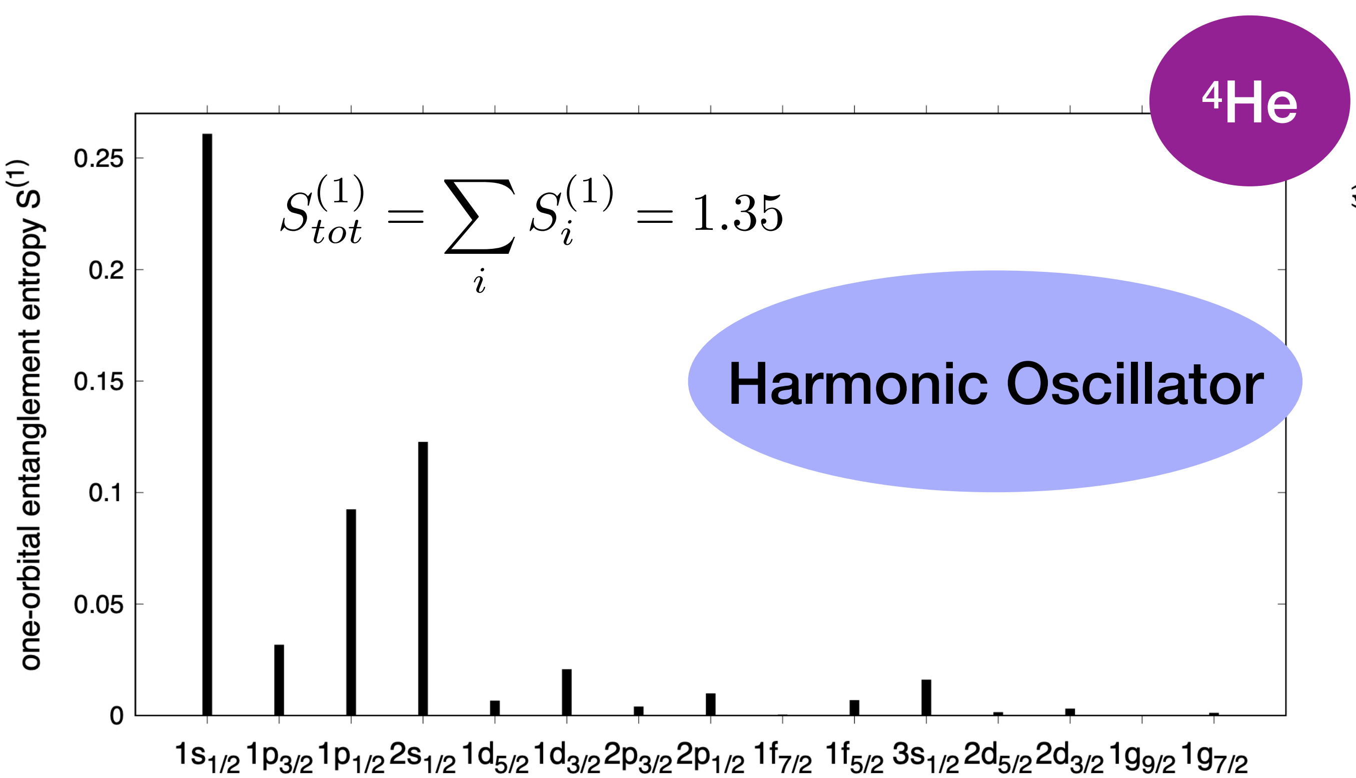
CR, Savage, Pillet, PRC 103, 034325 (2021)

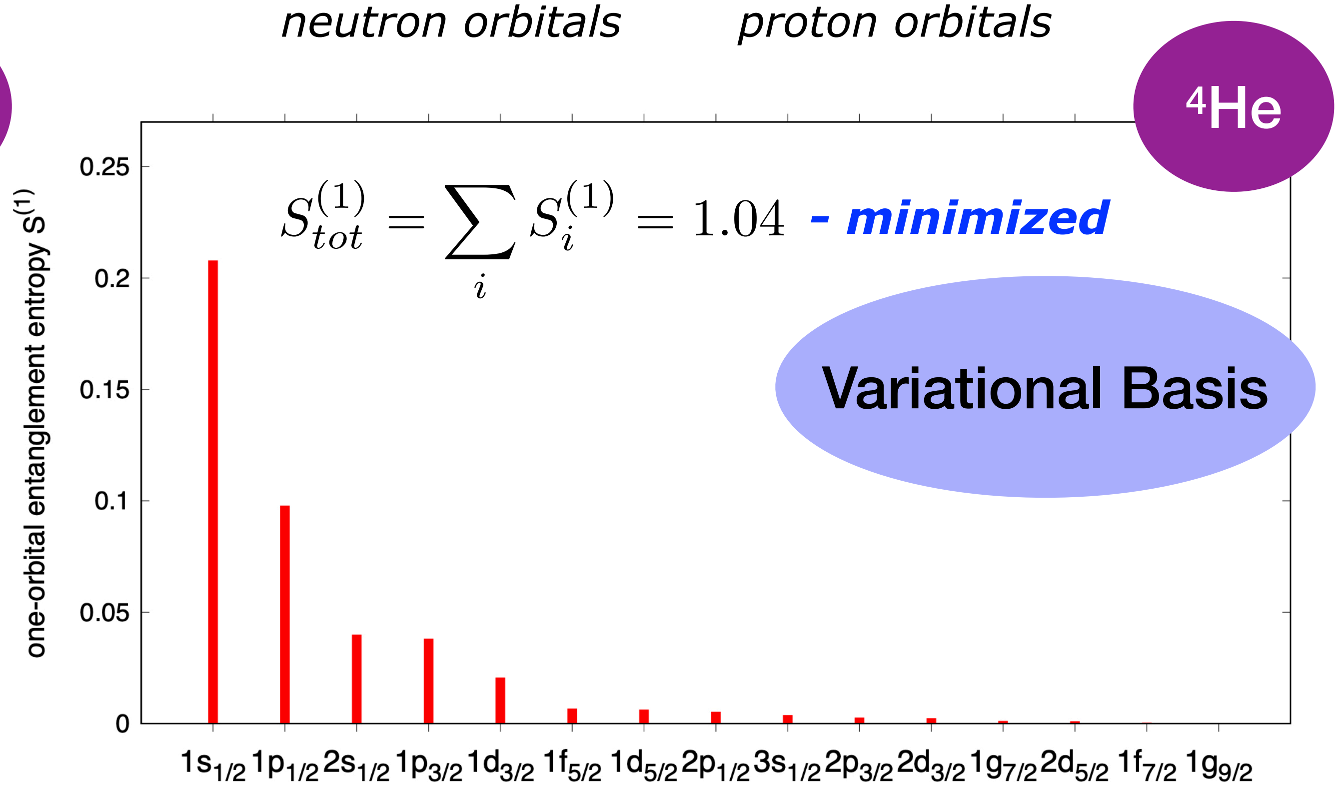
Single-orbital Von Neumann entropy:

$$S^{(1)}_{(i)} = -\mathrm{Tr}\left[\rho^{(i)} \ln \rho^{(i)}\right]$$

= measure of entanglement of one orbital with the rest of the system





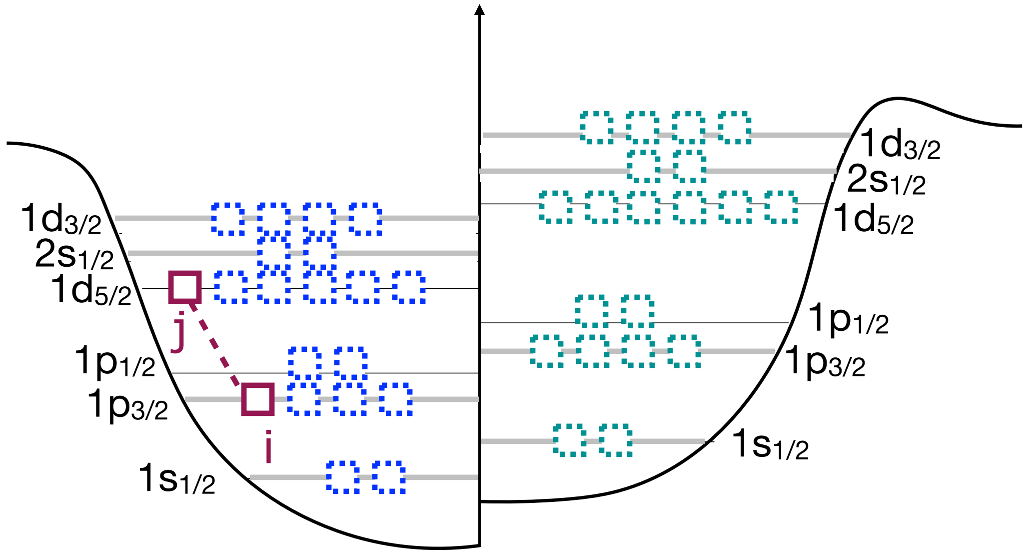


$$\hat{U} = e^{i\hat{T}}$$

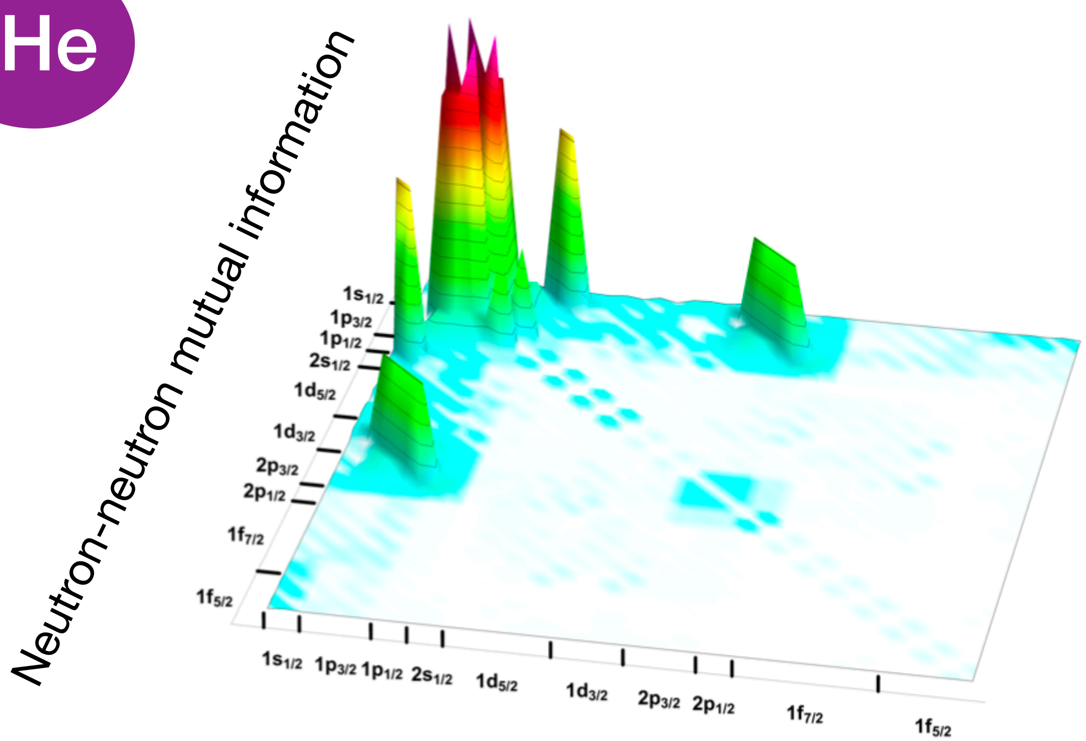
$\hat{T}$ = *1-body hermitian operator determined by a variational principle*

- **Mutual information** between orbitals

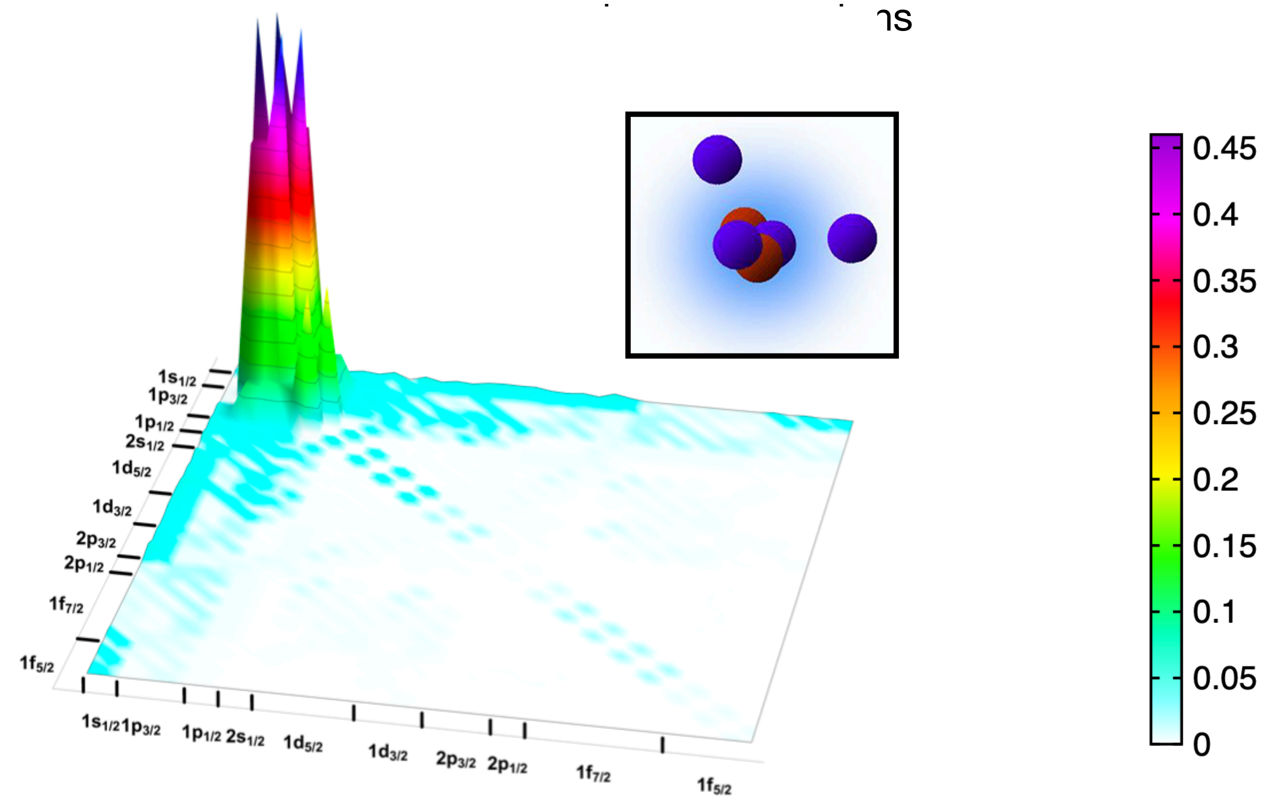
$$I_{ij} = -\left(S^{(2)}_{(ij)} - S^{(1)}_{(i)} - S^{(1)}_{(j)}\right)(1-\delta_{ij})$$



^6He



Harmonic oscillator orbitals



Variational orbitals

⇒ *emergence of ^4He-core + nn-valence structure*

CR, Savage, Pillet, PRC 103, 034325 (2021)

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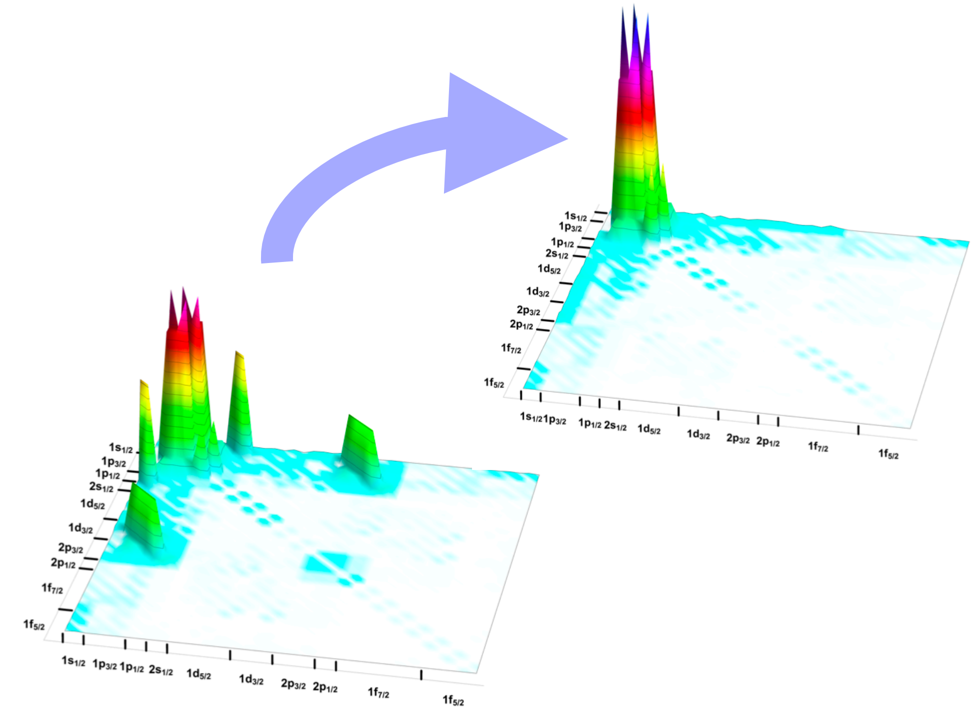
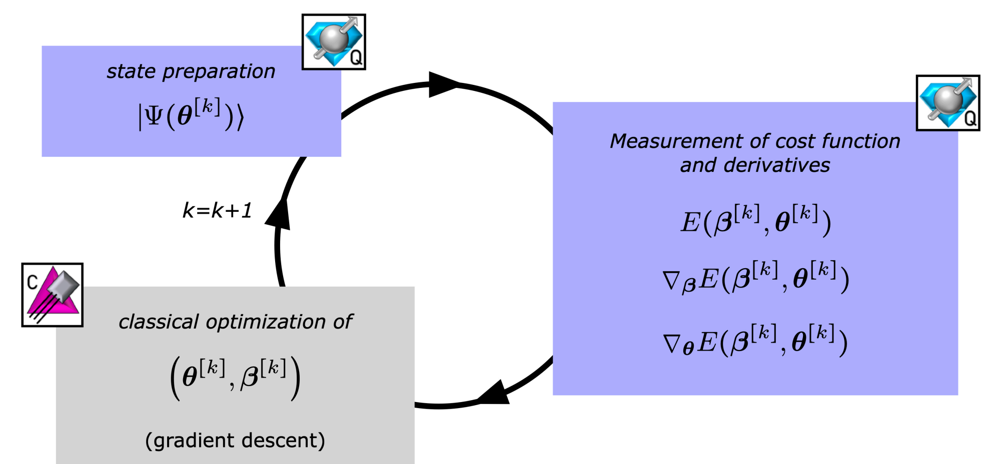
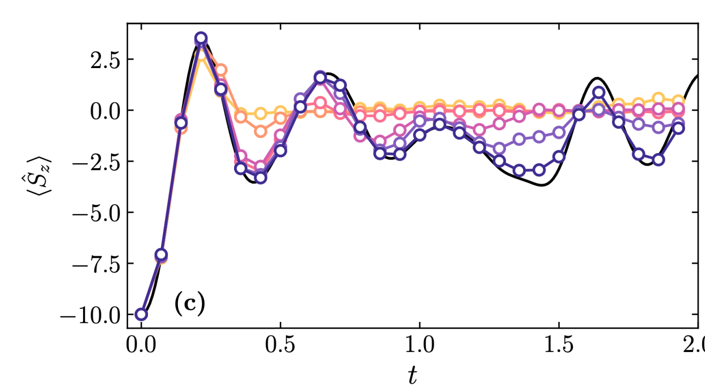


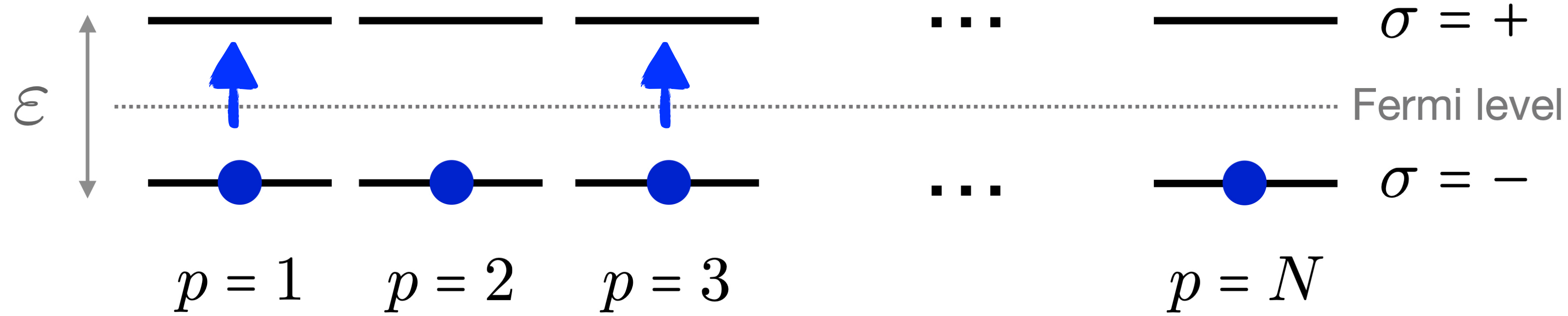


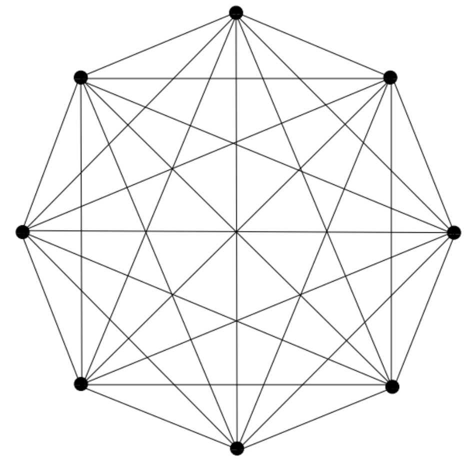


The Lipkin-Meshkov-Glick Model

Lipkin, Meshkov, Glick, Nucl. Phys. 62, 188 (1965)

- Relevance for nuclear physics, condensed matter, spin-squeezing, quantum sensing…
- Allows to study links between entanglement and quantum phase transitions





Simplex

$$H = \varepsilon J_z - \frac{V}{2}\left(J_+^2 + J_-^2\right)$$

$$J_z = \frac{1}{2}\sum_{p\sigma} \sigma c_{p\sigma}^{\dagger} c_{p\sigma}$$

$$J_+ = \sum_{p} \sigma c_{p+}^{\dagger} c_{p-}\ , \qquad J_- = (J_+)^{\dagger}$$

Phase Transition: doubly degenerate ground state of mixed parity (N→∞)

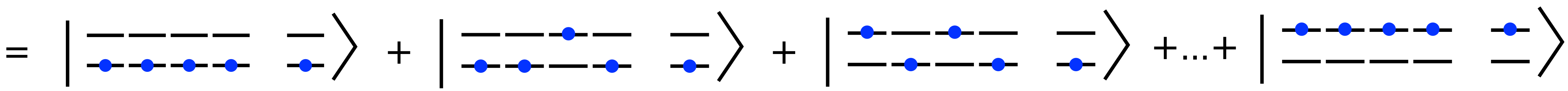
Benchmark for testing and comparing new quantum algorithms:

Cervia et al. PRC 104, 024305 (2021); Chikaoka & Liang, Chin. Phys. C 46 024106 (2022); Romero et al. PRC 105, 064317 (2022); Hlatshwayo et al. PRC 106, 024319 (2022)

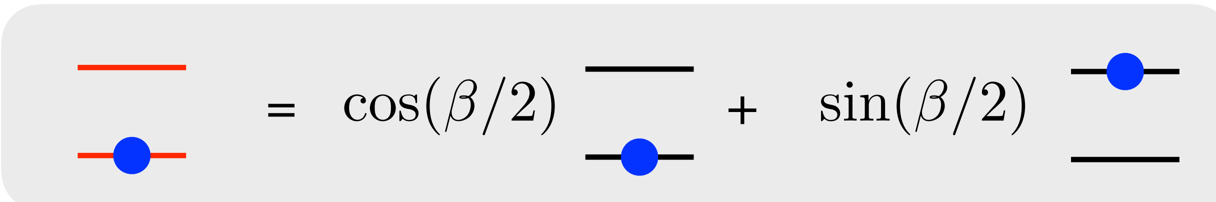
✳ Exact solution:

$$|\Psi\rangle = \sum_{M=-J}^{J} A_{J,M}|J,M\rangle \equiv \sum_{n=0}^{2J} A_n|n\rangle$$

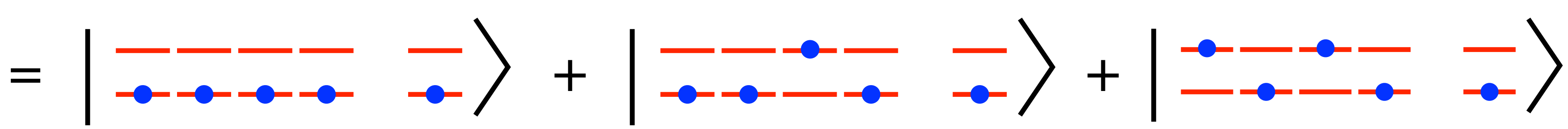
Eigenvector of H



✳ Effective description:



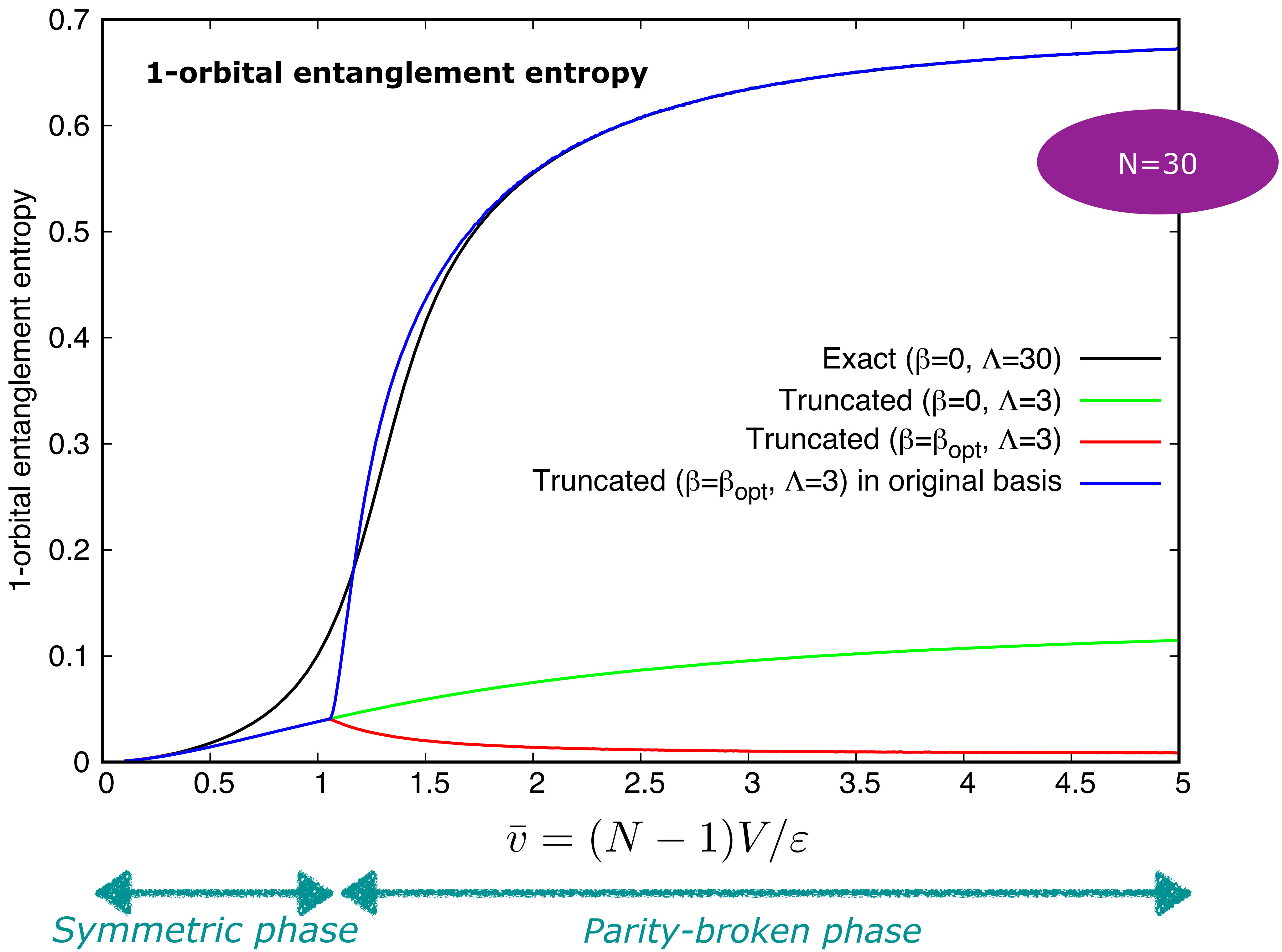
$$|\Psi\rangle^{\Lambda} = \sum_{n=0}^{\Lambda-1} A_n|n\rangle$$



Eigenvector of $H(\beta) = U(\beta)^{\dagger} H U(\beta)$

The LMG Model in effective model space: Entanglement

★ **Entanglement — preliminary work of Momme Hengstenberg (Uni Bielefeld)**



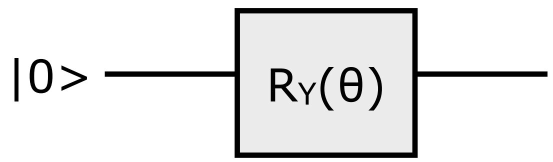
★ *Implementation on a digital quantum computer:*

Map the many-body states onto qubits, similarly to what is done in QFT

$$\Rightarrow \; \Lambda = 2^{n_{qubits}}$$

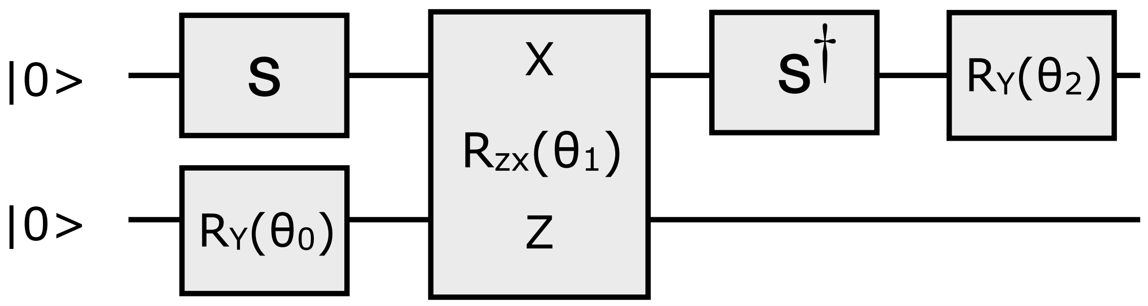
✳ 1 qubit ($\Lambda = 2$):

$$|\Psi(\theta)\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + \sin\left(\frac{\theta}{2}\right)|1\rangle$$



✳ 2 qubits ($\Lambda = 4$):

$$|\Psi(\theta_0, \theta_1, \theta_2)\rangle$$



CR, M. J. Savage arXiv:2301.05976 [quant-ph] (2023)

The LMG Model in effective model space: Quantum Simulations

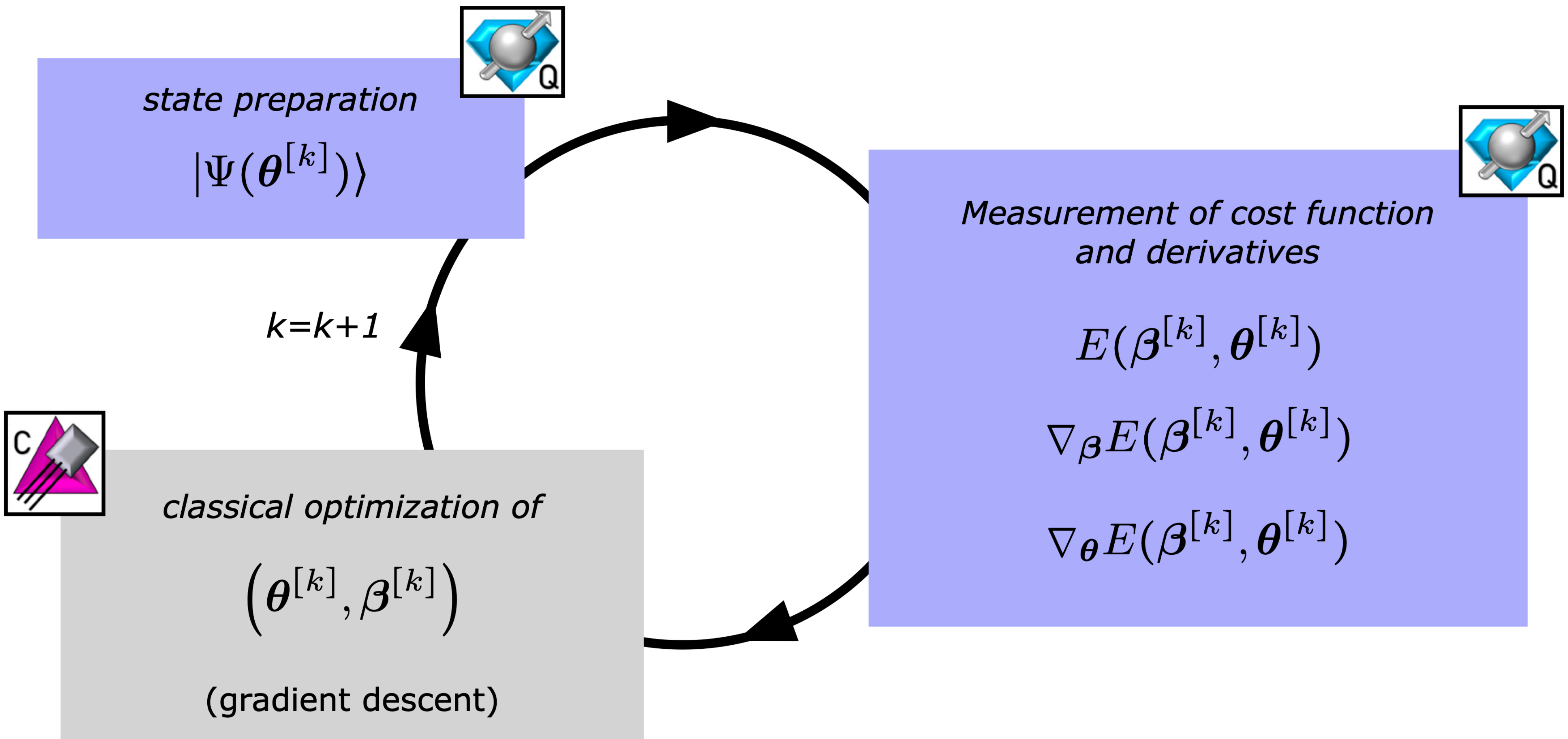
CR, M. J. Savage arXiv:2301.05976 [quant-ph] (2023)

★ Hamiltonian-Learning-VQE:

$$\overline{\sigma} = \{\hat{I}, \hat{X}, \hat{Y}, \hat{Z}\}$$

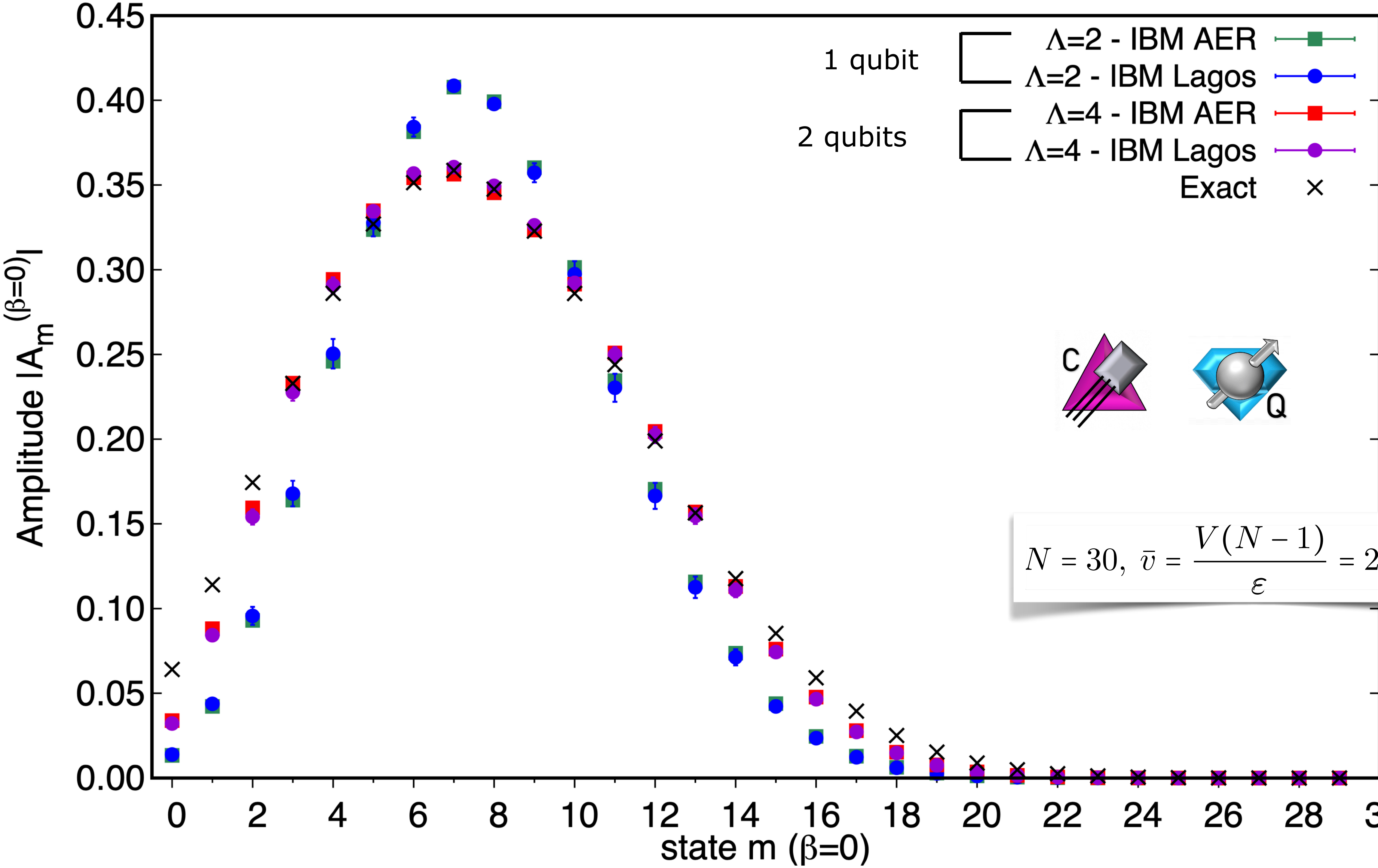
Cost function to minimize: $E(\beta, \boldsymbol{\theta}) = \langle \Psi(\boldsymbol{\theta}) | \hat{H}(\beta) | \Psi(\boldsymbol{\theta}) \rangle$

$$= \sum_{i_1, \ldots, i_{n_q}} h_{i_i, \ldots, i_{n_q}}(\beta) \, \langle \Psi(\boldsymbol{\theta}) | \overline{\sigma}_{i_1} \otimes \ \ldots \otimes \overline{\sigma}_{i_{n_q}} | \Psi(\boldsymbol{\theta}) \rangle$$



⇒ learns the effective Hamiltonian and identifies the associated ground state simultaneously

Wave function extracted from IBM quantum computer **(original basis $\beta=0$):**



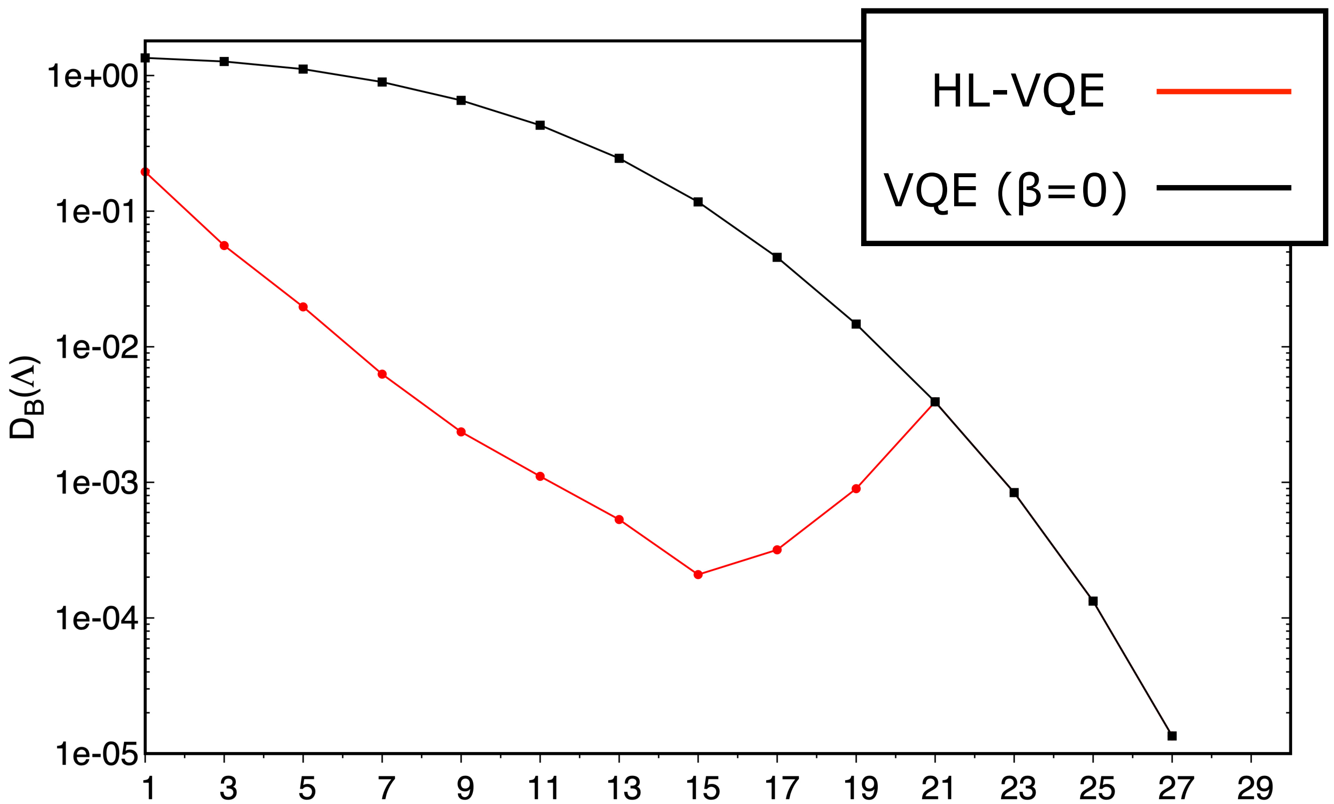
$$N = 30,\ \bar{v} = \frac{V(N-1)}{\varepsilon} = 2.0,\ \varepsilon = 1$$

CR, M. J. Savage arXiv:2301.05976 [quant-ph] (2023)

The LMG Model in effective model space

Distance between the exact and effective (truncated) wave function

$$D_B(\Lambda) = \sqrt{2(1 - |\langle\Psi(\Lambda)|\Psi_{ex}\rangle|)}$$

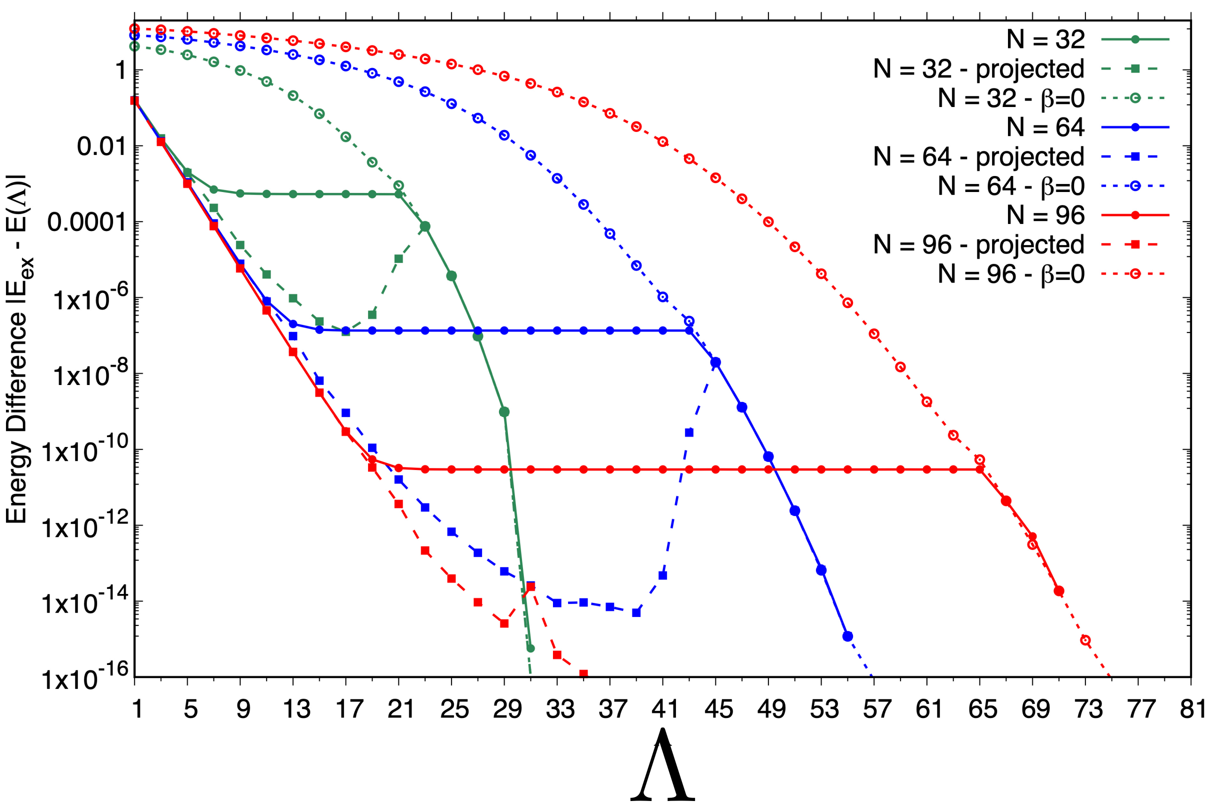


Size of the model space

$$\Lambda = 2^{n_{qubits}}$$

Energy difference:

$$|E_{ex} - E(\Lambda)|$$



exponential convergence in the symmetry-broken phase

CR, M. J. Savage arXiv:2301.05976 [quant-ph] (2023)

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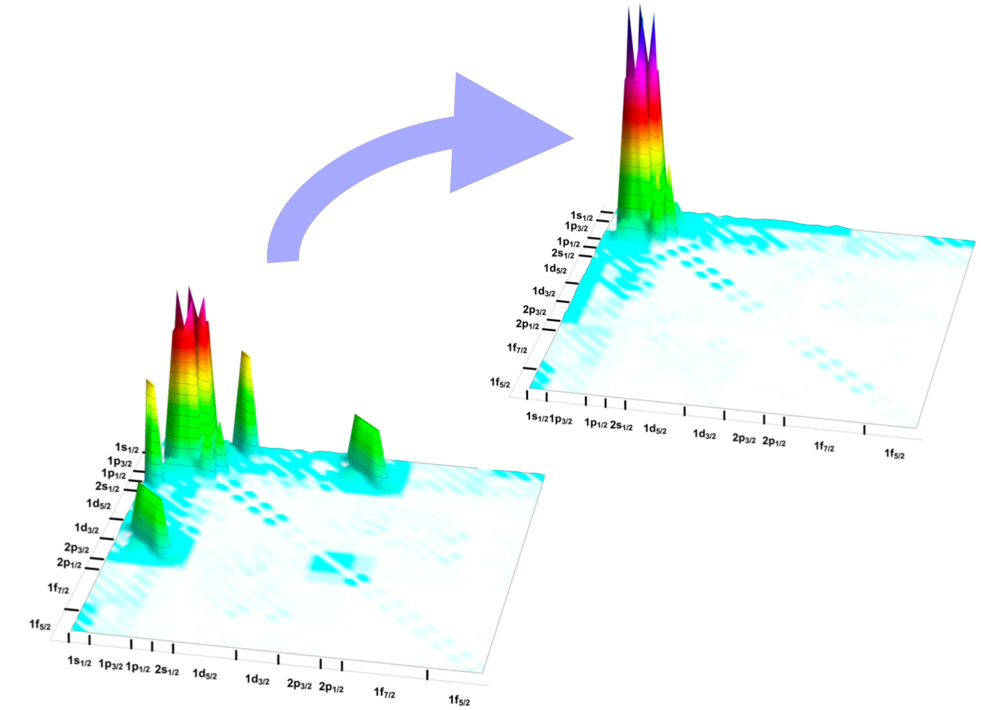

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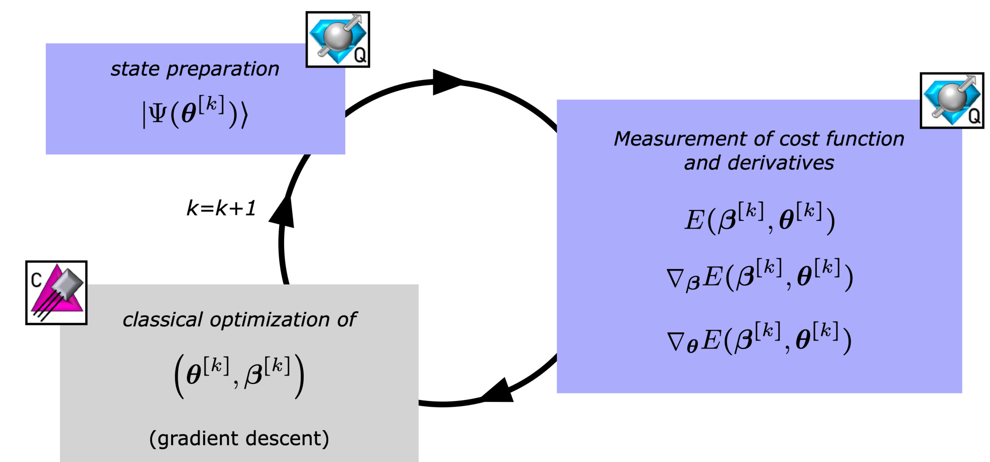

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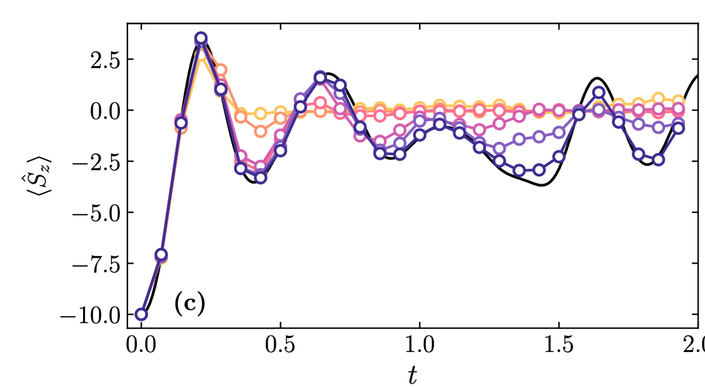
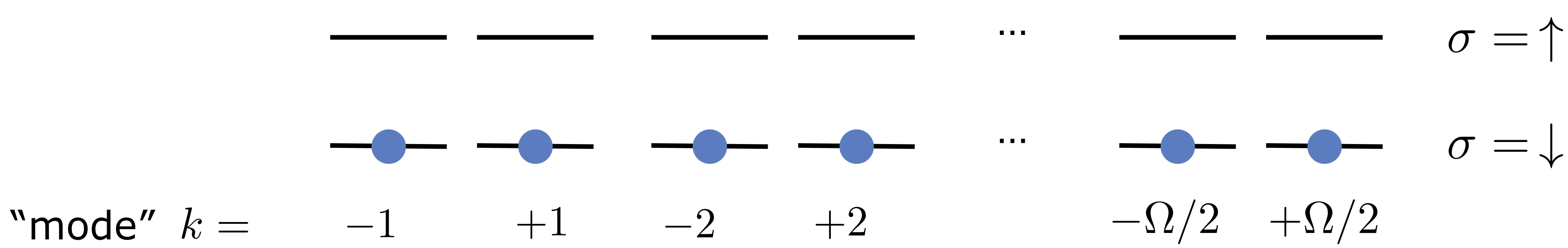
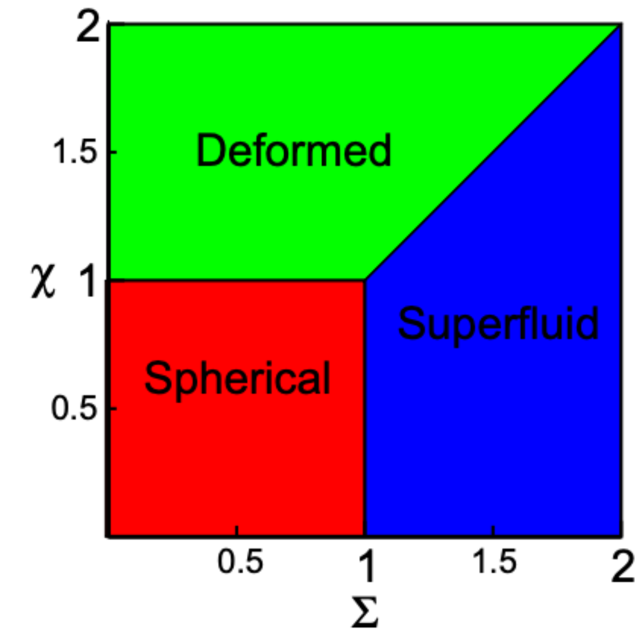


★The Agassi model

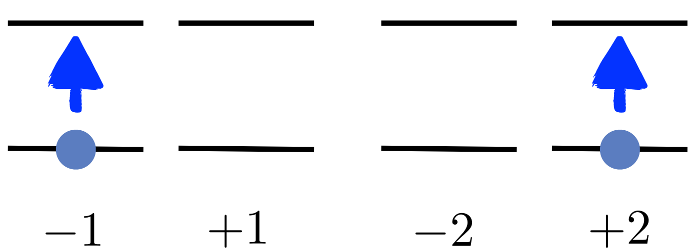
= extension of the LMG model with pairing interaction



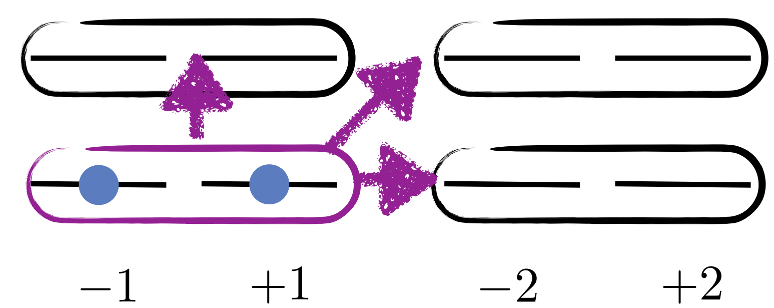


[Pérez-Fernández+ PLB 829 137133 (2022)]

$$\hat{H} = \varepsilon \hat{J}_z - \frac{V}{2}\left(\hat{J}_+^2 + \hat{J}_-^2\right) - g \sum_{\sigma\sigma'} \hat{B}_\sigma^\dagger \hat{B}_{\sigma'}$$



particle-hole interaction V



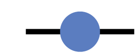
pairing interaction g

*D. Agassi, Nucl. Phys. A 116, 49 (1968)

Symmetry-guided mapping of the Agassi model onto qudit systems

- Previous quantum simulations of the Agassi model:

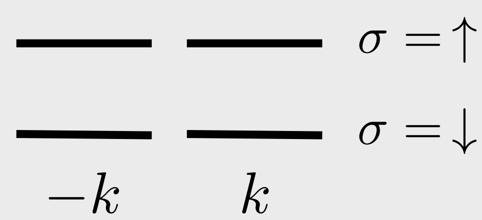
  Pérez-Fernández,et al. PLB 829, 137133 (2022); Sáiz, García-Ramos,et al. PRC 106, 064322 (2022): Ω=2 & 4 with 4 & 8 qubits

  Jordan-Wigner mapping of the sites (k, σ) onto qubits: ≡ $|0\rangle$  ≡ $|1\rangle$

- **Here we make use of the SO(5) symmetry:**

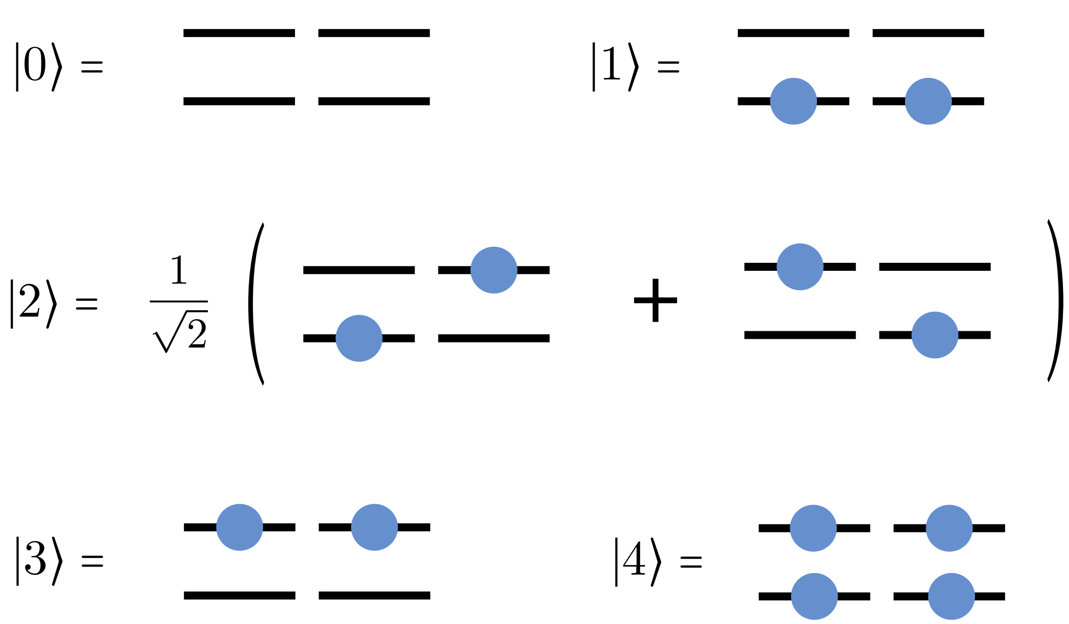
$J_z, J_\pm, B_{\uparrow,\downarrow}, B^\dagger_{\uparrow,\downarrow}$ = generators of SO(5)

Degrees of freedom = pairs of modes

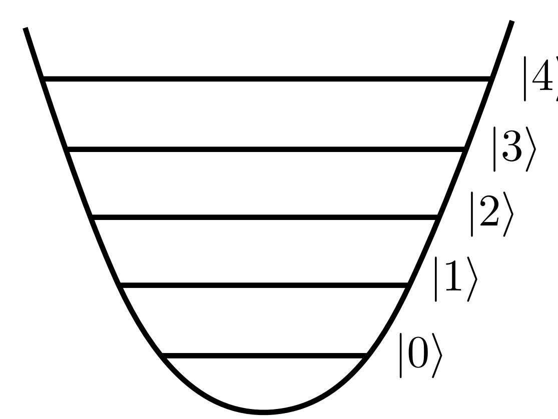


M. Illa, CR, M. J. Savage arXiv:2305.11941 [quant-ph] (2023)

⇒ 5 states:

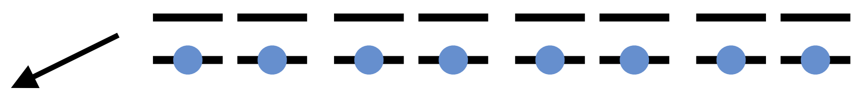


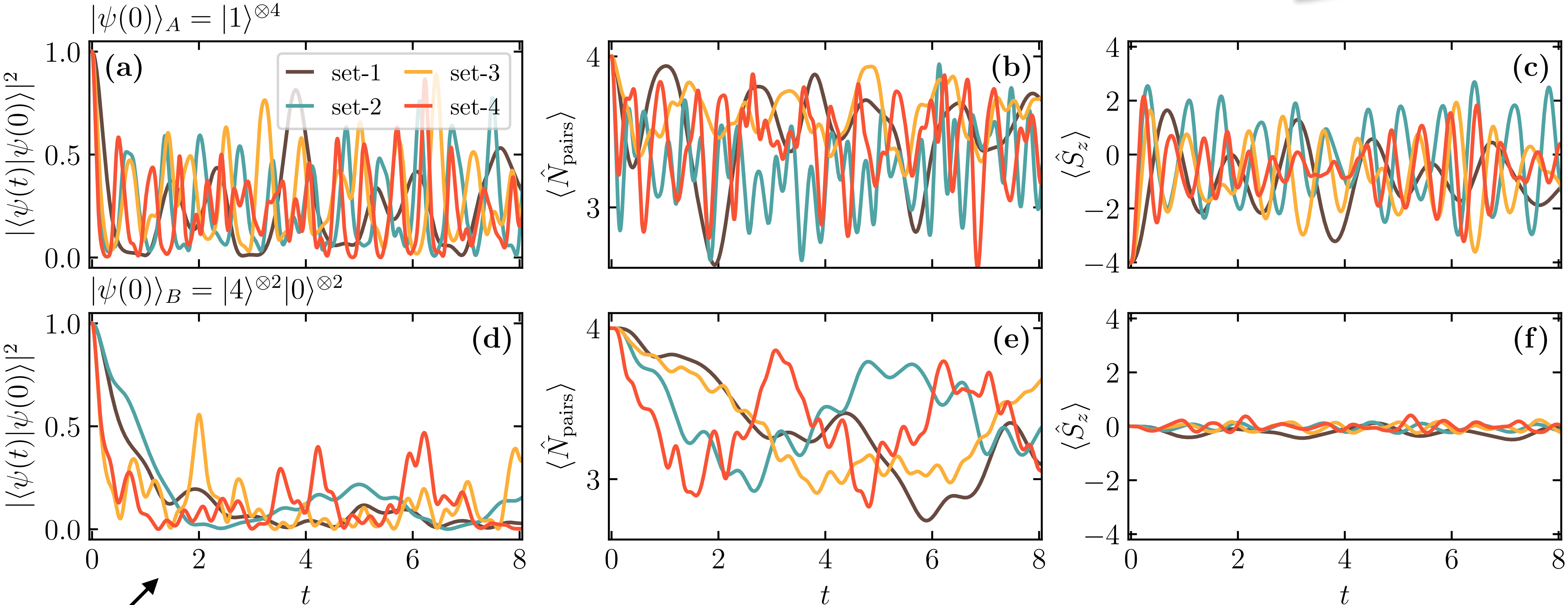
Naturally maps onto "qu5its" [qudits with d=5]

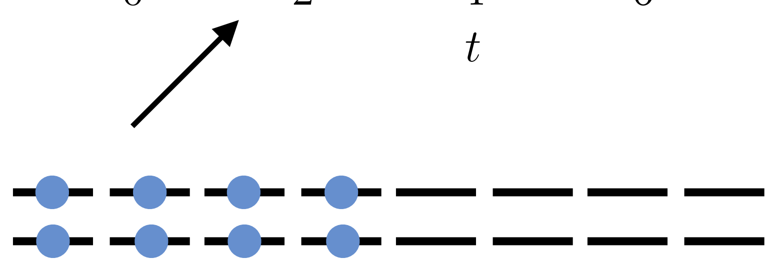


(ε, V, g) : set-0 = $(1.0, 0.0, 0.0)$
: set-1 = $(1.0, 0.5, 0.5)$
: set-2 = $(1.0, 1.5, 0.5)$
: set-3 = $(1.0, 0.5, 1.5)$
: set-4 = $(1.0, 1.5, 1.5)$

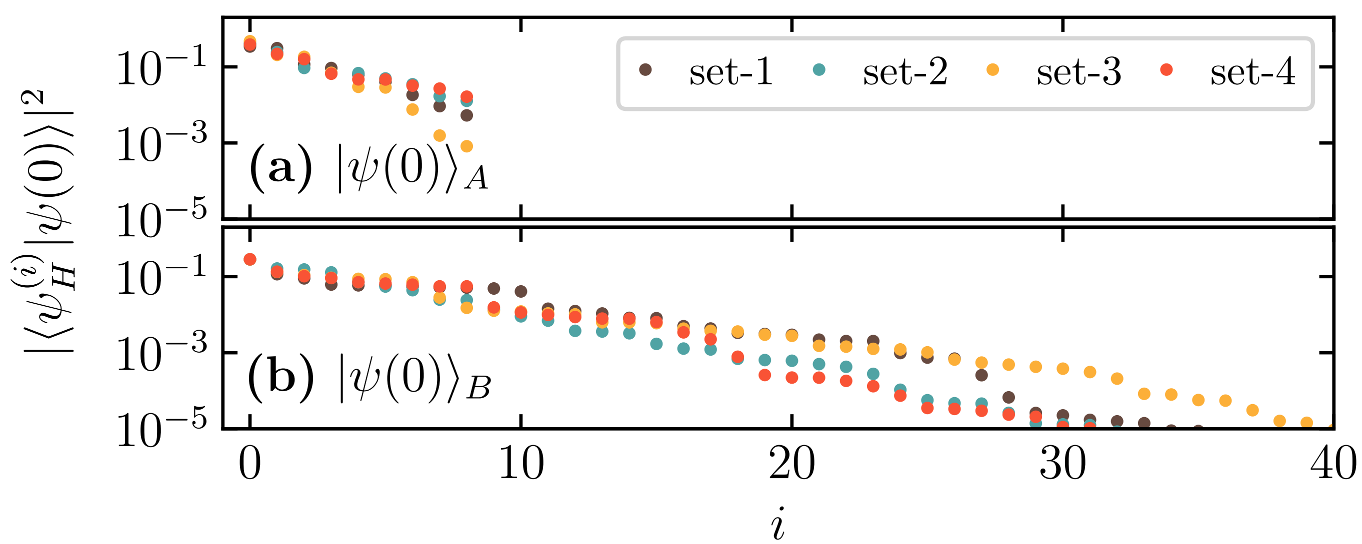
★ *Time evolution — exact exponentiation* $|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$







$\Omega = 8$



Symmetry-guided mapping of the Agassi model onto qudit systems

★ Time evolution — circuits for simulations using qu5its

- **Hamiltonian mapping to qu5its:**

$$\hat{H} = \sum_{j=1}^{\Omega/2} \sum_{j'\neq j=1}^{\Omega/2} H^{(2)}_{(jj')}$$

Acts on 2 qu5its j, j'

$$\begin{aligned} H^{(2)} &\equiv \sum_a \hat{H}^{(2,a)} \\ &= \left[\varepsilon\, \hat{j}_z - (V+g)\hat{\mathcal{X}}_{13} - g\hat{N}_{\text{pairs}}\right] \otimes \hat{I}_5 \\ &\quad + \hat{I}_5 \otimes \left[\varepsilon\, \hat{j}_z - (V+g)\hat{\mathcal{X}}_{13} - g\hat{N}_{\text{pairs}}\right] \\ &\quad - V \sum_{r,s\in\{(12),(23)\}} \left(\hat{\mathcal{X}}_r \otimes \hat{\mathcal{X}}_s - \hat{\mathcal{Y}}_r \otimes \hat{\mathcal{Y}}_s\right) \\ &\quad - \frac{g}{2} \sum_{\substack{r,s\in\{(01),(03),\\ -(14),-(34)\}}} \left(\hat{\mathcal{X}}_r \otimes \hat{\mathcal{X}}_s + \hat{\mathcal{Y}}_r \otimes \hat{\mathcal{Y}}_s\right) \end{aligned}$$

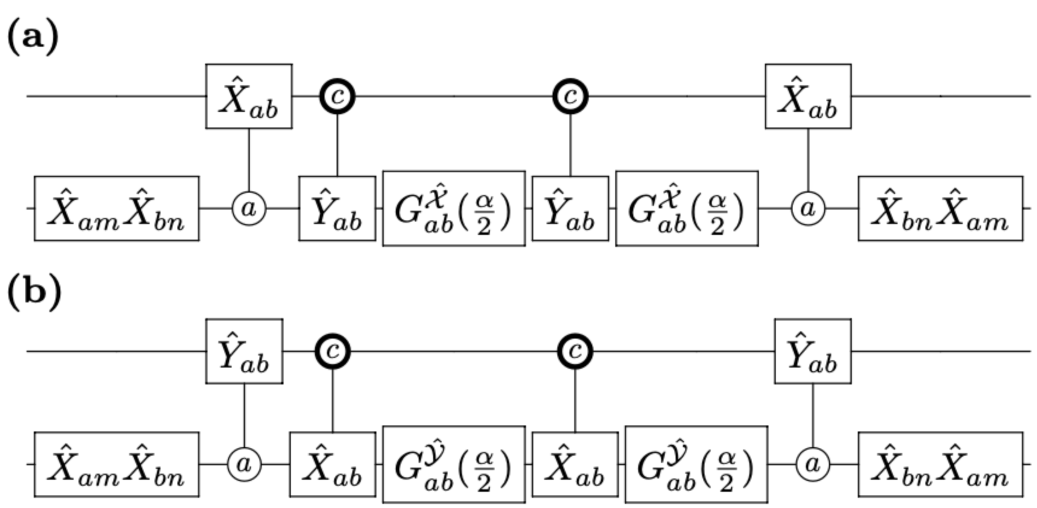
generators of Givens rotations

$$G^{\mathcal{X}\mathcal{X}}_{abmn}(\alpha) \qquad G^{\mathcal{Y}\mathcal{Y}}_{abmn}(\alpha)$$

- **Trotter decomposition at leading order:**

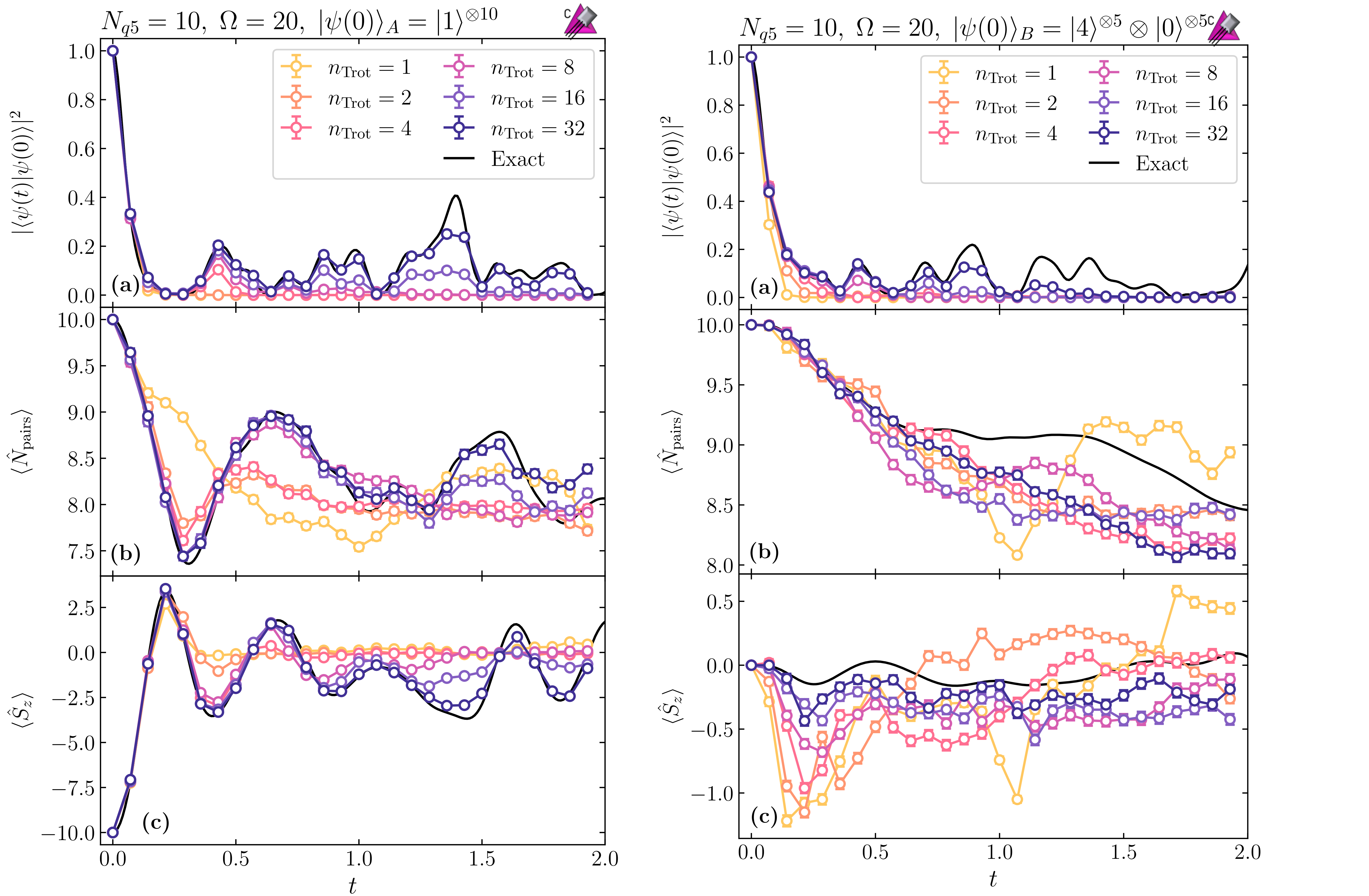
$$\hat{U}(t) = e^{-i\hat{H}t} \simeq \left(e^{-i\hat{H}\Delta t}\right)^{n_{Trot}}$$

$$e^{-i\hat{H}\Delta t} = e^{-i\sum_{jj'} \hat{H}^{(2)}_{jj'}\Delta t} \simeq \prod_{jj'} \prod_{a} e^{-i\hat{H}^{(2,a)}_{jj'}\Delta t}$$



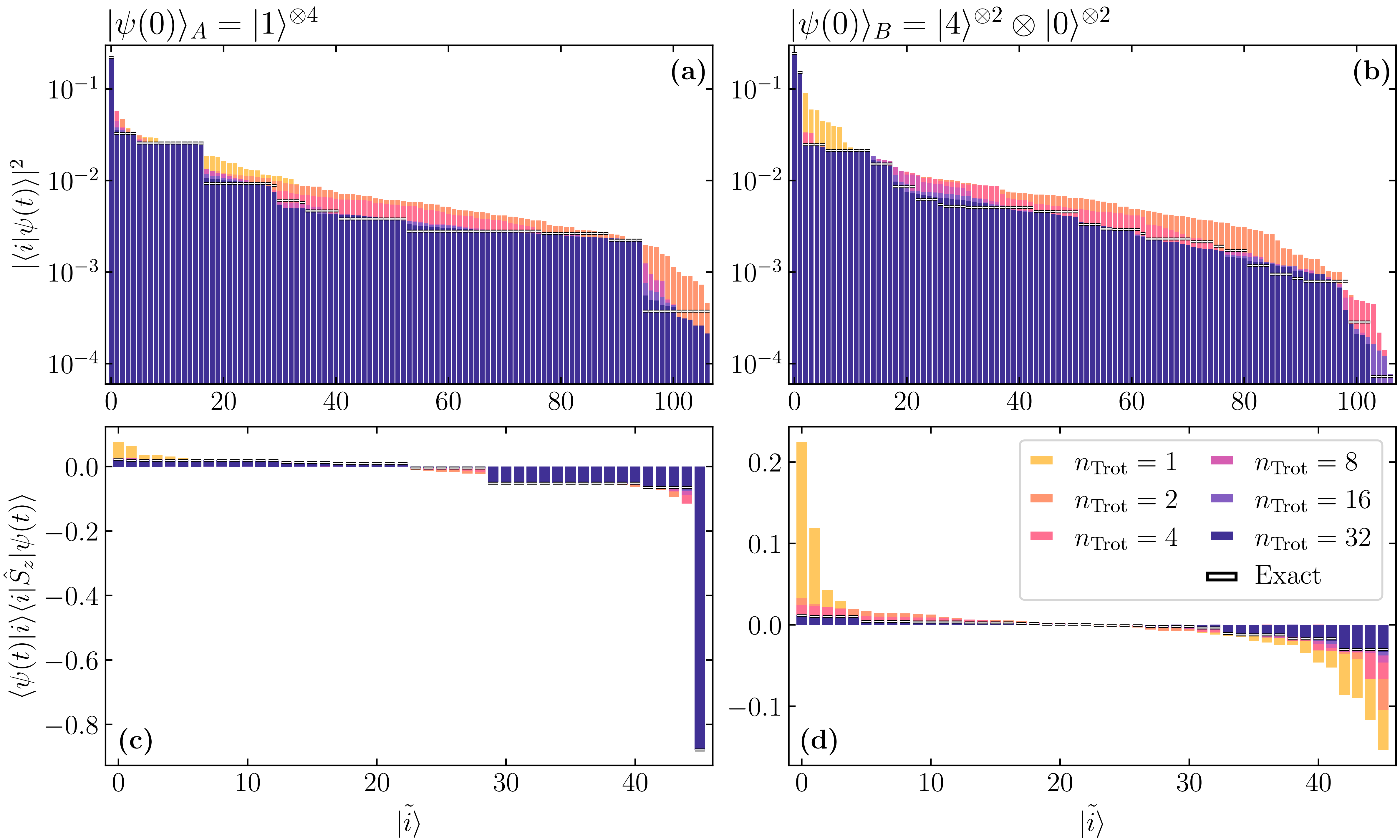
Circuits for $G^{\mathcal{X}\mathcal{X}}_{abmn}(\alpha)$ and $G^{\mathcal{Y}\mathcal{Y}}_{abmn}(\alpha)$

★ ***Developed a qudit-system simulator using Google's `cirq` software:*** [interaction set-3]



Symmetry-guided mapping of the Agassi model onto qudit systems

★ ***A new sign problem:*** $|\psi(0)\rangle = \sum_i c_i(0)|i\rangle$ ← Computational-basis states

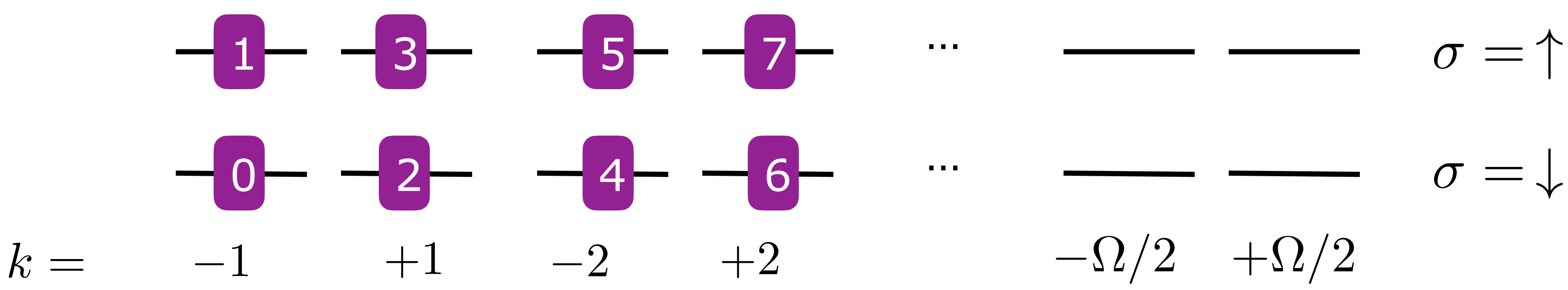


★ Resource requirements and comparison with mappings onto qubits

A) "Physics-Aware" Jordan-Wigner (paJW) mapping

— $\equiv |0\rangle$ —●— $\equiv |1\rangle$

Organization in terms of mode-pairs:



Bosonization made explicit

Similar to D. Lacroix's JW mapping of the Richardson model

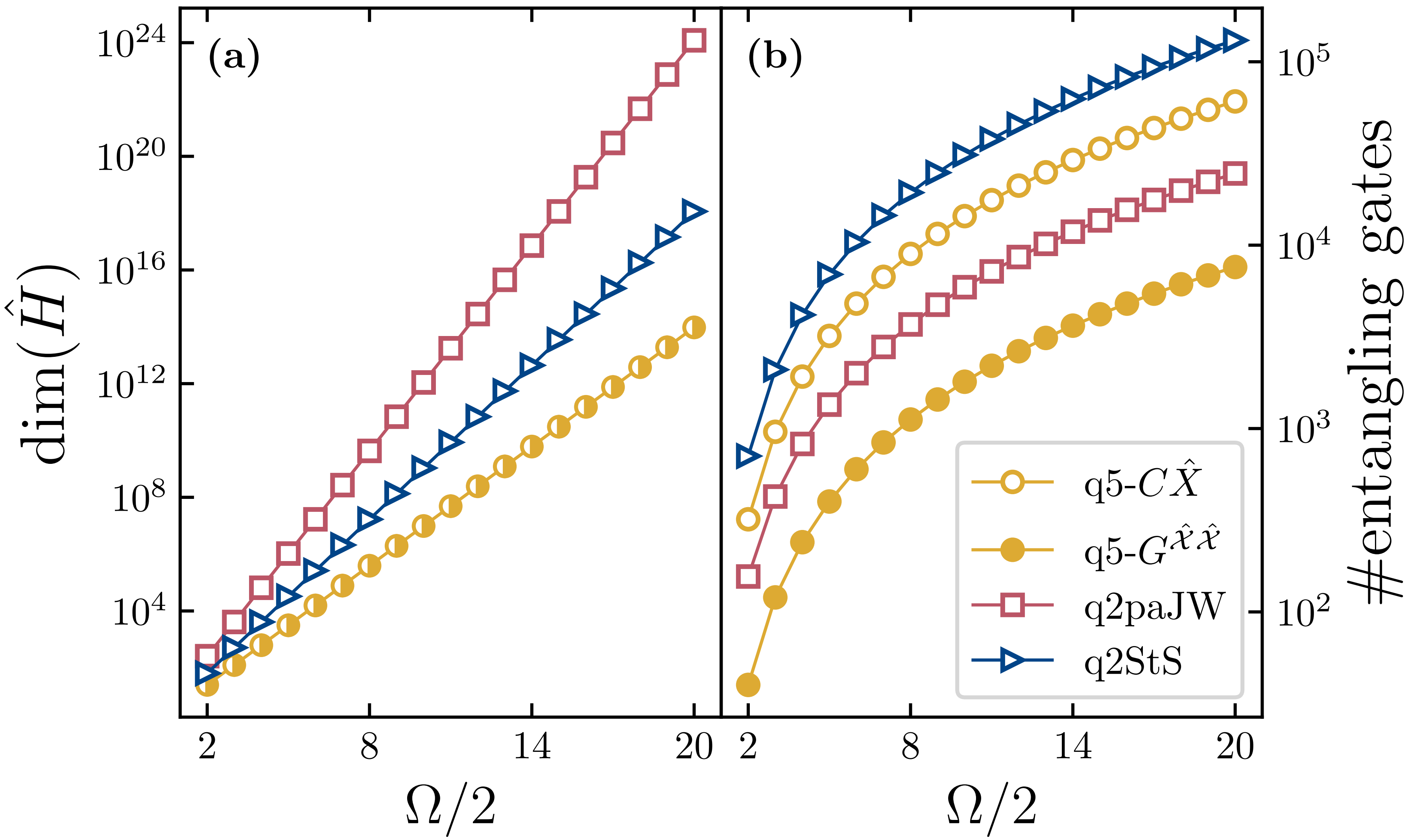
→ minimizes the number of phase operators Z
→ 4 qubits per mode pair

B) State-to-state (StS) qubit-qu5it mapping

→ 3 qubits are used to map the 5 states of one mode pair

$$|0\rangle = |000\rangle \ , \quad |1\rangle = |001\rangle \ , \quad |2\rangle = |010\rangle \ , \quad |3\rangle = |011\rangle \ , \quad |4\rangle = |100\rangle$$

★ *Resource requirements and comparison with mappings onto qubits*



q5-$\hat{G}^{\mathcal{X}\mathcal{X}}$: Two-qu5it Givens rotations $G^{\mathcal{X}\mathcal{X}}_{pq,rs}(\alpha) = e^{-i\alpha\mathcal{X}_{pq}\otimes\mathcal{X}_{rs}}$ are available on the device

q5-$C\hat{X}$: They are implemented via generalized CX, CY

Conclusion

* Entanglement rearrangement and wave-function localization in the Hilbert space appear crucial for fast convergence of classical calculations and efficient quantum computations, as demonstrated with the LMG model.

* **Physics-informed mappings to qubits/qudits and entanglement-driven algorithms could be key for future developments of efficient quantum simulations of many-body systems**

➔ Next: adapt and apply these concepts to more general nuclear interactions and systems

* Entanglement is a useful tool for exploration of the nuclear wave function and to reveal physical phenomena

  ➔ **link with emergence of degrees of freedom?**

  ➔ **Could entanglement (minimization) be a fundamental organizational principle of matter?**

BACKUP

Single-orbital entanglement

- Single-orbital Von Neumann entropy: $S^{(1)}_{(i)} = -\mathrm{Tr}\left[\rho^{(i)} \ln \rho^{(i)}\right]$

  = measure of entanglement of one orbital with the rest of the system

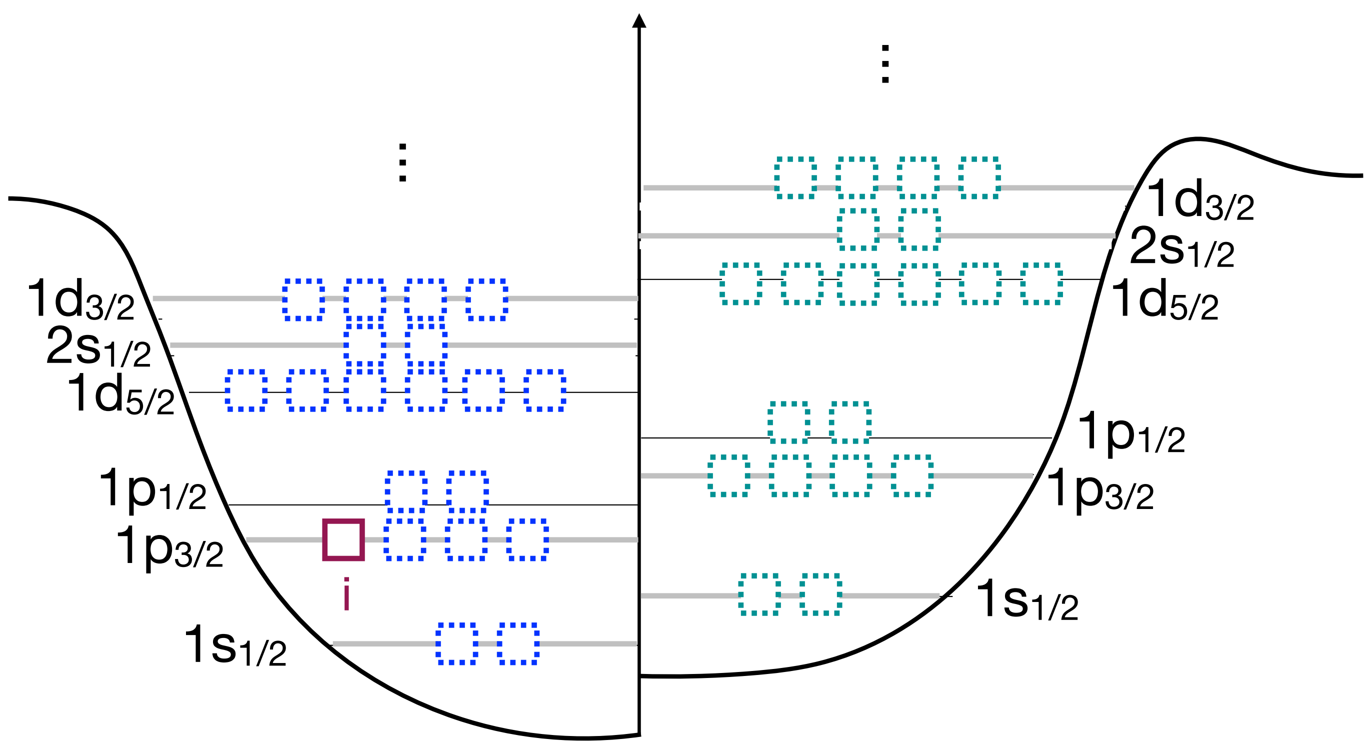
$$(i) \equiv \{n_i, l_i, j_i, m_i, \tau_i\}$$

$\rho^{(i)}$ is the one-orbital reduced density matrix:

$$\gamma_{ii} = \langle \Psi | a_i^\dagger a_i | \Psi \rangle$$

occupation numbers

$$\rho^{(i)} = \mathrm{Tr}_{(n_1,\ldots,n_{i-1},n_{i+1},\ldots n_N)} |\Psi\rangle\langle\Psi| = \begin{pmatrix} 1-\gamma_{ii} & 0 \\ 0 & \gamma_{ii} \end{pmatrix}$$

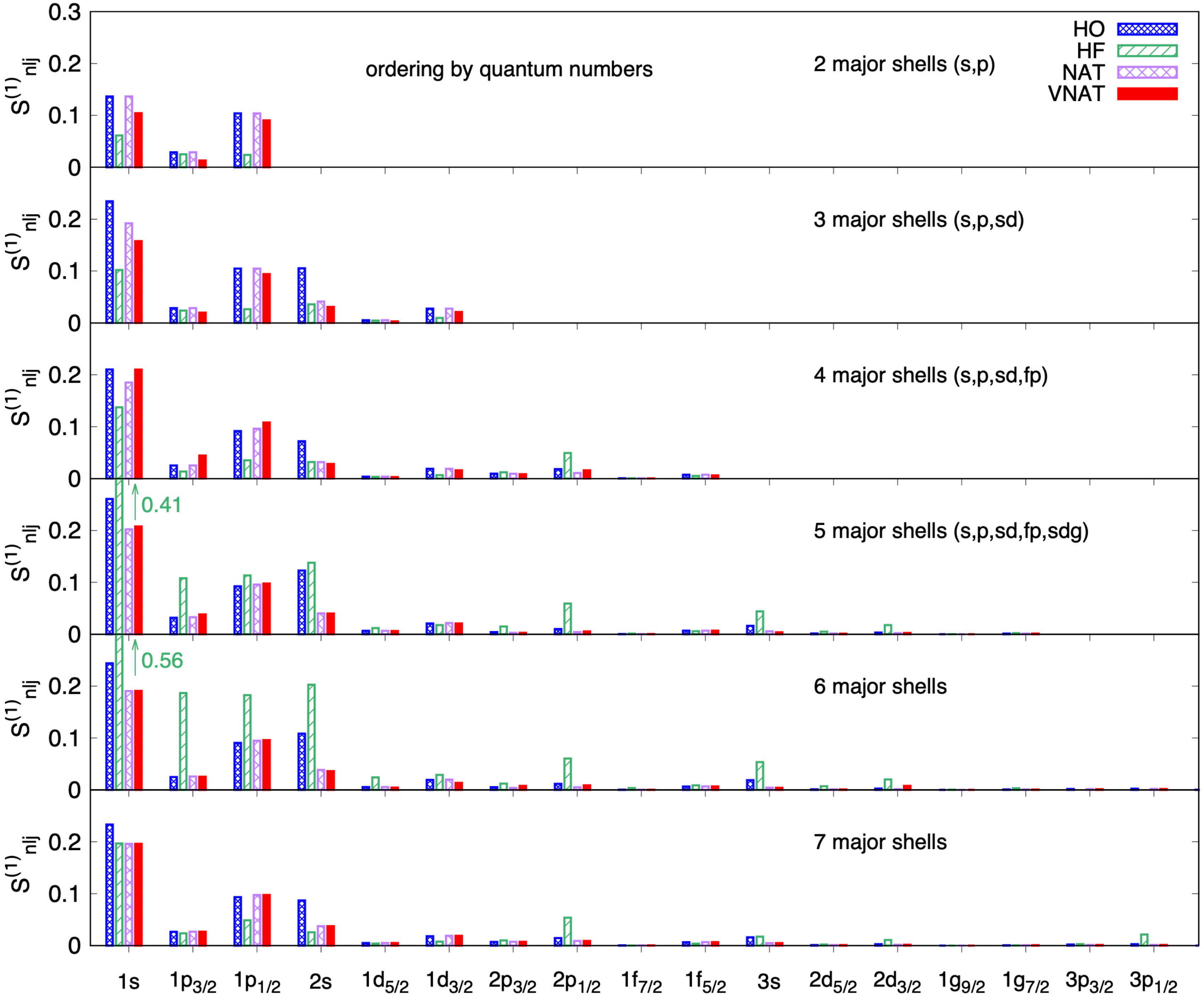


neutron orbitals *proton orbitals*

Single-orbital entanglement in ^{4}He

- Convergence of the single-orbital Von Neumann entropy:

$$S^{(1)}_{tot} = \sum_i S^{(1)}_i$$



N_{tot}	HO	HF	NAT	VNAT
2 shells	0.596	0.270	0.596	0.441
3 shells	1.143	0.487	0.929	0.746
4 shells	1.065	0.686	0.928	1.063
5 shells	1.348	2.327	1.036	1.042
6 shells	1.264	3.434	0.972	0.963
7 shells	1.217	1.069	1.006	1.006

✳ *HF bad convergence properties also reflected on entanglement*

$$2-4 \text{ shells}: |\Psi_{HF}\rangle \simeq 94-98\% \text{ SD}$$

$$5 \text{ shells}: |\Psi_{HF}\rangle \simeq 70\% \text{ SD}$$

$$6 \text{ shells}: |\Psi_{HF}\rangle \simeq 56\% \text{ SD}$$

$$7 \text{ shells}: |\Psi_{HF}\rangle \simeq 91\% \text{ SD}$$

✳ *NAT & VNAT typically have similar entanglement patterns*

Two-orbital entanglement

- Two-orbital Von Neumann entropy: $S^{(2)}_{(ij)} = -\mathrm{Tr}\left[\rho^{(ij)} \ln \rho^{(ij)}\right]$

  = measure of entanglement of two orbitals with the rest of the system

$$\gamma_{ijij} = \langle \Psi | a_i^\dagger a_j^\dagger a_j a_i | \Psi \rangle$$

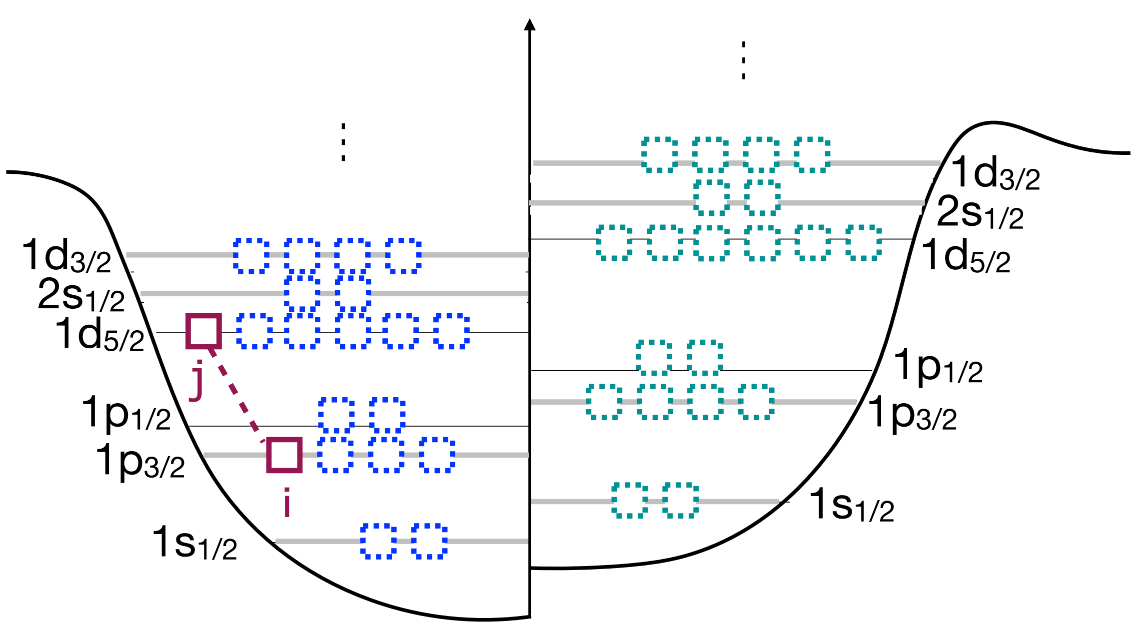
two-nucleon density

$\rho^{(ij)}$ is the two-orbital reduced density matrix:

$$\rho^{(ij)} = \mathrm{Tr}_{n_1,\ldots,n_{i-1},n_{i+1},\ldots n_{j-1},n_{j+1},\ldots,n_N} |\Psi\rangle\langle\Psi| = \begin{pmatrix} 1-\gamma_{ii}-\gamma_{jj}+\gamma_{ijij} & 0 & 0 & 0 \\ 0 & \gamma_{jj}-\gamma_{ijij} & \gamma_{ji} & 0 \\ 0 & \gamma_{ij} & \gamma_{ii}-\gamma_{ijij} & 0 \\ 0 & 0 & 0 & \gamma_{ijij} \end{pmatrix}$$

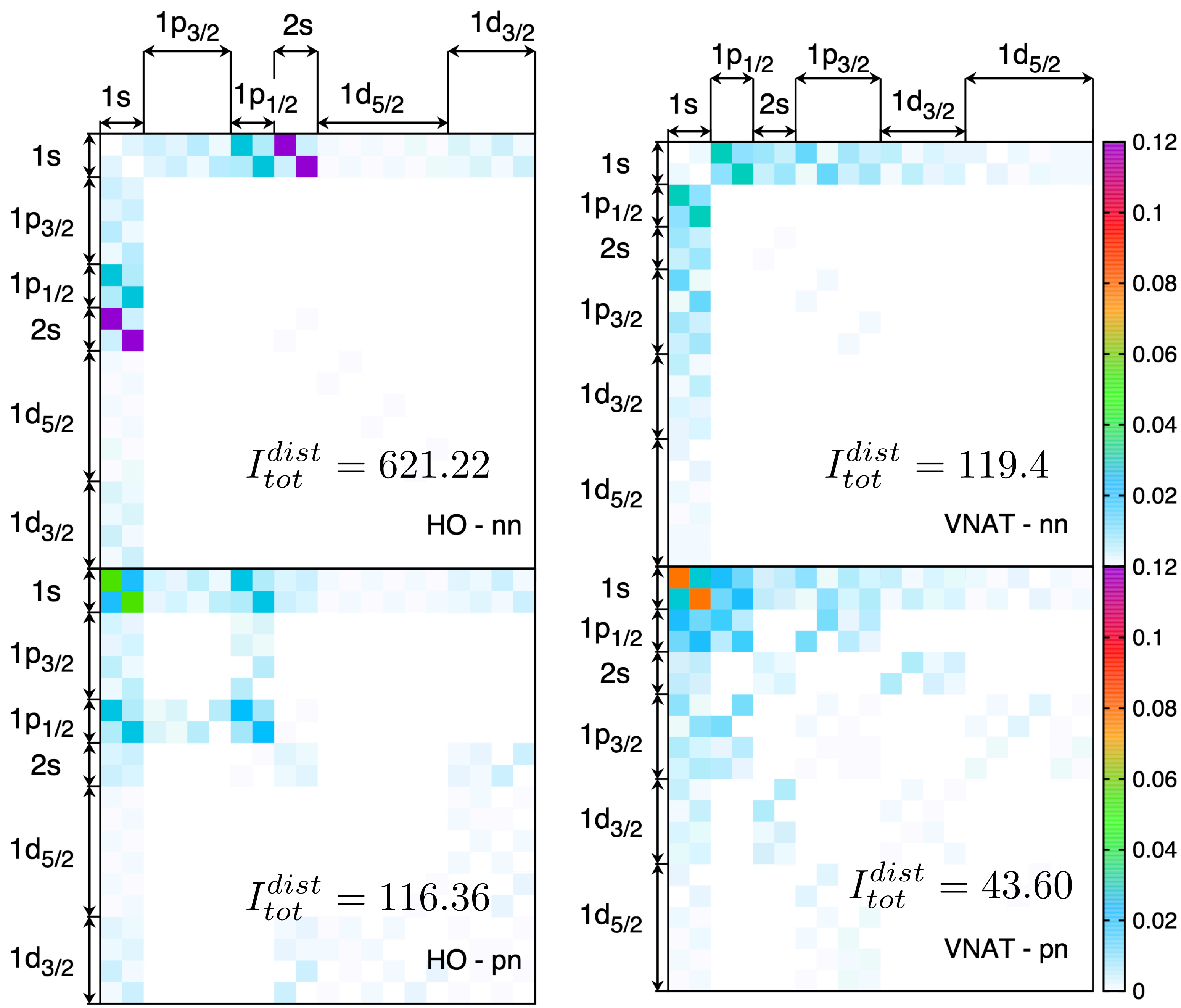
- Mutual information between two orbitals embedded in the nucleus $I_{ij} = -\left(S^{(2)}_{(ij)} - S^{(1)}_{(i)} - S^{(1)}_{(j)}\right)(1-\delta_{ij})$

  = measure of both quantum and classical correlations



Two-orbital mutual information in ^{4}He

"localization of correlations" in the basis - ordering of the calculations



"Entanglement distance":

$$I_{ij}^{dist} = I_{ij} \times |i-j|^2$$

$$I_{tot}^{dist} = \sum_{ij} I_{ij}^{dist}$$

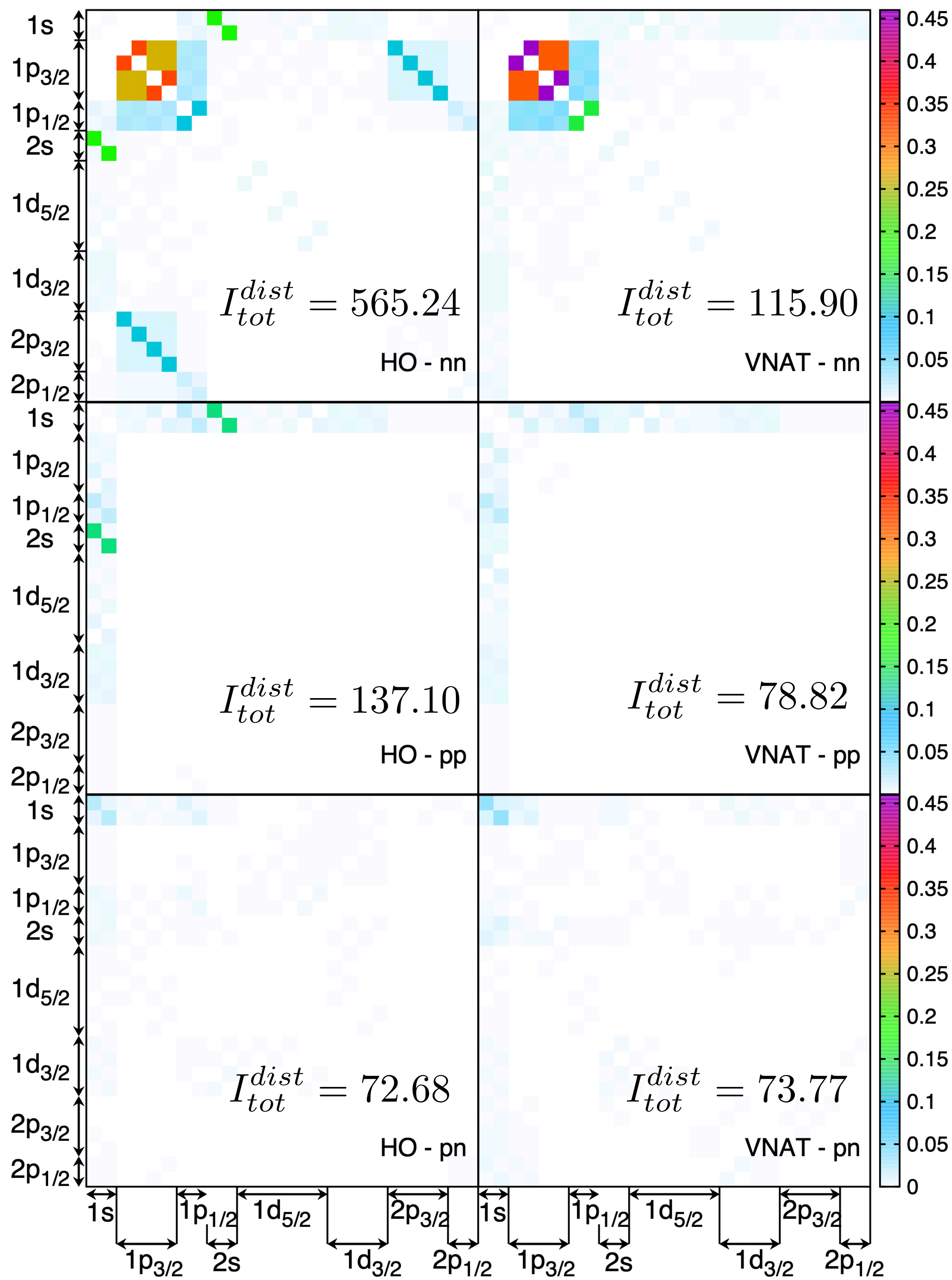
- In DMRG the entanglement distance is used to group the most interacting orbitals together, here such grouping occurs naturally

Two-orbital mutual information in ^{6}He

neutron-neutron MI:

proton-proton MI:

proton-neutron MI:



Entanglement distance:

$$I^{dist}_{ij} = I_{ij} \times |i - j|^2$$

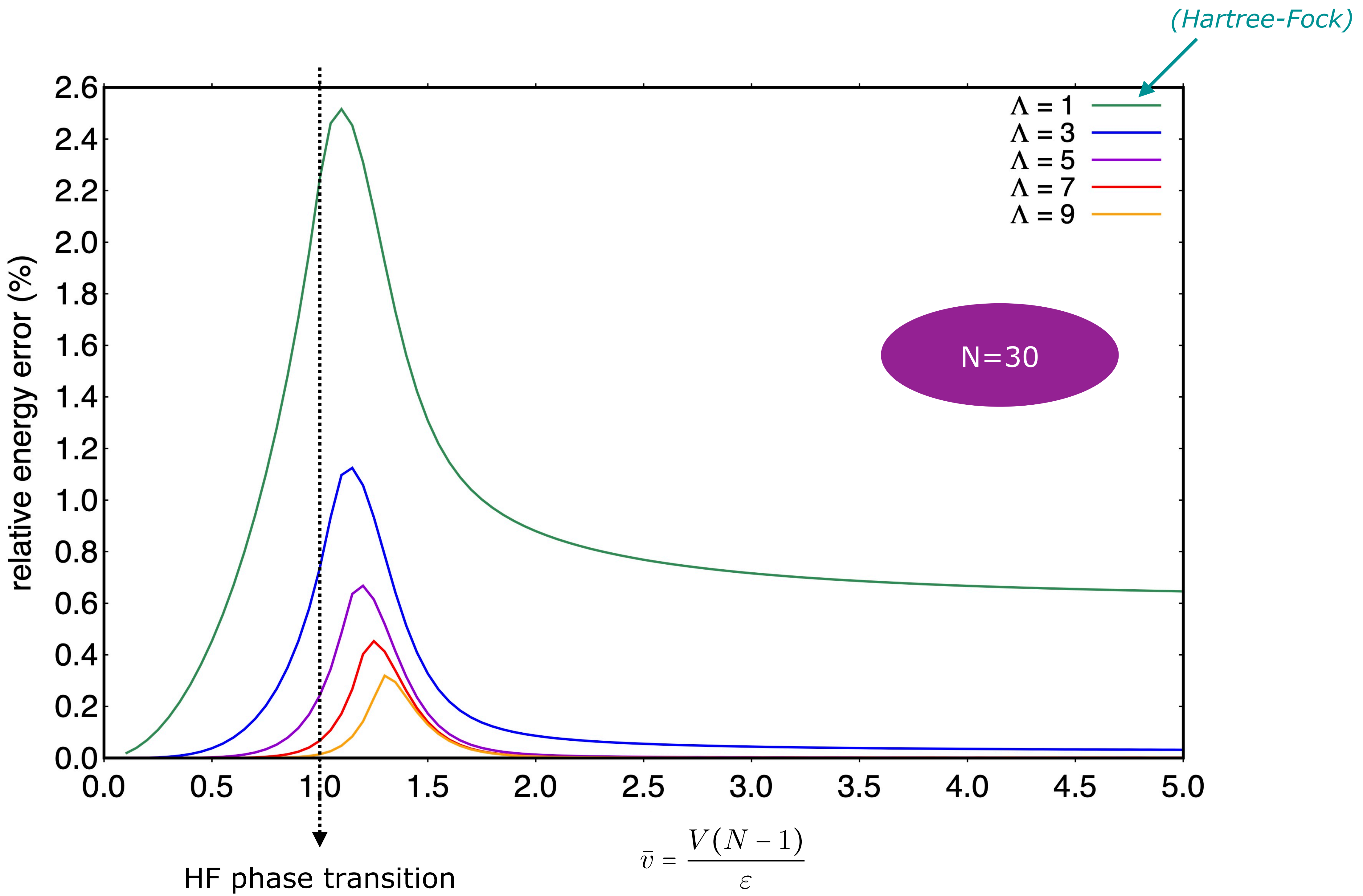
$$I^{dist}_{tot} = \sum_{ij} I^{dist}_{ij}$$

Correlations among neutron orbitals are the dominant ones

The Lipkin-Meshkov-Glick Model in effective model space

★**Energy**

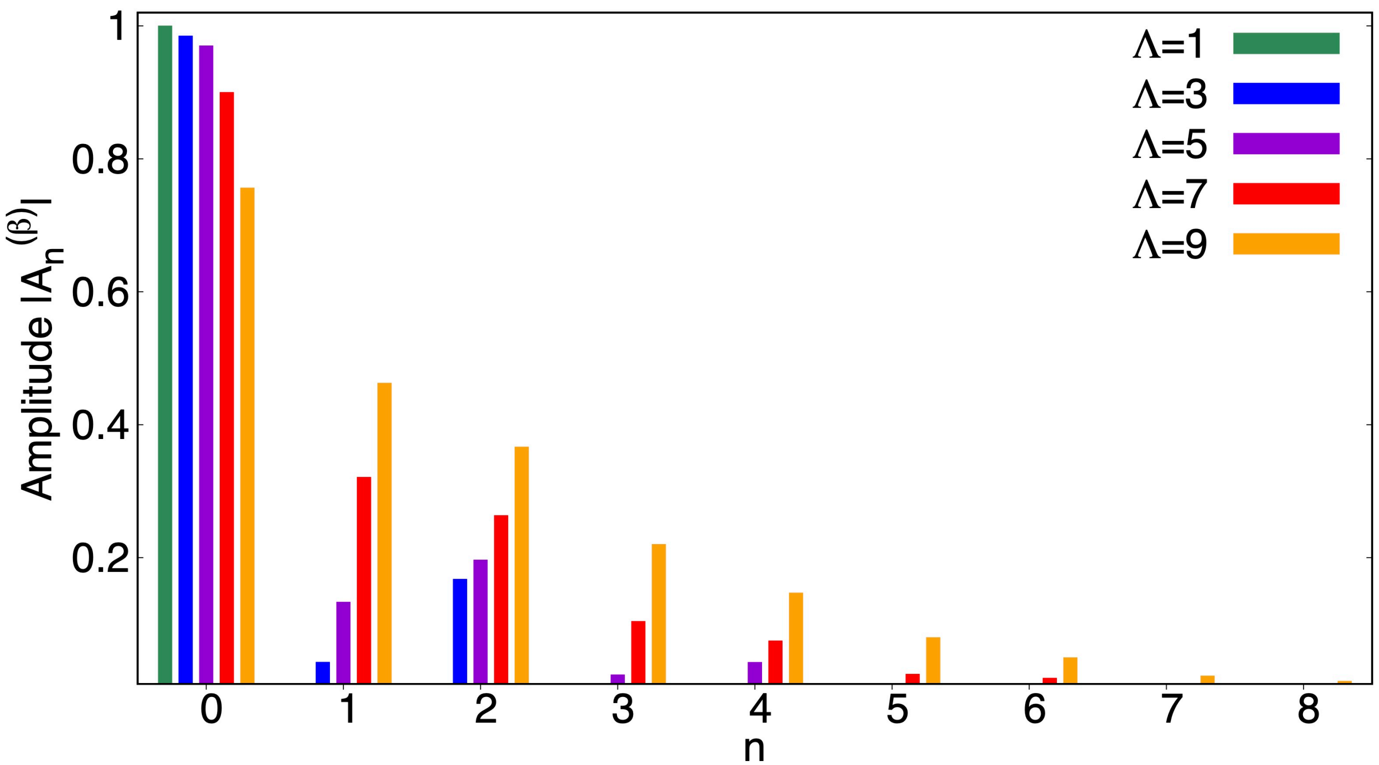
$$\frac{|E_{ex} - E|}{|E_{ex}|}$$



$$\bar{v} = \frac{V(N-1)}{\varepsilon}$$

The Lipkin-Meshkov-Glick Model in effective model space

✳ ***Effective wave function (rotated basis):***



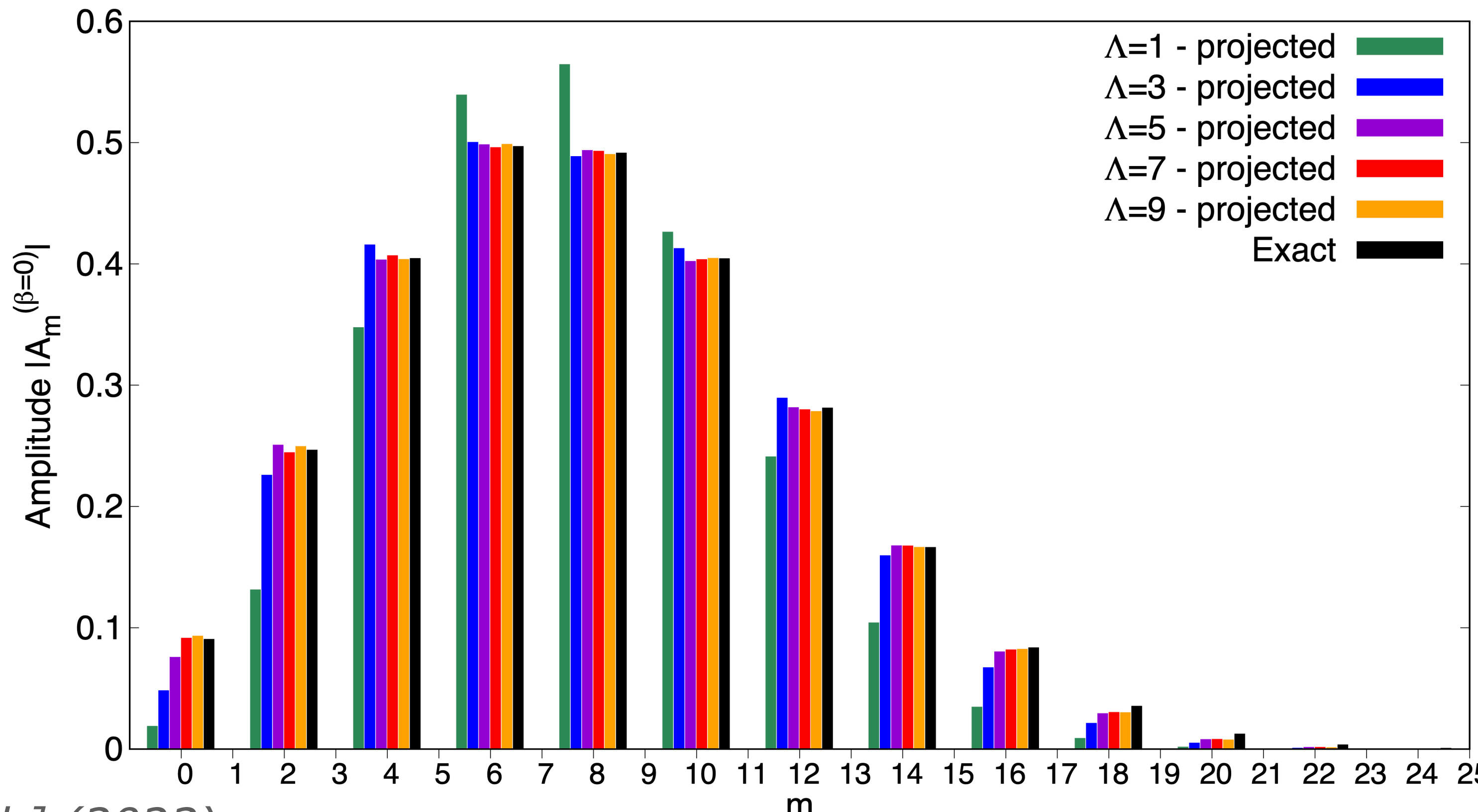
$$N = 30,\ \bar{v} = \frac{V(N-1)}{\varepsilon} = 2.0,\ \varepsilon = 1$$

wave function is localized in the effective model space

➔ fall-off will increase the efficiency of quantum simulations

Λ	β	Λ	β
1,2	1.047	17,18	0.289
3,4	1.016	19,20	0.150
5,6	0.977	21,22	0.0
7,8	0.906	23,24	0.0
9,10	0.791	25,26	0.0
11,12	0.664	27,28	0.0
13,14	0.538	29,30	0.0
15,16	0.415	31	0.0

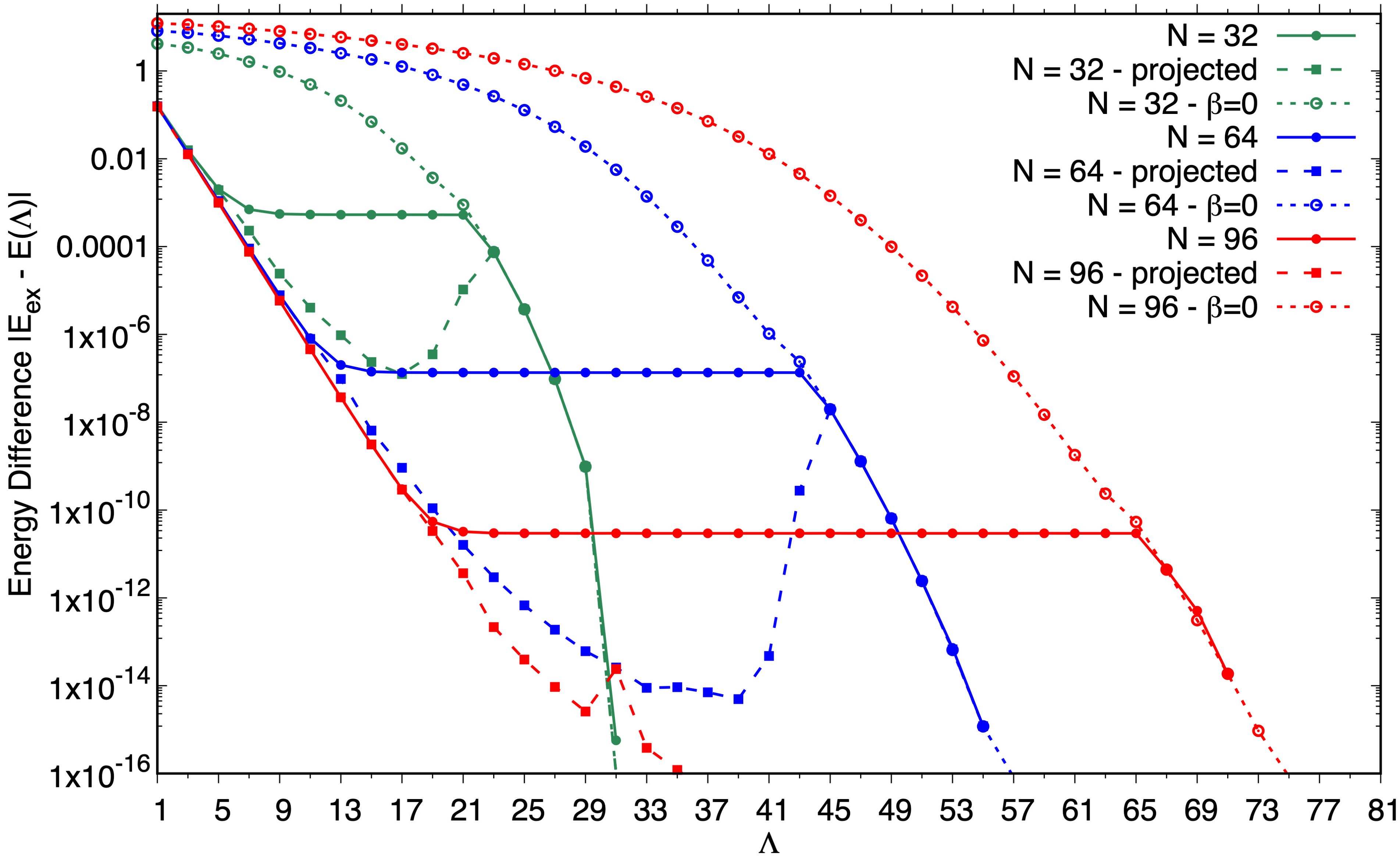
✳ ***Effective wave function (original basis β=0):***



CR, M. J. Savage arXiv:2301.05976 [quant-ph] (2023)

The Lipkin-Meshkov-Glick Model in effective model space

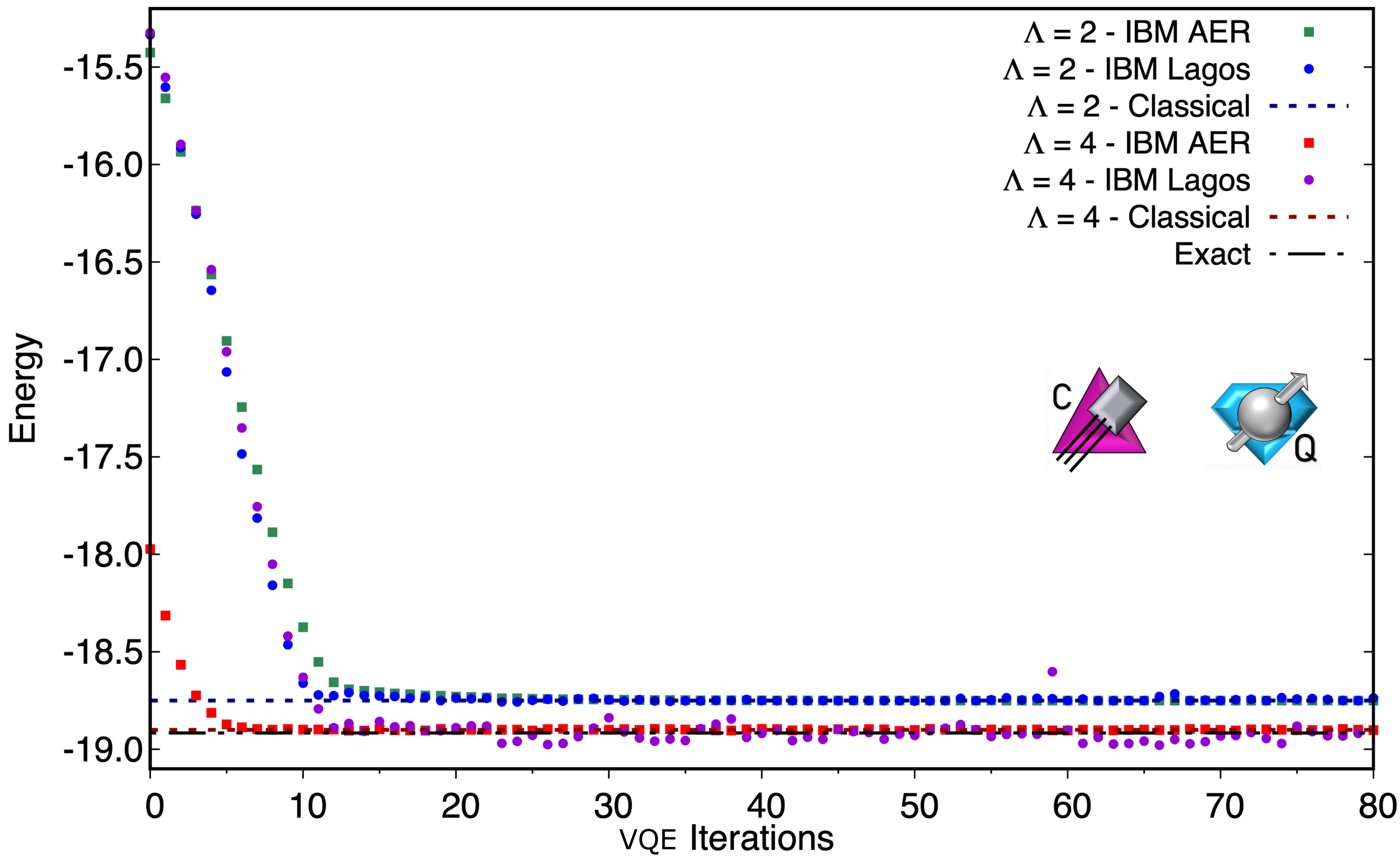
★ ***Convergence for different particle numbers:***



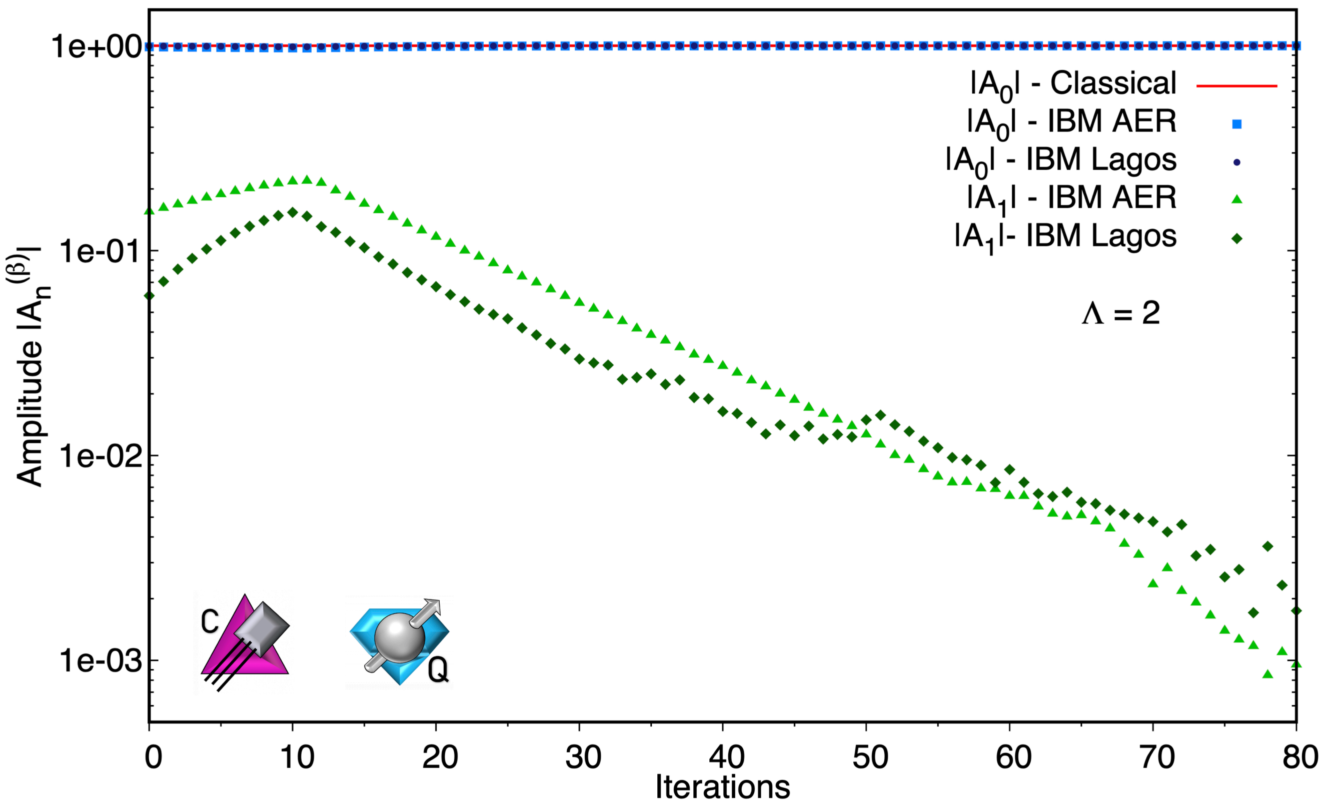
→ consistent with an exponential improvement of the convergence in the symmetry-broken phase, which is sustained further by the projection

The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

★***Energies:*** $N = 30,\ \bar{v} = \dfrac{V(N-1)}{\varepsilon} = 2.0,\ \varepsilon = 1$

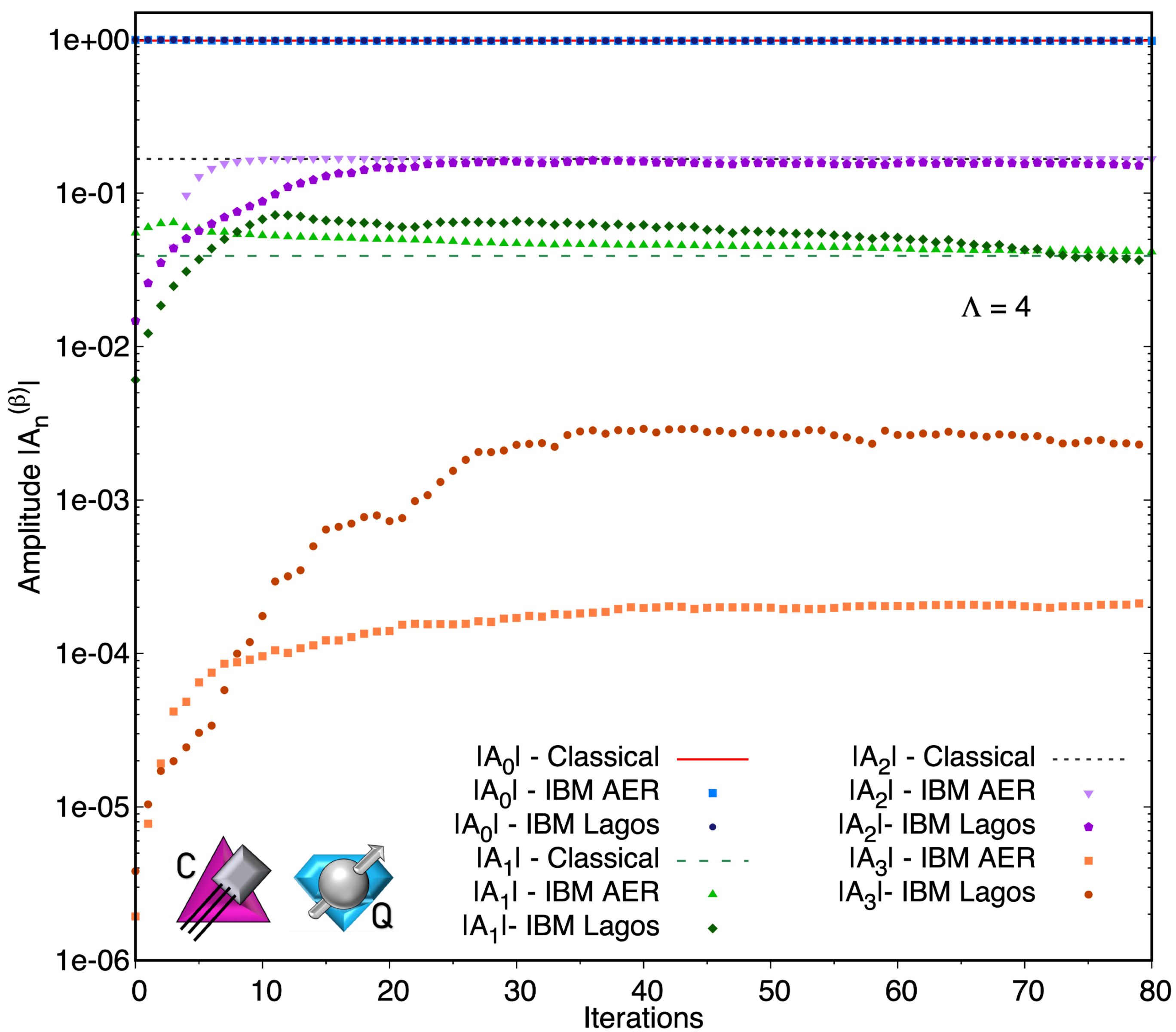


★ ***Wave functions (in the optimized basis):***



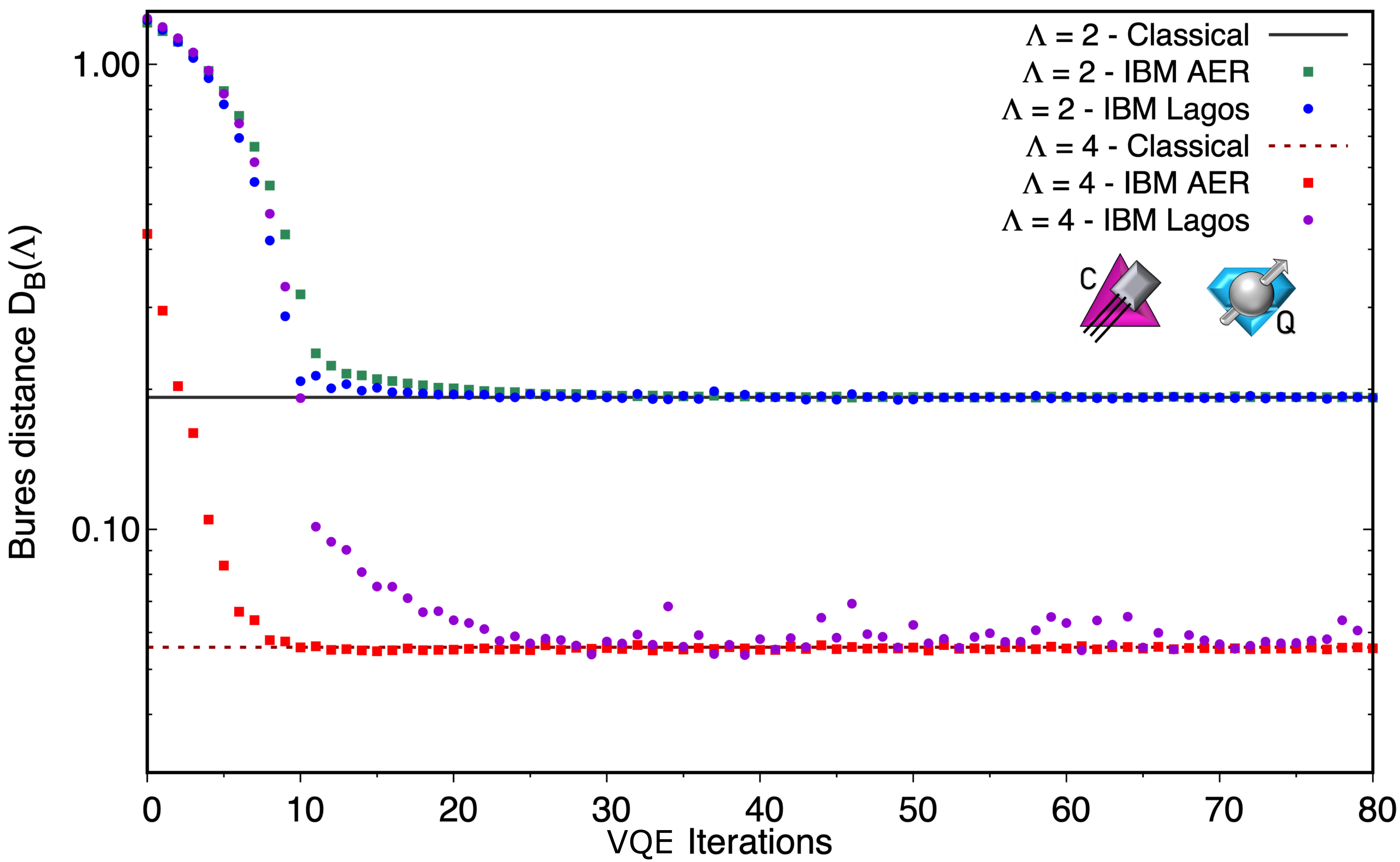
$$|\Psi\rangle = A_0|0\rangle + A_1|1\rangle$$

$$|\Psi\rangle = \sum_{n=0}^{3} A_n|n\rangle$$



The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

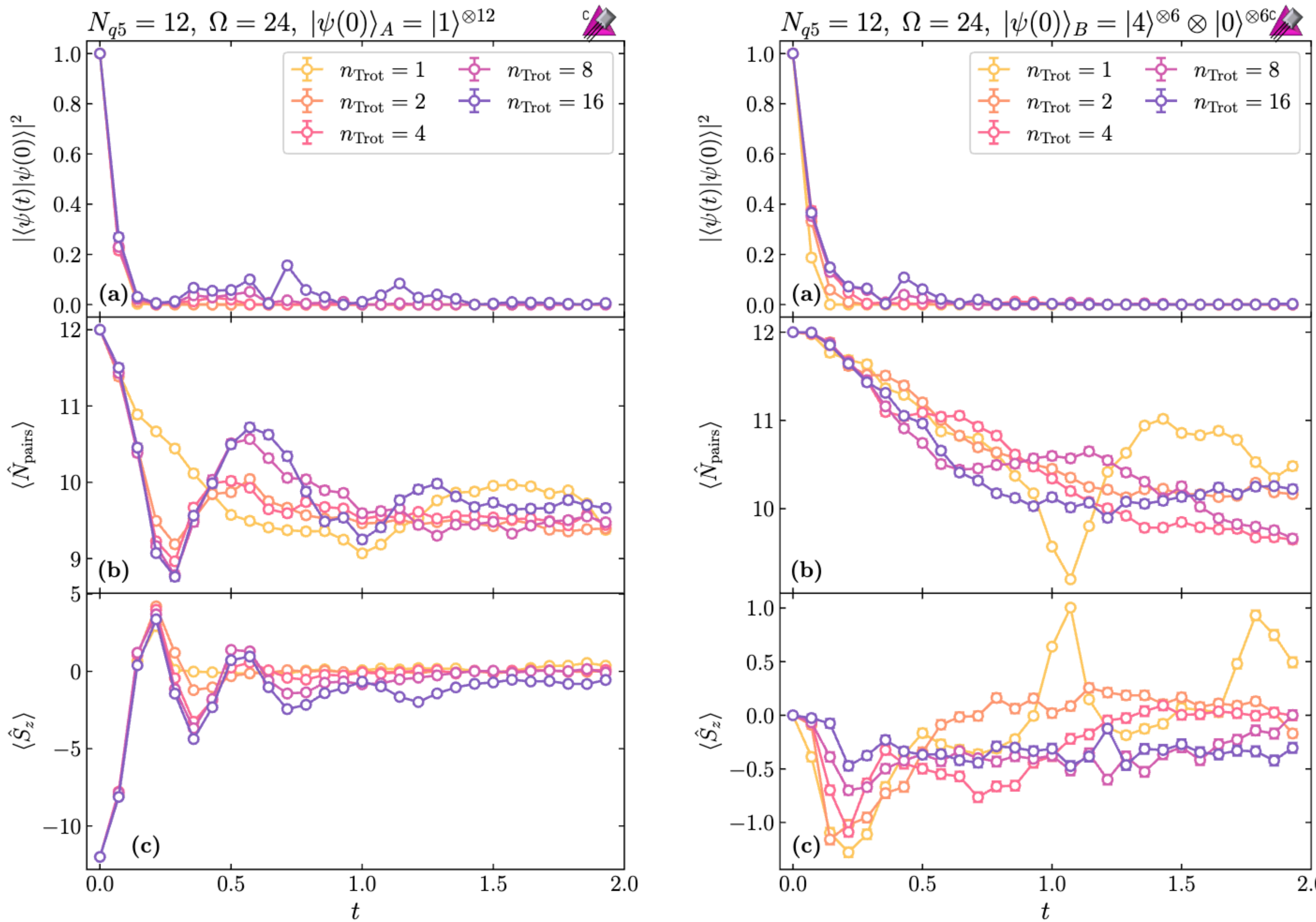
★ ***Bures distance:*** $D_B(\Lambda) = \sqrt{2(1-|\langle\Psi(\Lambda)|\Psi_{ex}\rangle|)}$



Symmetry-guided mapping of the Agassi model onto qudit systems

★ ***Implementations on Google's `cirq` simulator*** (with interaction set-3)

Ω = 24



M. Illa, CR, M. J. Savage arXiv:2305.11941 [quant-ph] (2023)