

*Quantum Computing for Many-Body problems (QCMB): atomic nuclei,
neutrinos, and other strongly correlated Fermi systems*

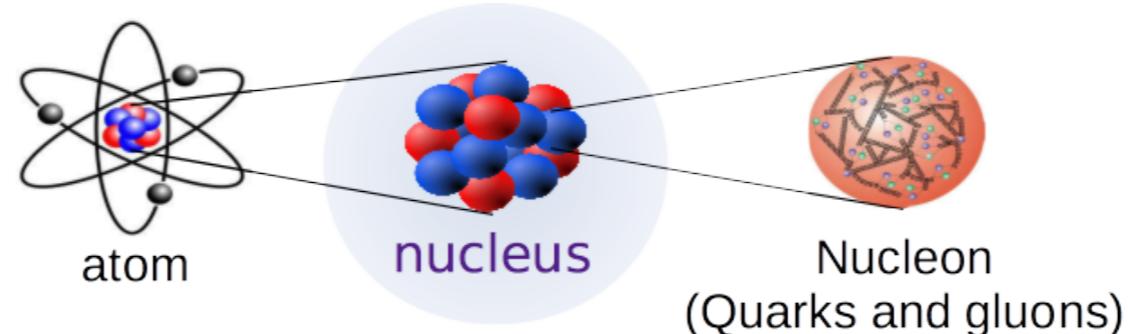
Orsay, November 24, 2022

Entanglement and Hamiltonian-Learning VQE in
quantum simulations of effective model spaces for
nuclear physics

Caroline Robin

*Fakultät für Physik, Universität Bielefeld, Germany
GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany*

Introduction



One of the goals of low-energy nuclear theory is to solve the nuclear many-body problem

- specific features: the nuclear force is not fully known, non-perturbative, two species of non-elementary particles...
- one feature that is shared with other quantum many-body systems is **entanglement**

$$|\Psi\rangle = \sum_n^{\sim 2^N} A_n |\Phi_n\rangle$$

→ see talks by T. Papenbrock
and L. Robledo on Tuesday

☞ Understanding the entanglement structure of many-body systems can guide:

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

density matrix renormalization group (DMRG), tensor networks...

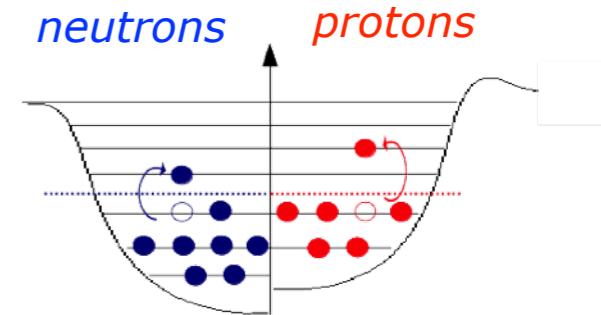
→ see talk by T. Ayral on Tuesday

- ▶ The development of quantum computations of physical systems

Introduction

Classical and Quantum Computations of nuclei currently require to truncate the Hilbert space

$$|\Psi\rangle = \sum_{\pi\nu \in \mathcal{H}_{trunc}} A_{\pi\nu} |\Phi_\pi\rangle \otimes |\Phi_\nu\rangle$$



Then one has to make up for the truncation.

For example, one can optimize the single-particle states (orbitals) via a variational principle:

$$\delta \left(\frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right)_{\{\varphi_i\}} = 0$$

This can be seen as modifying the Hamiltonian as $\hat{H} \rightarrow \hat{H}_{eff} = e^{iT} \hat{H} e^{-iT}$

where T is the one-body operator transforming the orbitals obtained from the variational principle

$$c_i^\dagger \rightarrow a_i^\dagger = e^{iT} c_i^\dagger e^{-iT}$$

☞ Approach known as “Multi-Configuration Self-Consistent Field Method” in quantum chemistry

Outline

- ★ Entanglement in light nuclei: How does the entanglement structure evolve with the Hamiltonian transformation?

CR, M. J. Savage, N. Pillet, PRC 103, 034325 (2021)

- ★ Exploration of effective model spaces to describe systems using Hamiltonian-learning-VQE: application to the Lipkin-Meshkov-Glick model

in collaboration with Martin J. Savage (IQuS, UW Seattle)

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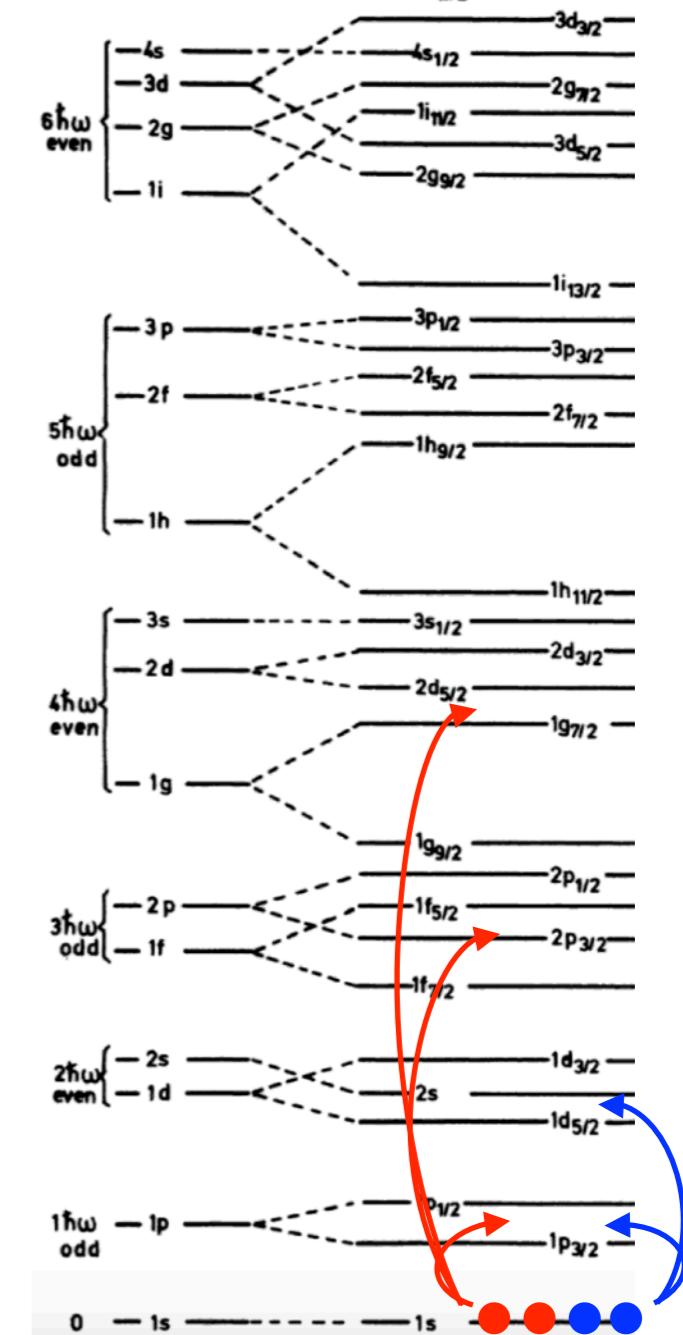
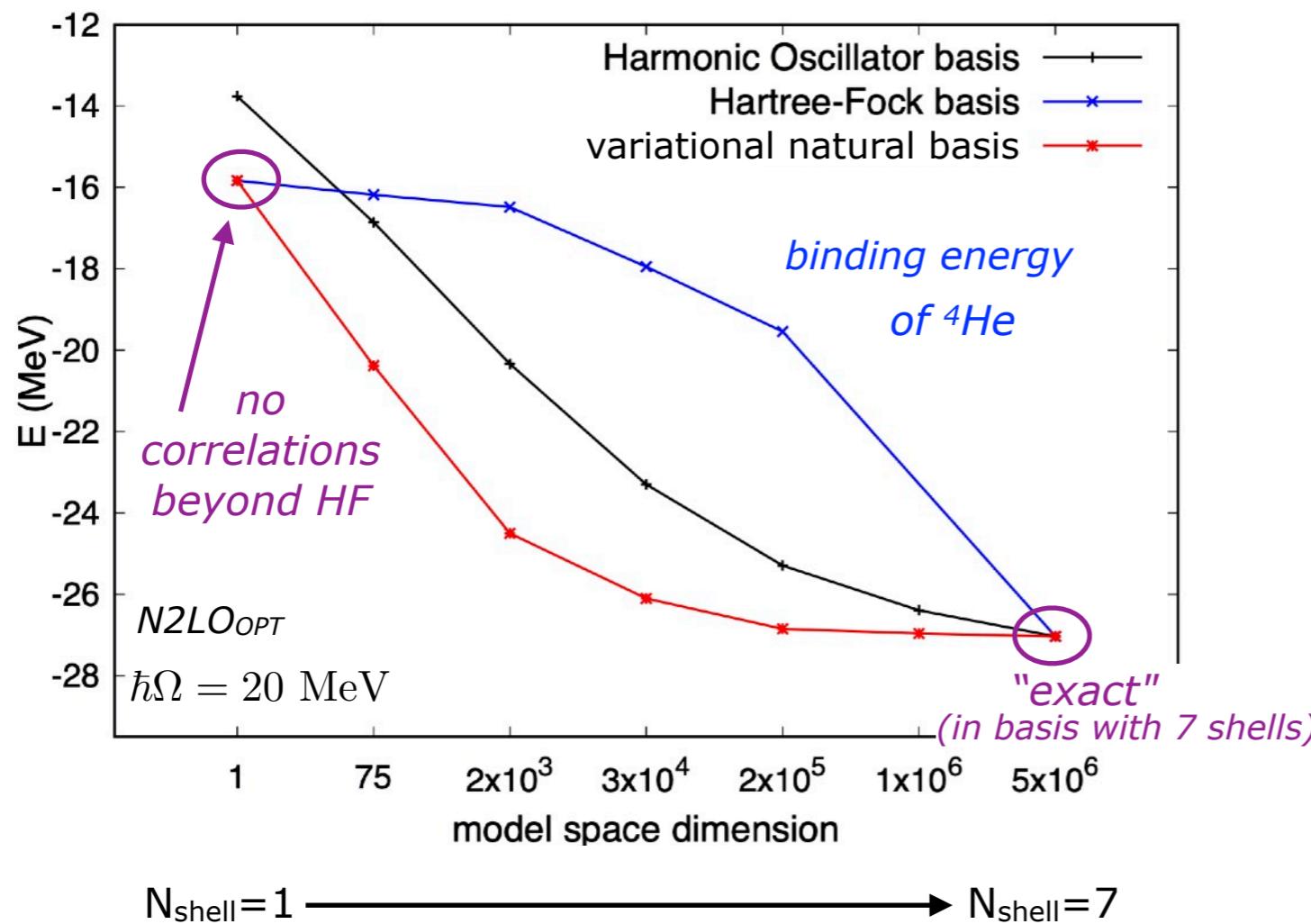
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Entanglement of single-particle orbitals in the nuclear ground state

★ **application to ${}^4\text{He}$ with a chiral interaction** (2-body force $\text{N}2\text{LO}_{\text{opt}}$ [Ekström et al. PRL 110 192502 (2013)])

single-particle bases expanded on 7 HO major shells
full diagonalization in active space with $N_{\text{shell}} \leq 7$

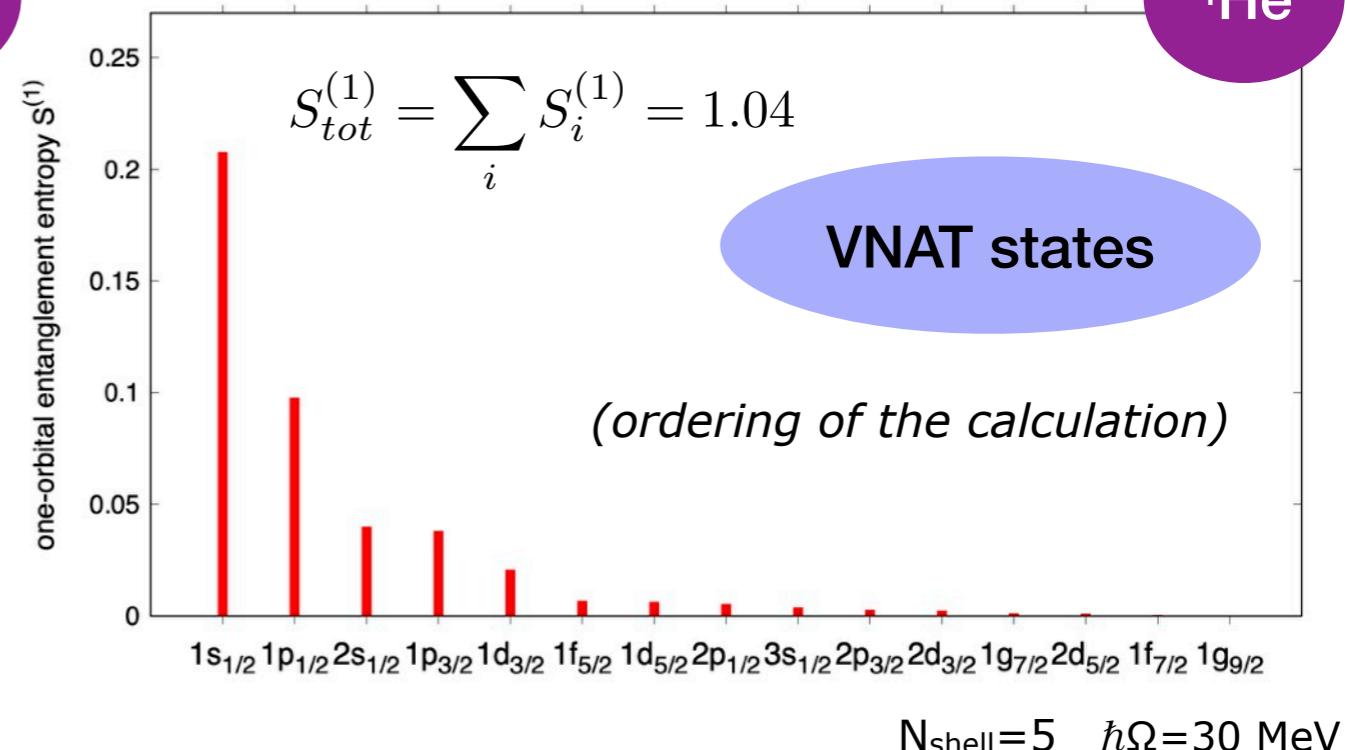
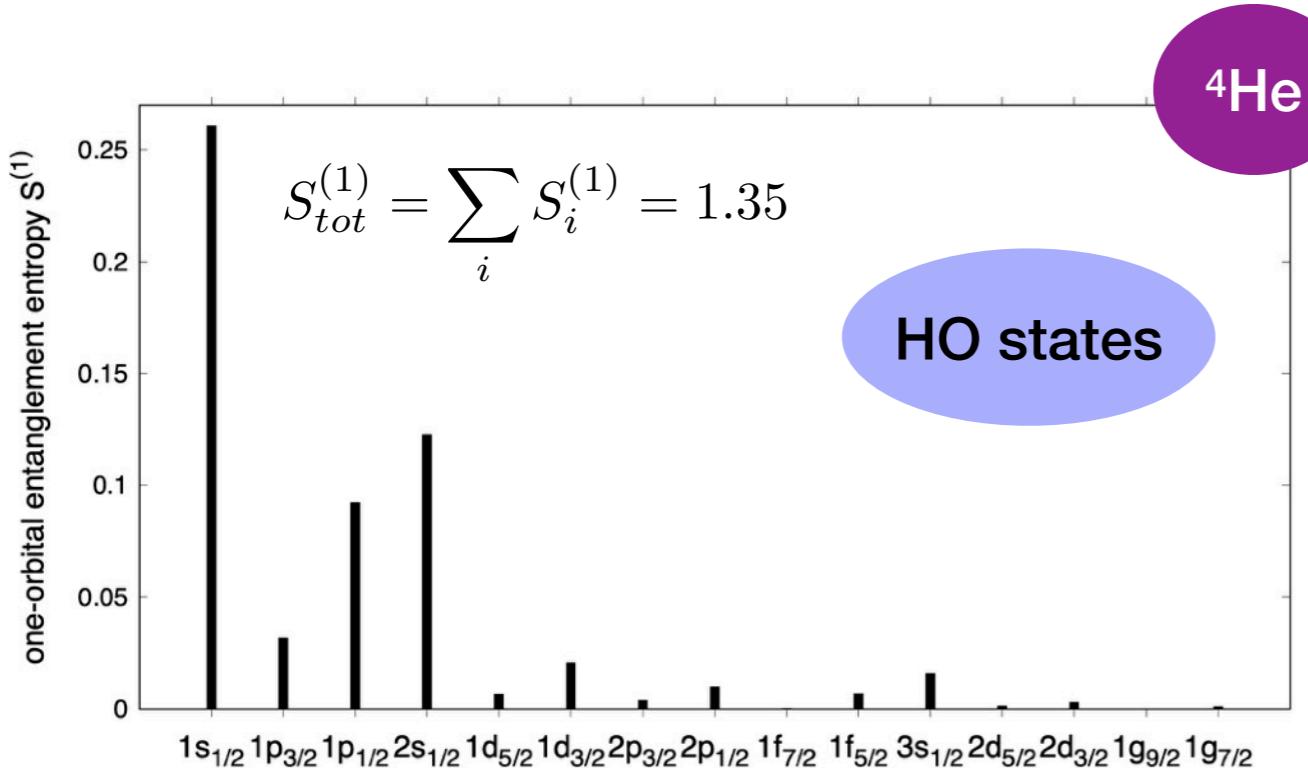
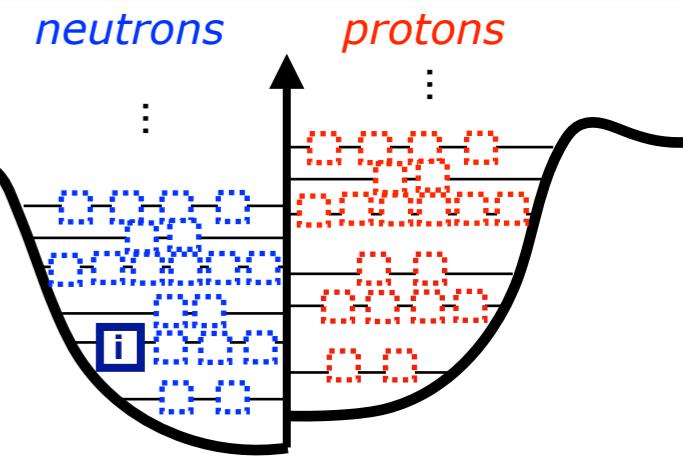


Single-orbital entanglement in ^4He

- ▶ Single-orbital Von Neumann entropy: $S_{(i)}^{(1)} = -\text{Tr} [\rho^{(i)} \ln \rho^{(i)}]$
= measure of entanglement of one orbital with the rest of the system

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

$$\rho^{(i)} = \text{Tr}_{(n_1, \dots, n_{i-1}, n_{i+1}, \dots, n_N)} |\Psi\rangle\langle\Psi|$$

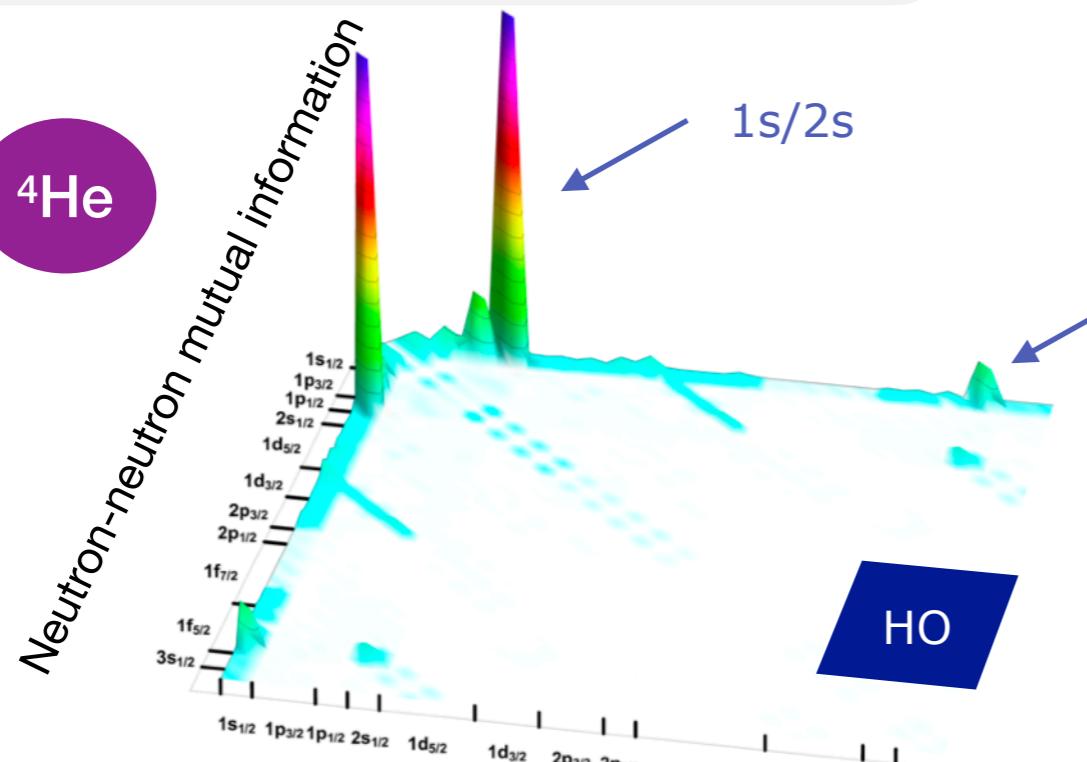


- the VNAT basis is naturally ordered by decreasing entanglement entropy
- $S_{tot}^{(1)}$ is in fact minimized in the (V)NAT basis [Gigena and Rossignoli, PRA 92, 042326 (2015)]

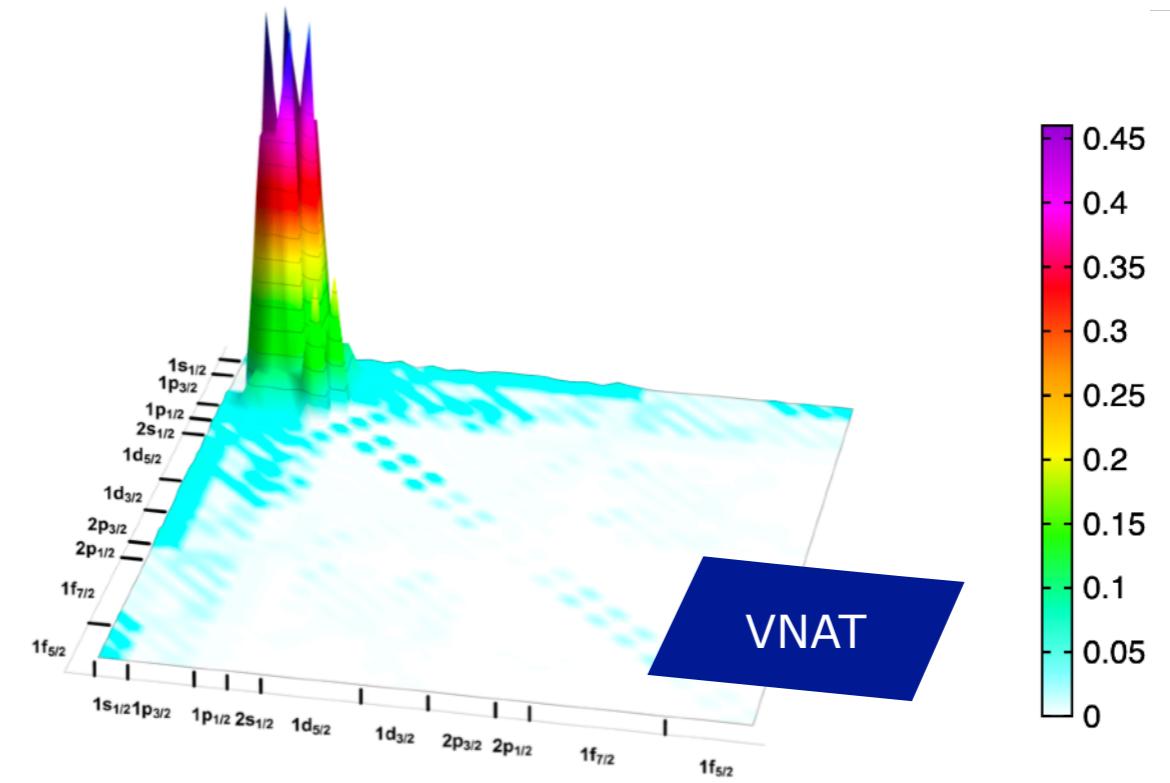
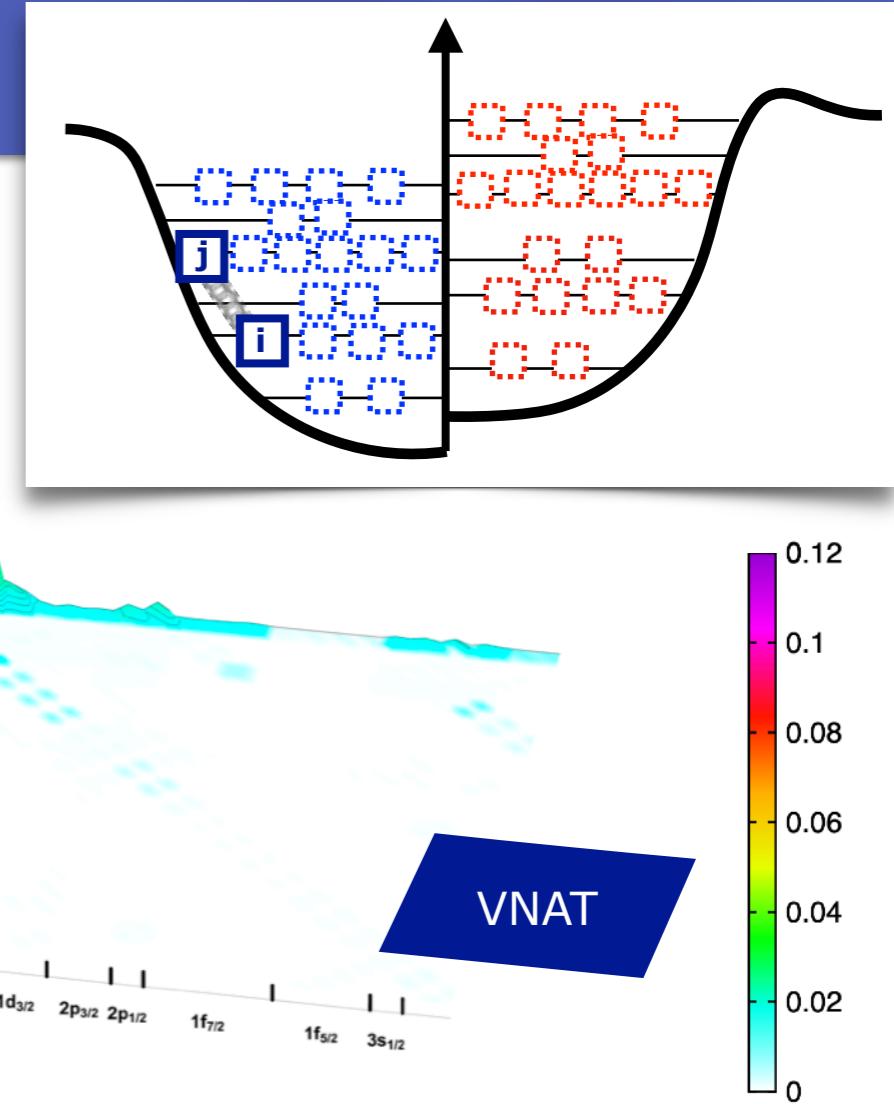
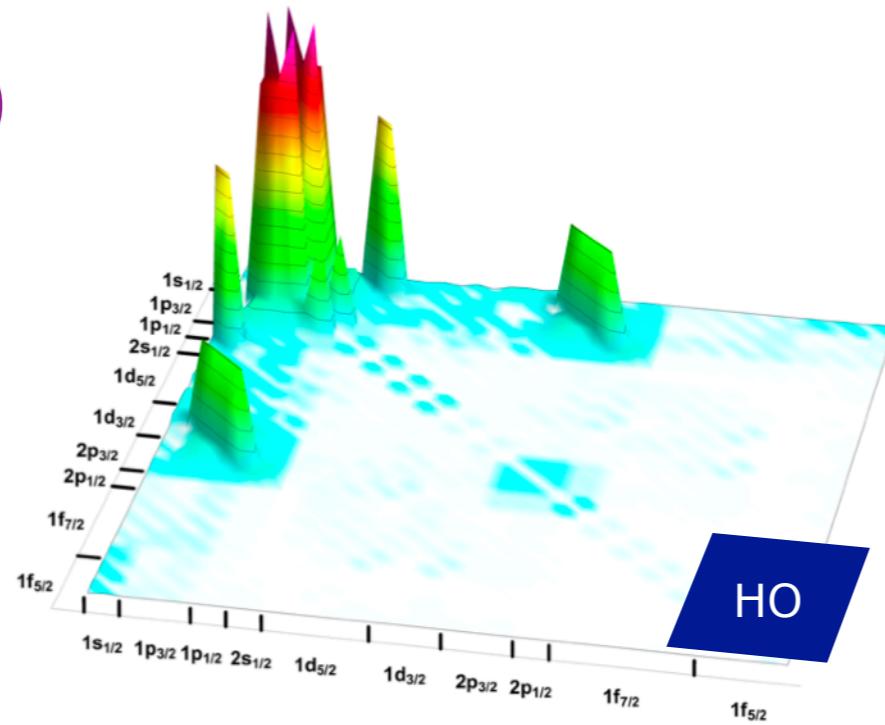
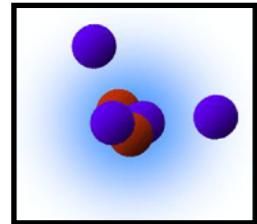
Mutual information

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

^4He



^6He



- ▶ localization of correlations in the VNAT basis \Rightarrow emergence of ^4He -core + nn-valence structure

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Several previous studies of Lipkin Model on quantum computers:

Lipkin model on a quantum computer, M.J. Cervia et al. PRC 104, 024305 (2021)

Quantum computing for the Lipkin model with unitary coupled cluster and structure learning ansatz, A. Chikaoka, H. Liang, Chin. Phys. C 46 024106 (2022)

Solving nuclear structure problems with the adaptive variational quantum algorithm, A.M. Romero et al. PRC 105, 064317 (2022)

Simulating excited states of the Lipkin model on a quantum computer, M. Q. Hlatshwayo et al. PRC 106, 024319 (2022)

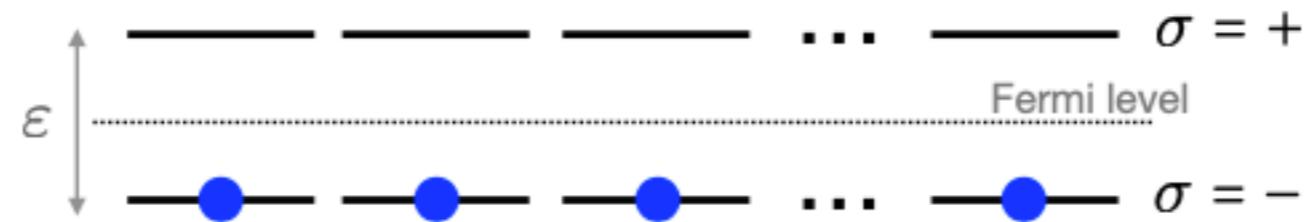
⇒ good benchmark for comparing different methods

The Lipkin-Meshkov-Glick Model - exact solutions

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

N particles distributed on two N-fold degenerate levels

and interacting via a monopole-monopole interaction that scatters pairs of particles:



$$H = \frac{\epsilon}{2} \sum_{\sigma p} \sigma c_{p\sigma}^\dagger c_{p\sigma} - \frac{V}{2} \sum_{pq\sigma} c_{p\sigma}^\dagger c_{q\sigma}^\dagger c_{q-\sigma} c_{p-\sigma}$$

$$= \epsilon J_z - \frac{V}{2} (J_+^2 + J_-^2)$$

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

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

exact solutions: $|\Psi_{ex}^{(J)}\rangle = \sum_{M=-J}^J A_{J,M} |J, M\rangle \equiv \sum_{n=0}^{2J} A_n |n\rangle$

\downarrow
np-nh excitation

Parity symmetry $\Pi = \exp\left(i\pi \sum_p c_{p+}^\dagger c_{p+}\right) \propto (-1)^{\text{number of particles in the upper level}}$

\Rightarrow the ground state ($J=N/2$) only contains even n

The Lipkin-Meshkov-Glick Model in truncated space

Effective wave function: $|\Psi\rangle = \sum_{n=0}^{\Lambda-1} A_n^{(\beta)} |n, \beta\rangle$

Λ = cut-off on the np-nh excitations

β = rotation angle of the single-particle states

$$\begin{pmatrix} c_{p+}(\beta) \\ c_{p-}(\beta) \end{pmatrix} = \begin{pmatrix} \cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2) \end{pmatrix} \begin{pmatrix} c_{p+} \\ c_{p-} \end{pmatrix}$$

governed by an effective Hamiltonian:

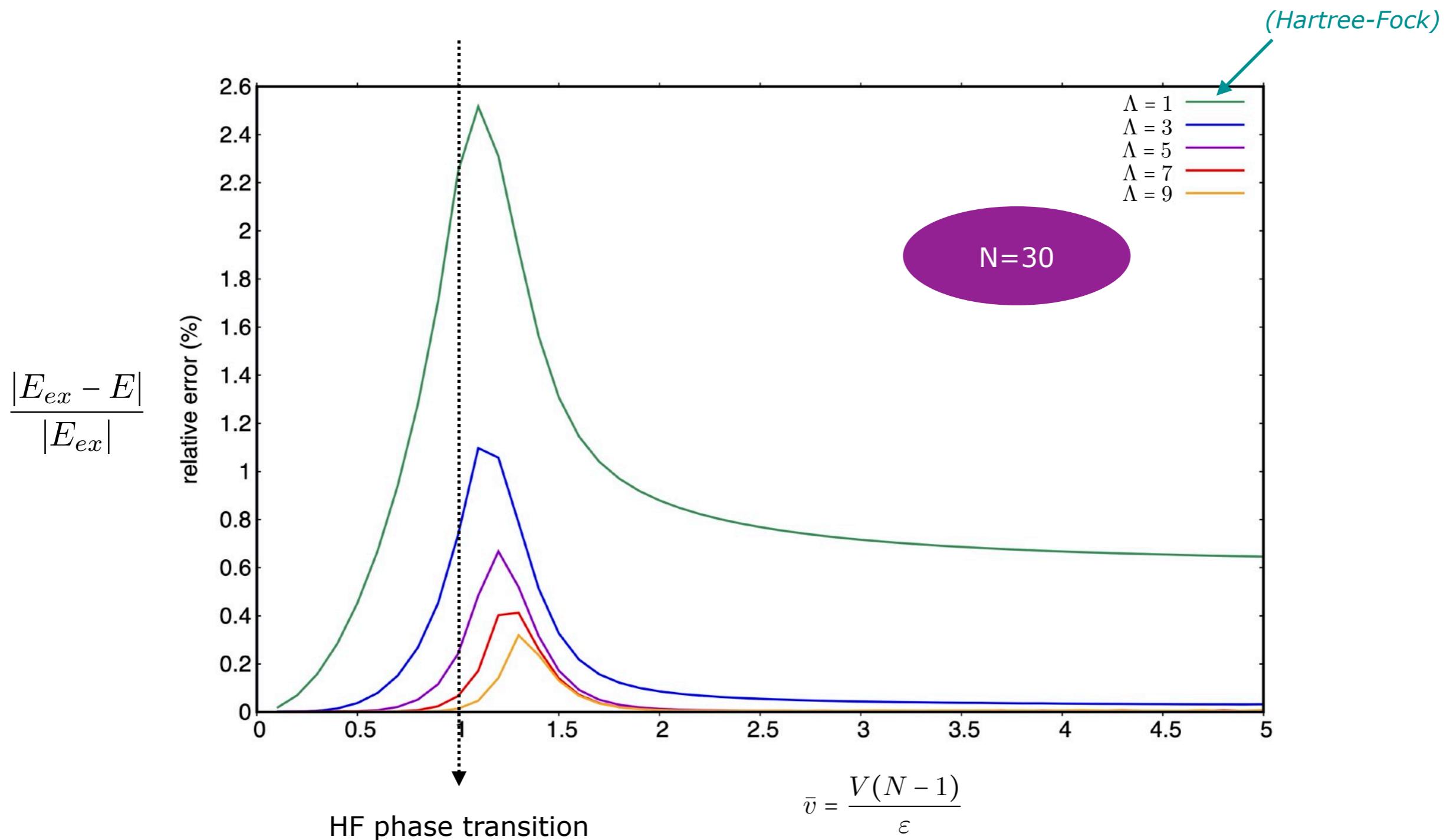
$$\begin{aligned} H(\beta) = & \varepsilon \left[\cos \beta J_z(\beta) + \frac{1}{2} \sin \beta (J_+(\beta) + J_-(\beta)) \right] \\ & - \frac{V}{4} \left[\sin^2 \beta (4 J_z(\beta)^2 - \{J_+(\beta), J_-(\beta)\}) + (1 + \cos^2 \beta) (J_+(\beta)^2 + J_-(\beta)^2) \right. \\ & \quad \left. - 2 \sin \beta \cos \beta (\{J_z(\beta), J_+(\beta)\} + \{J_z(\beta), J_-(\beta)\}) \right] \end{aligned}$$

The parameters $(\{A_n^{(\beta)}\}, \beta)$ are determined by minimizing $\langle \Psi(\{A_n^{(\beta)}\}) | H(\beta) | \Psi(\{A_n^{(\beta)}\}) \rangle$

The Lipkin-Meshkov-Glick Model in truncated space: Classical Results

C.R., M.J. Savage, in prep.

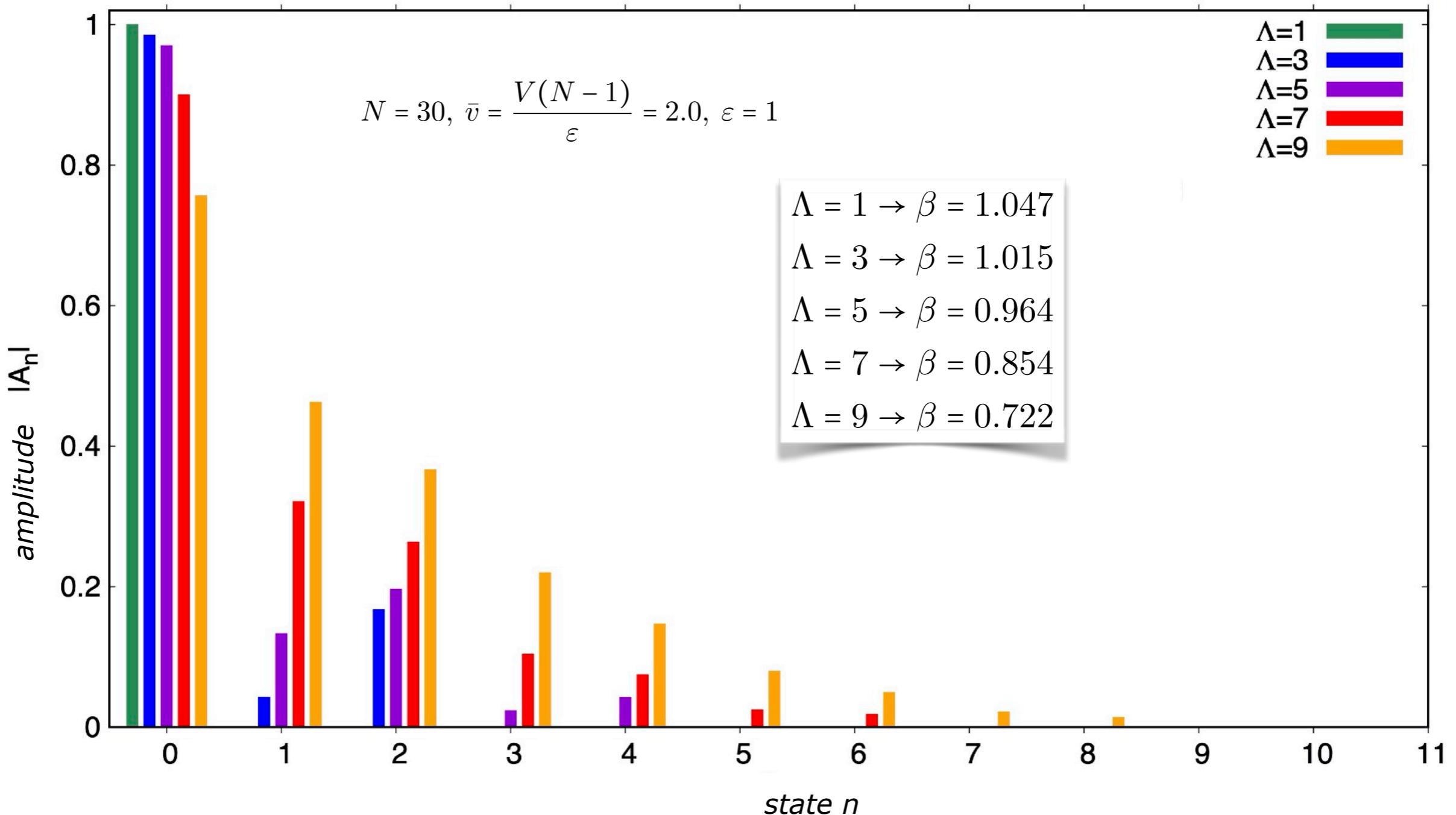
★Energy



The Lipkin-Meshkov-Glick Model in truncated space

C.R., M.J. Savage, in prep.

★ Wave function in the optimized (rotated) basis:

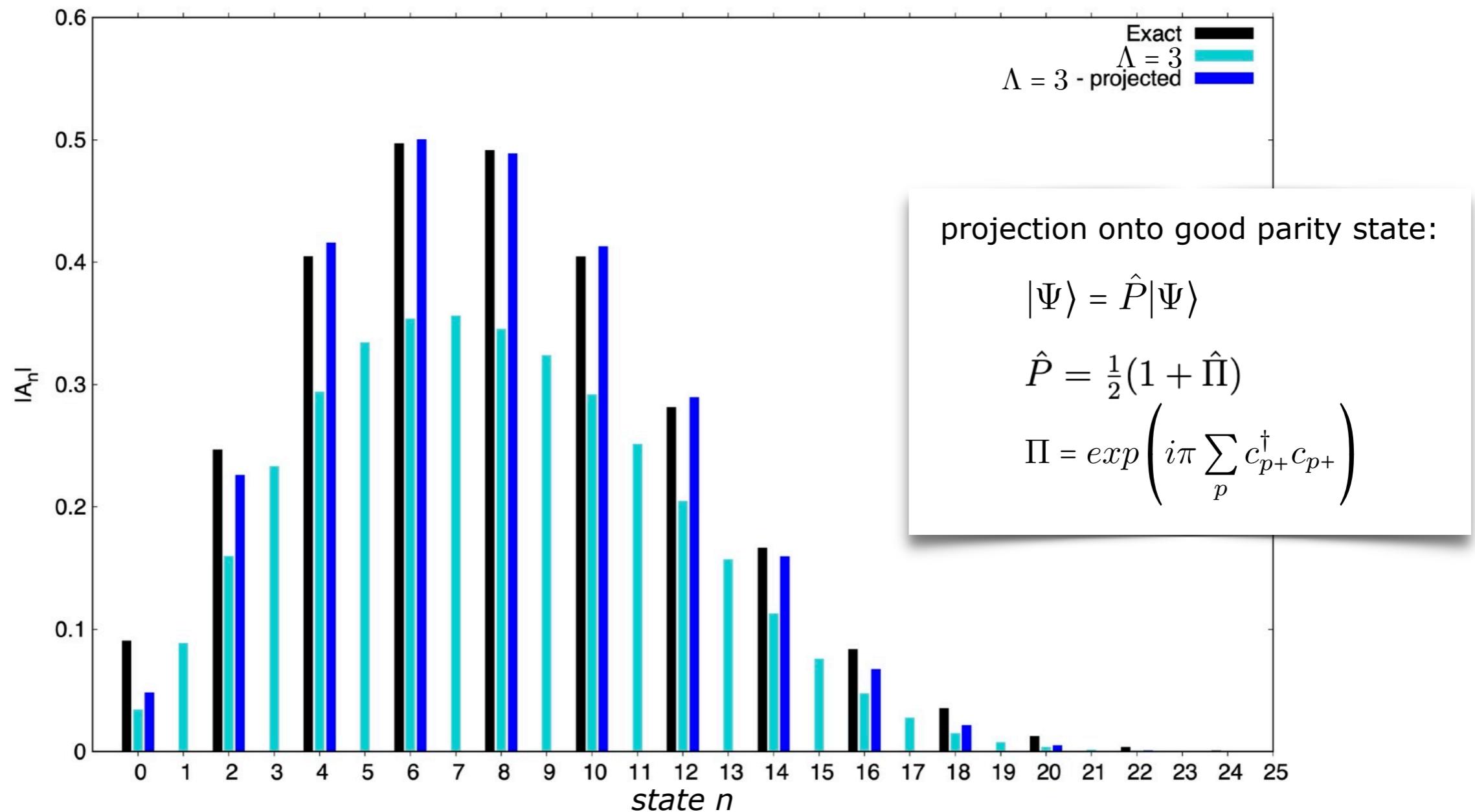


- wave function is localized in the effective model space → fall-off will increase the efficiency of quantum simulations
- β decreases as model space increases and tends to exact (full-model-space) solution

The Lipkin-Meshkov-Glick Model in truncated space

C.R., M.J. Savage, in prep.

★ Wave function in the initial basis ($\beta=0$):

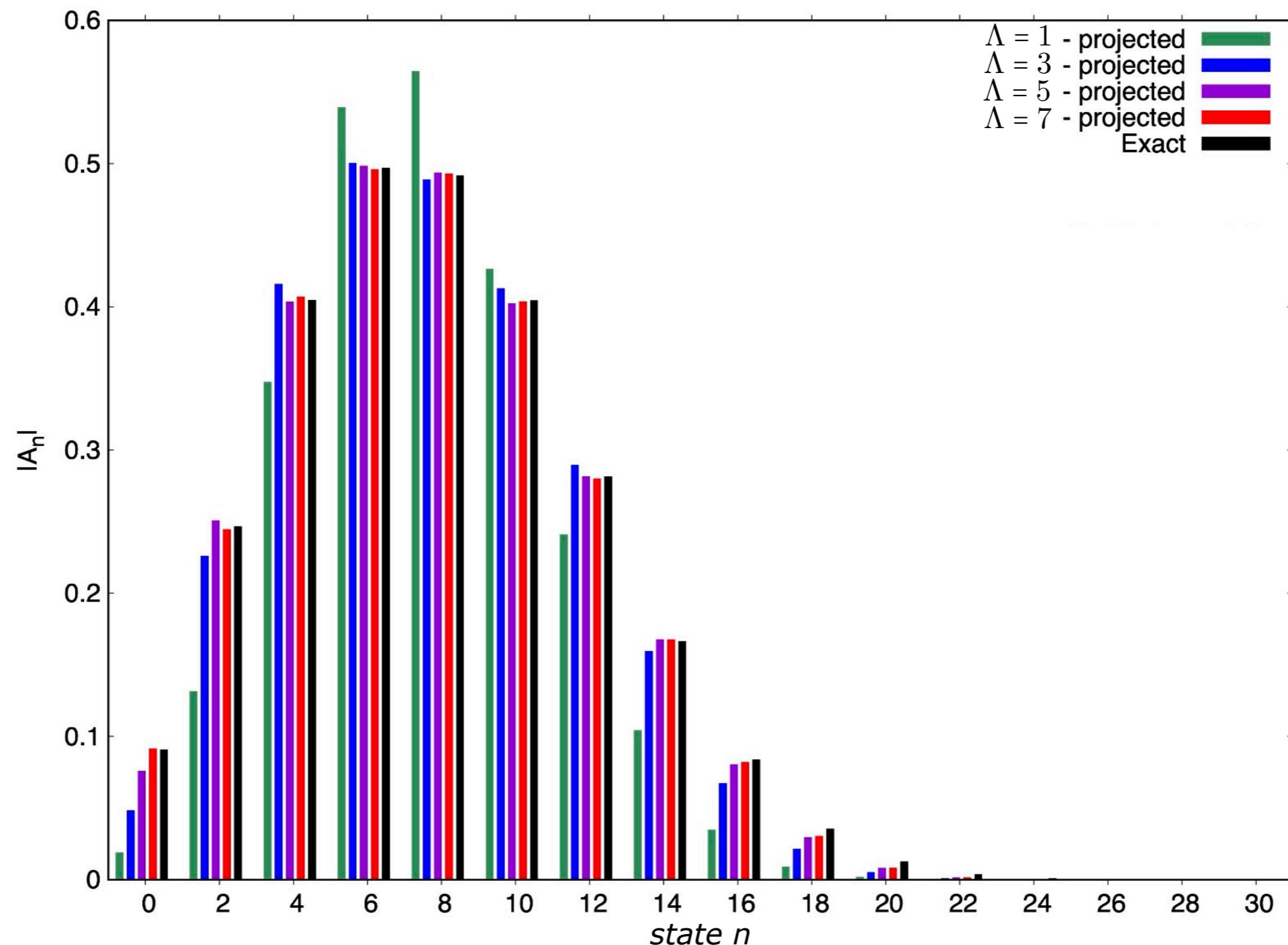


- The orbital rotation breaks parity symmetry \Rightarrow projection needed (here “projection after variation”)
- For these parameters, three configurations in the rotated basis can well reproduce the exact wave function

The Lipkin-Meshkov-Glick Model in truncated space

C.R., M.J. Savage, in prep.

★ Wave function in the initial basis ($\beta=0$) - convergence:

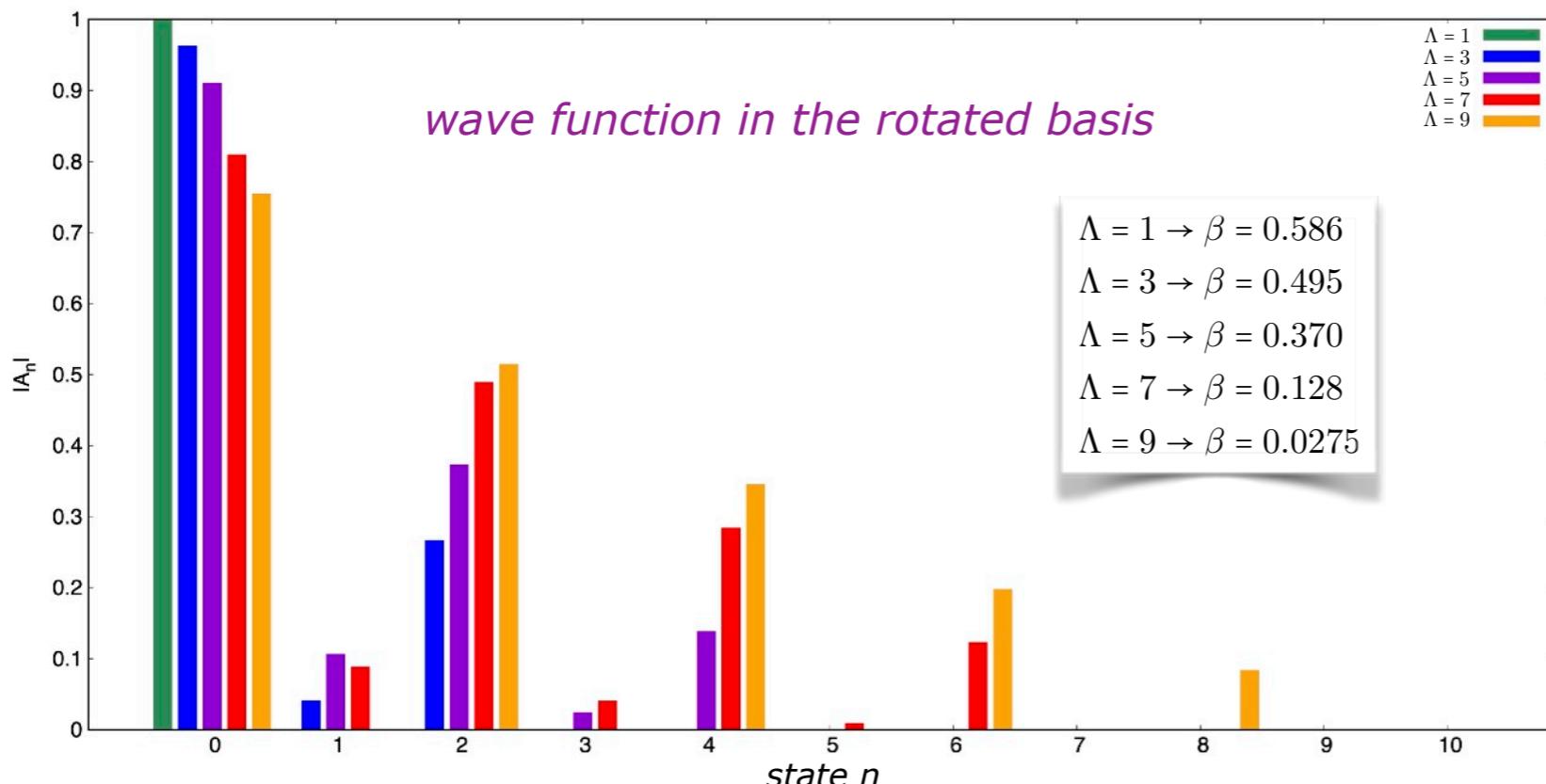
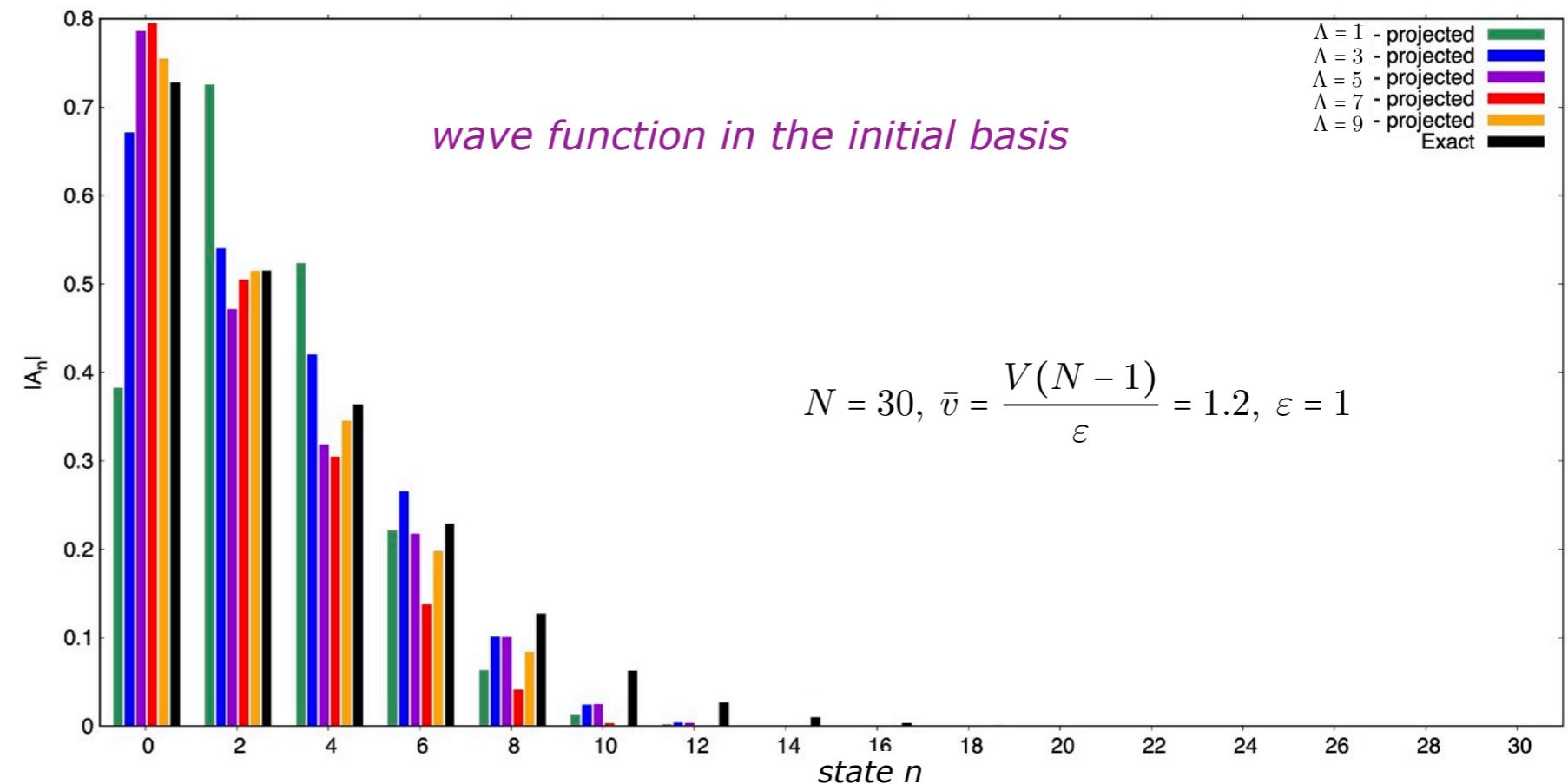


The Lipkin-Meshkov-Glick Model in truncated space

★Near the phase transition:

Closer to the phase transition
the exact wave function is
already localized near $n=0$

→ no “scale separation”



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

C.R., M.J. Savage, in prep.

★ Implementation on a digital quantum computer:

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

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

- * n_{qubits} determined by number of states, not by particle number N
- * localization of the effective wave function around $n=0$ ($0p0h$) reduces the number of required qubits for given desired precision
- * The (real) effective wave function can be parametrized by $\Lambda-1$ angles and can be implemented by unitary operators

* see e.g. Klco and Savage *PRA* 99, 052335 (2019); *PRA* 102, 012612 (2020), ...

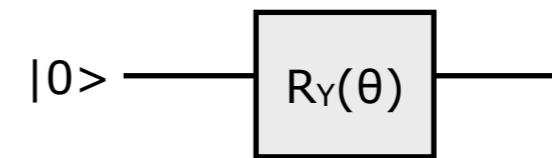
The Lipkin-Meshkov-Glick Model in truncated space: Quantum Simulations

C.R., M.J. Savage, in prep.

Examples:

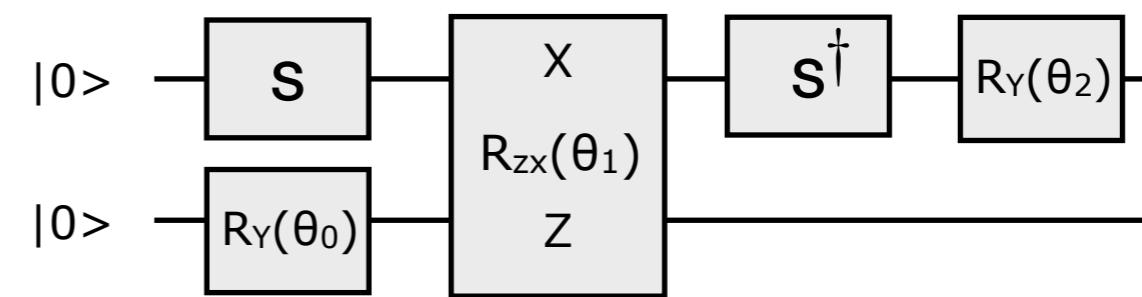
* 1 qubit ($\Lambda = 2$):

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



* 2 qubits ($\Lambda = 4$):

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



$$R_{ZX}(\theta) = e^{-i\frac{\theta}{2}\hat{X}\otimes\hat{Z}}$$

native IBM gate

→ replaces at least 3 CNOTs

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

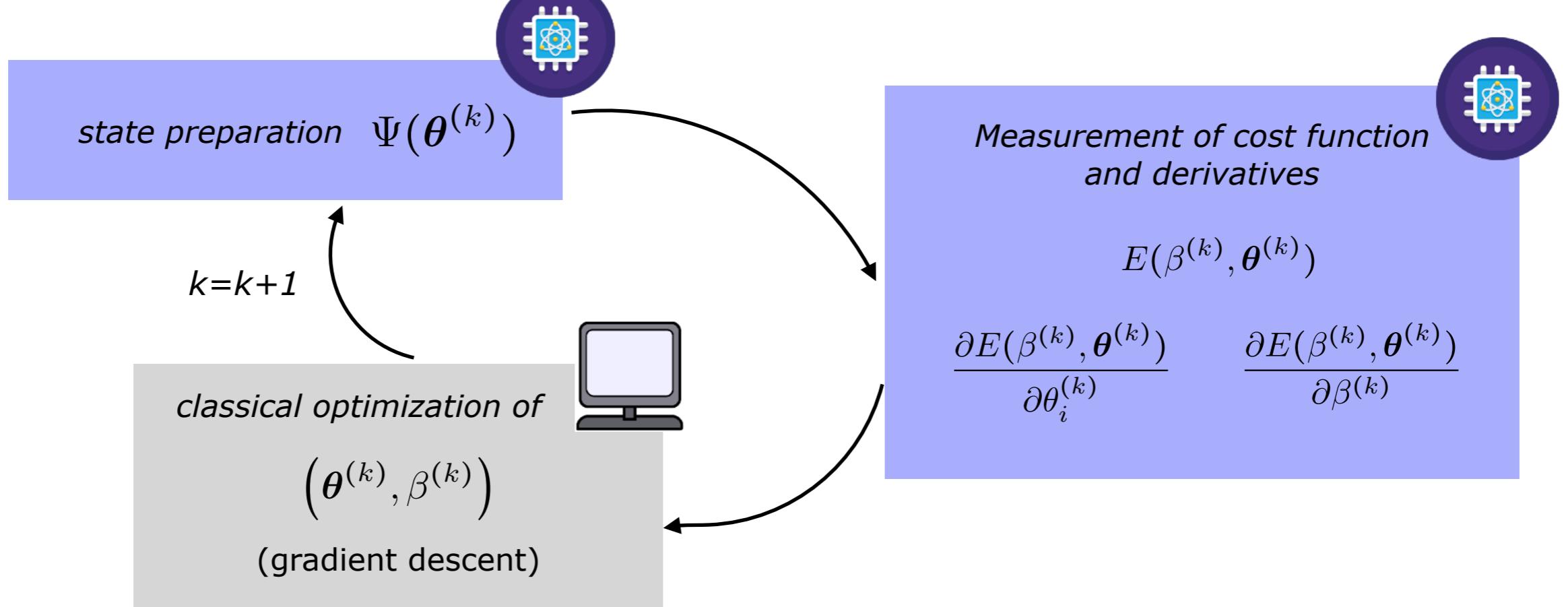
C.R., M.J. Savage, in prep.

★Hamiltonian-Learning-VQE:

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

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

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



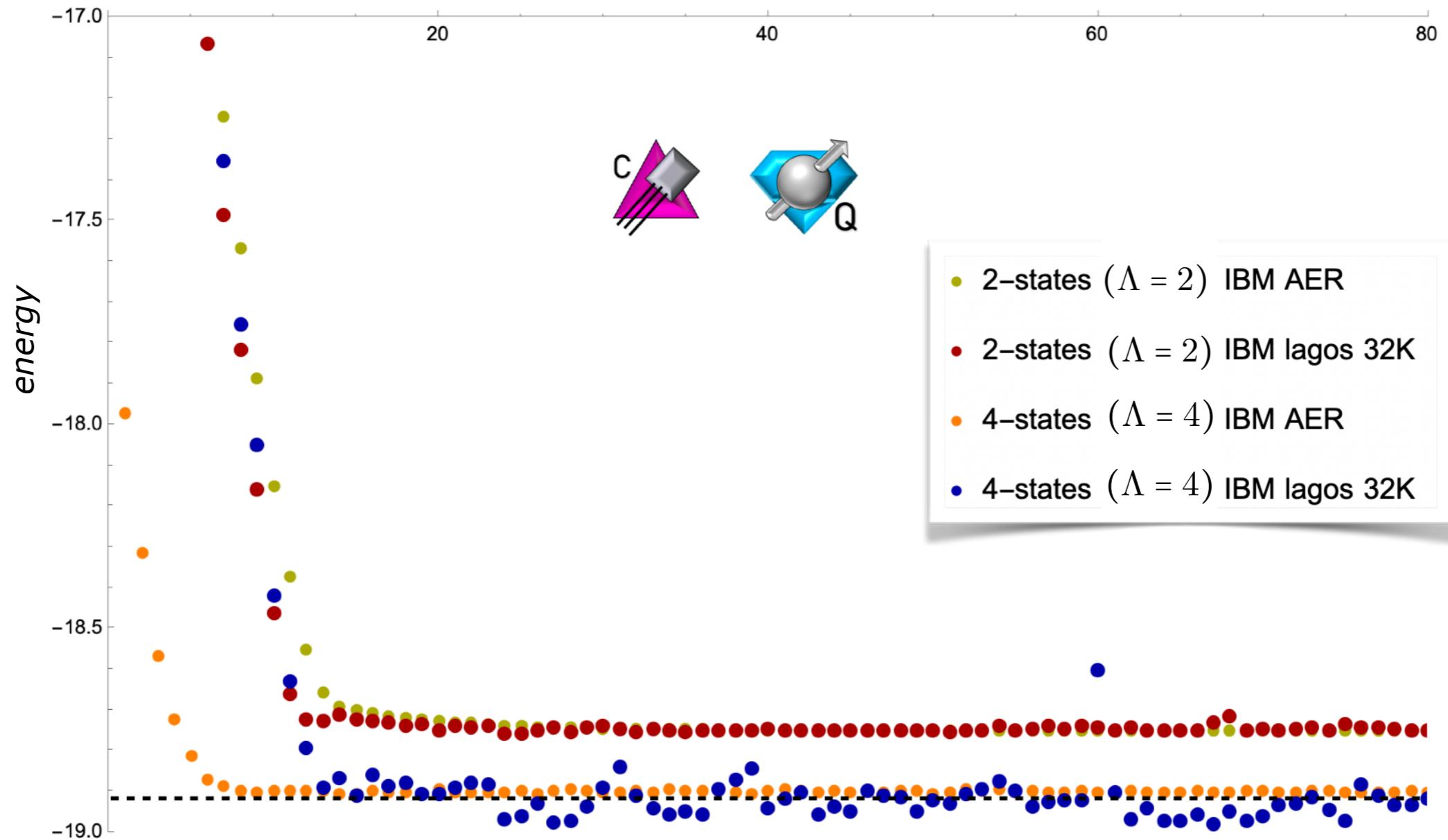
⇒ learns the effective Hamiltonian and identifies the associated ground state simultaneously

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

C.R., M.J. Savage, in prep.

★Energies:

VQE iterations



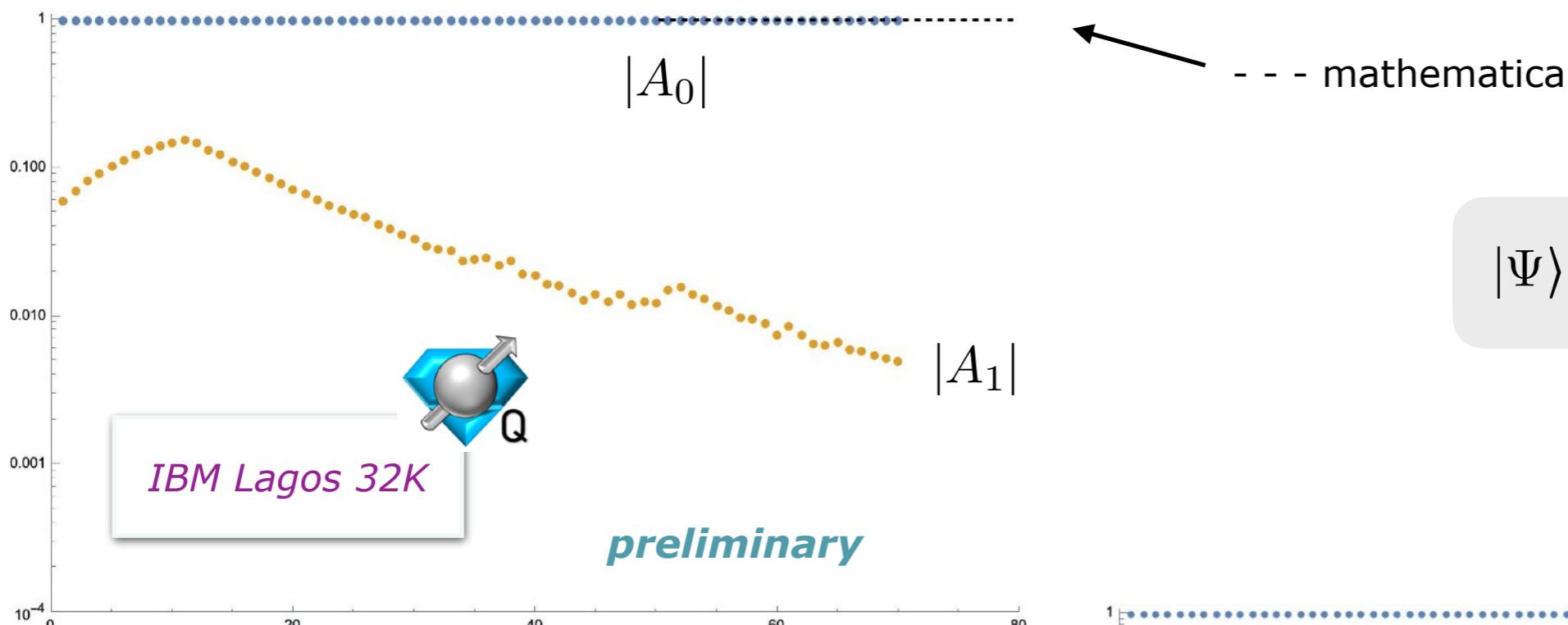
$$N = 30, \bar{v} = \frac{V(N-1)}{\varepsilon} = 2.0, \varepsilon = 1$$

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

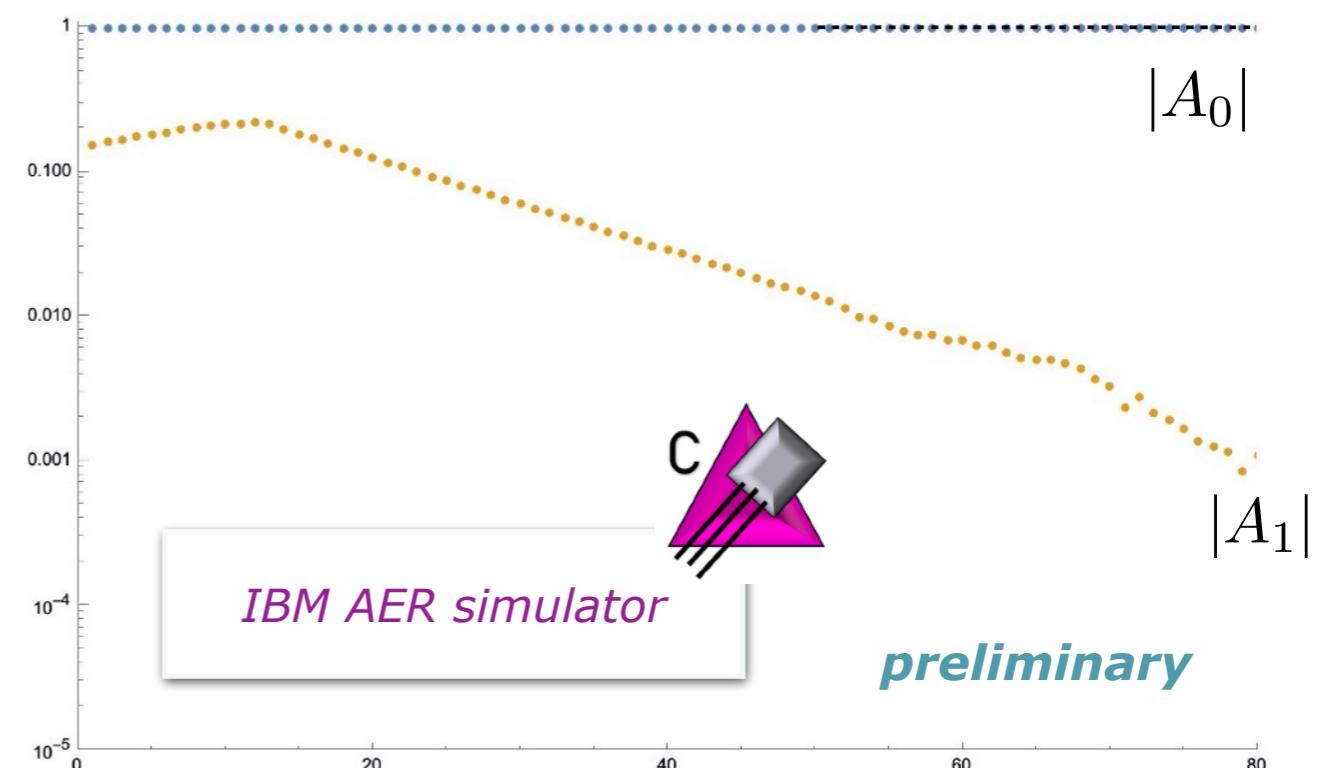
C.R., M.J. Savage, in prep.

★ Wave functions (in the optimized basis):

Results for 1 qubit ($\Lambda=2$)



0p-0h (HF) state does not couple to 1p-1h
⇒ $A_1 = 0$

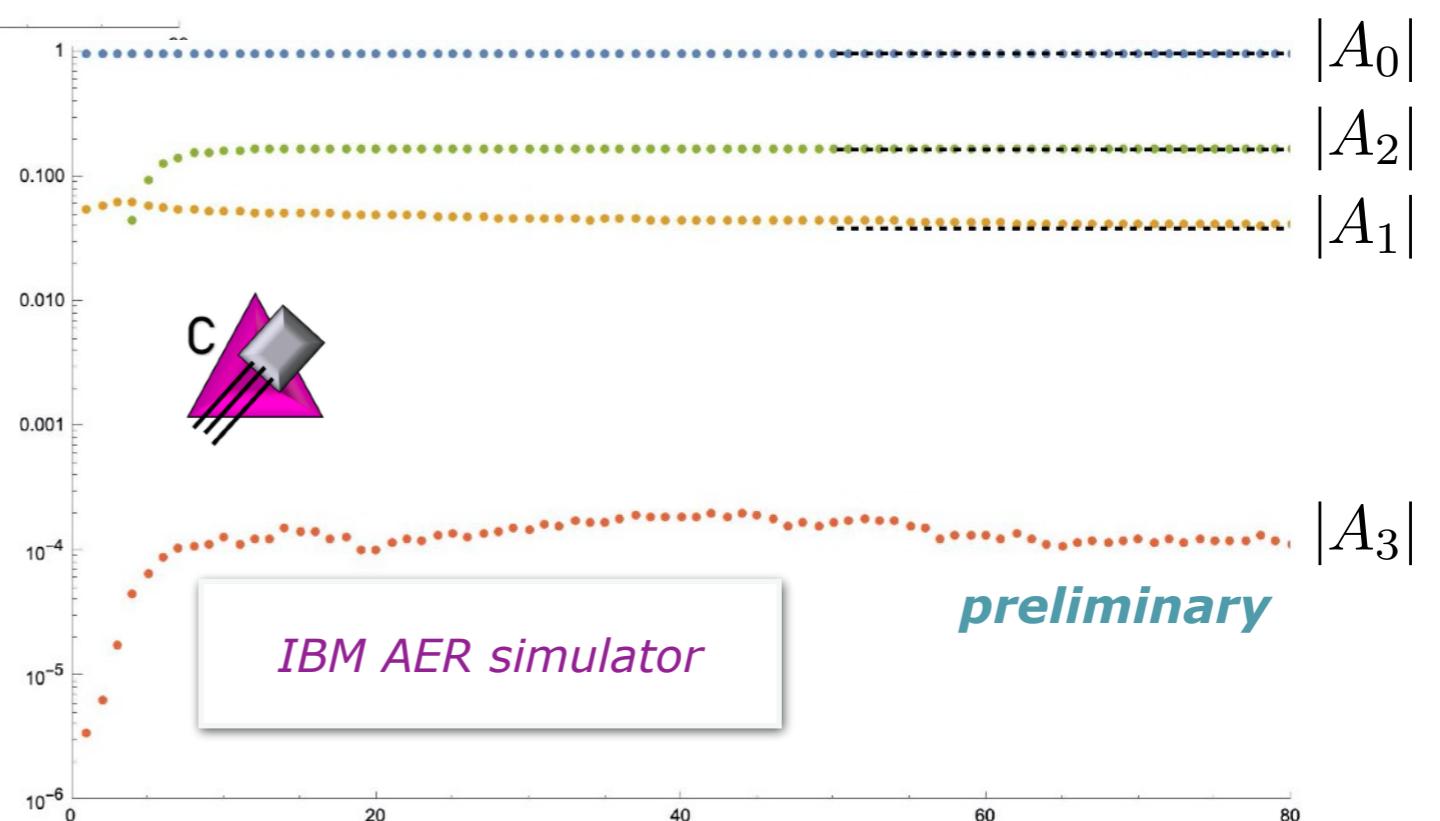
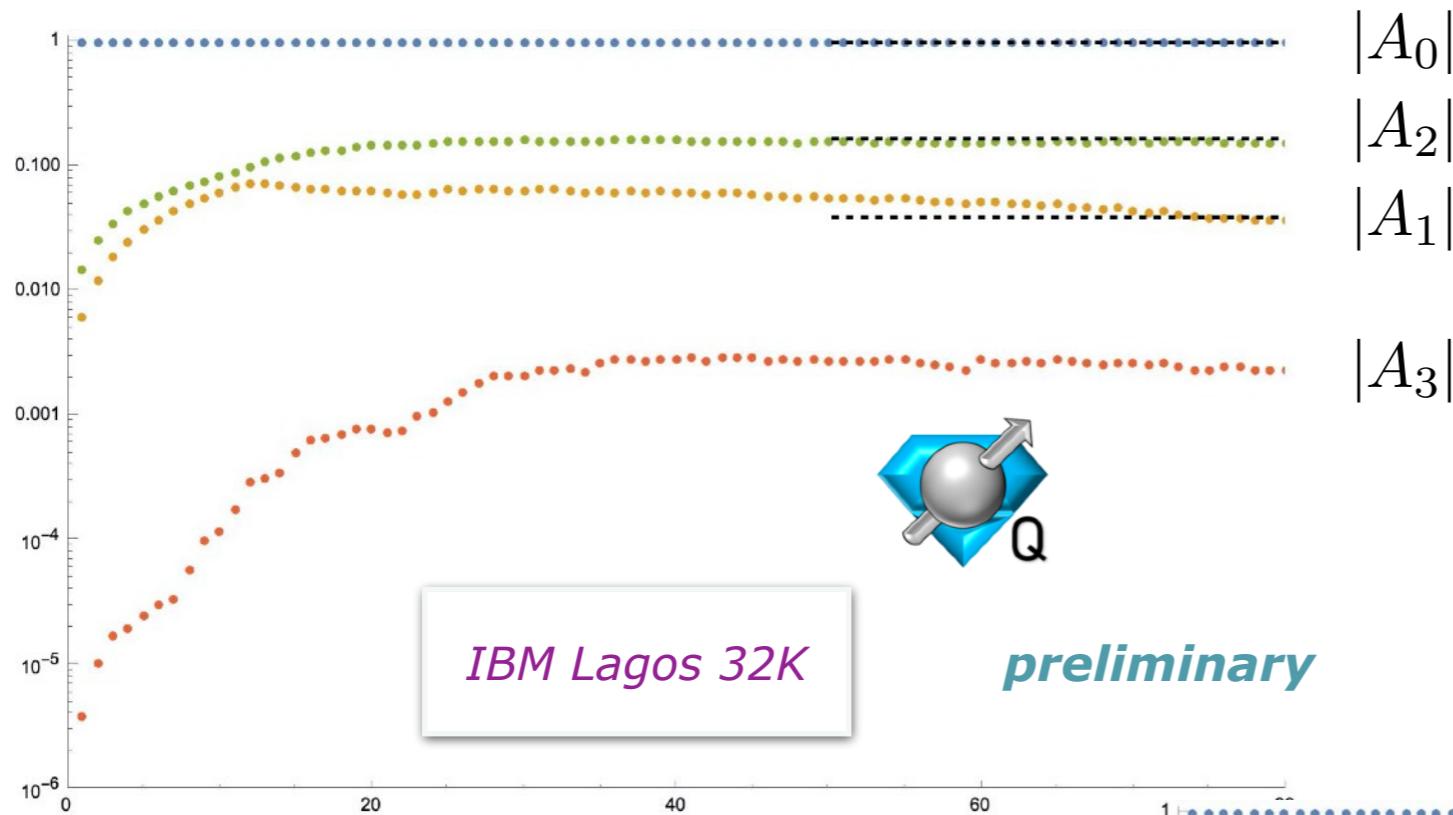


The Lipkin-Meshkov-Glick Model in truncated space: Quantum Simulations

C.R., M.J. Savage, in prep.

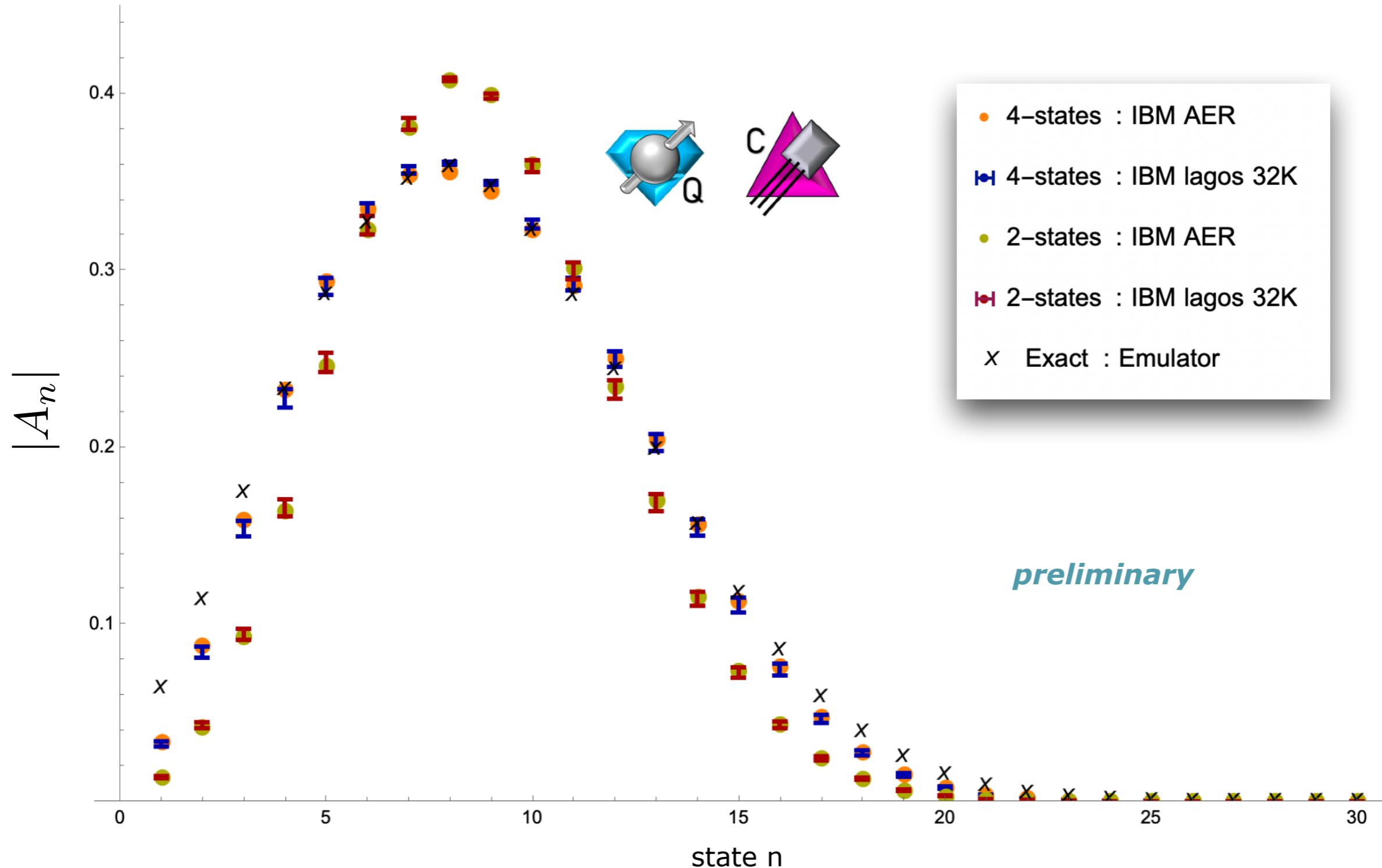
★ Wave functions (in the optimized basis):

Results for 2 qubits ($\Lambda=4$)



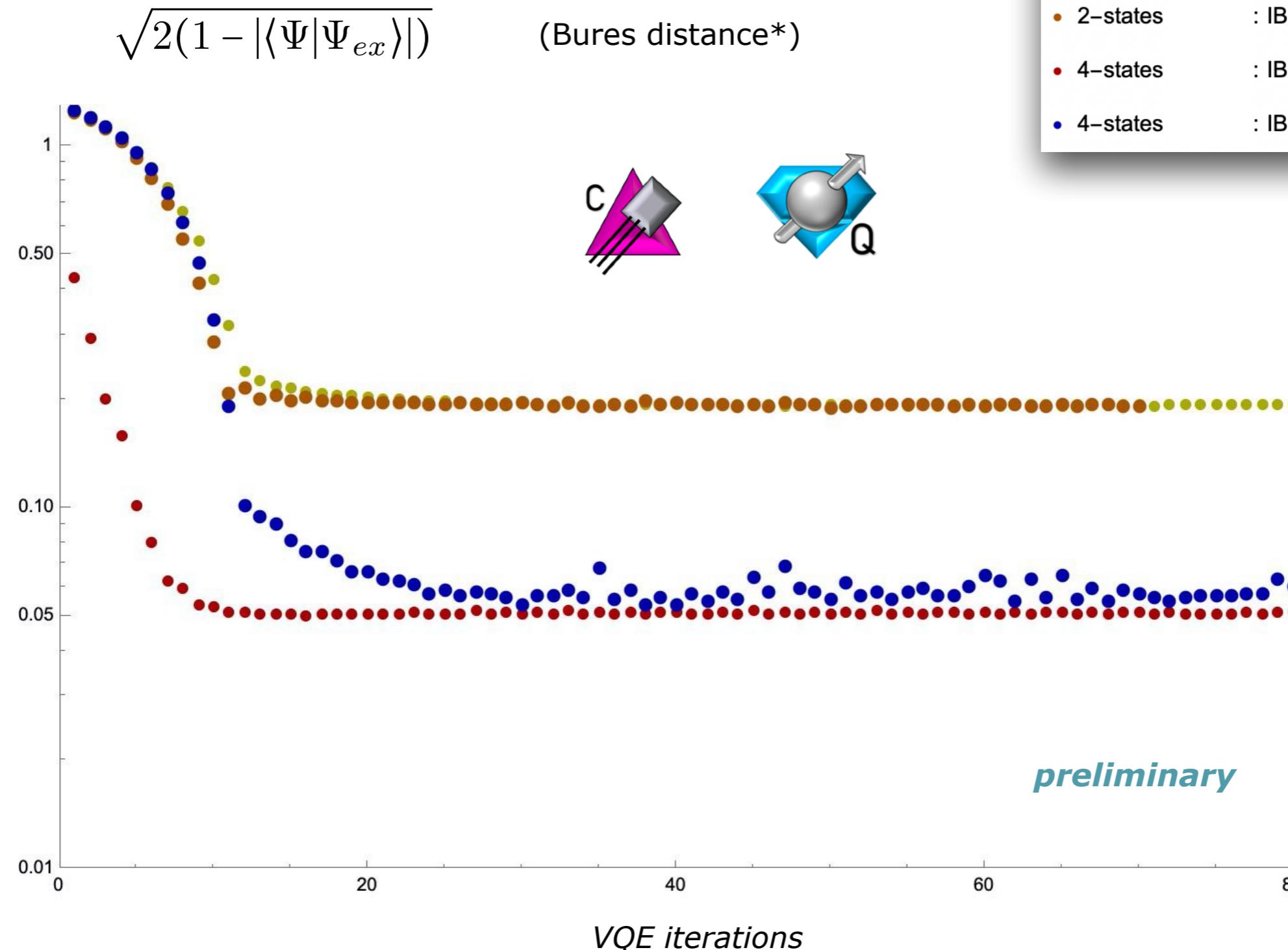
The Lipkin-Meshkov-Glick Model in truncated space: Quantum Simulations

★ Wave functions (in the initial basis):



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

★ Fidelity



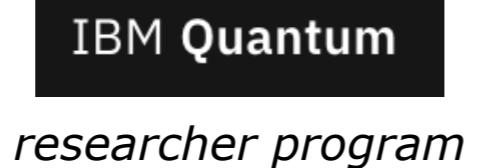
*Bures, American Mathematical Society (AMS). 135: 199 (1969)

Conclusion

- * Entanglement is a useful tool for exploration of the nuclear wave function and to reveal physical phenomena
- * Entanglement rearrangement and wave-function localization appear crucial for fast convergence of classical calculations and efficient quantum computations.
- * We have developed a Hamiltonian-Learning-VQE procedure to be used with quantum computers, to simultaneously determine the Hamiltonian and ground-state wave function in effective model spaces. Good results were obtained for the Lipkin model.
→ Next: adapt and apply this procedure to more general nuclear interactions and systems

Thank you!

and thanks to



& the organizers of the workshop!

for support

Backups

Multi-configuration self-consistent field method

$$|\Psi\rangle = \sum_{n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots} C_{n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots} |n_{\pi_1} n_{\pi_2} \dots n_{\nu_1} n_{\nu_2} \dots\rangle \quad \text{- truncated!}$$

Variational principle determines:

★ The expansion coefficients:



$$\begin{pmatrix} H \\ C \end{pmatrix} = E \begin{pmatrix} C \end{pmatrix}$$

Large-scale
diagonalization

to introduce explicit correlations in the truncated configuration space

★ The single-particle states:



general mean field
(→ single-particle energies)

$$[\hat{h}(\gamma), \hat{\gamma}] = \hat{G}(\sigma)$$

Source term
 σ = two-body correlation matrix

$$\sigma_{kilm} = \langle \Psi | a_k^\dagger a_m^\dagger a_l a_i | \Psi \rangle - (\gamma_{ki} \gamma_{lm} - \gamma_{km} \gamma_{li})$$

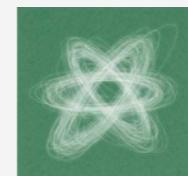
One-nucleon density

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

(→ single-particle states)

Generalized
mean-field
equation

⇒ “variational natural orbitals” (VNAT)



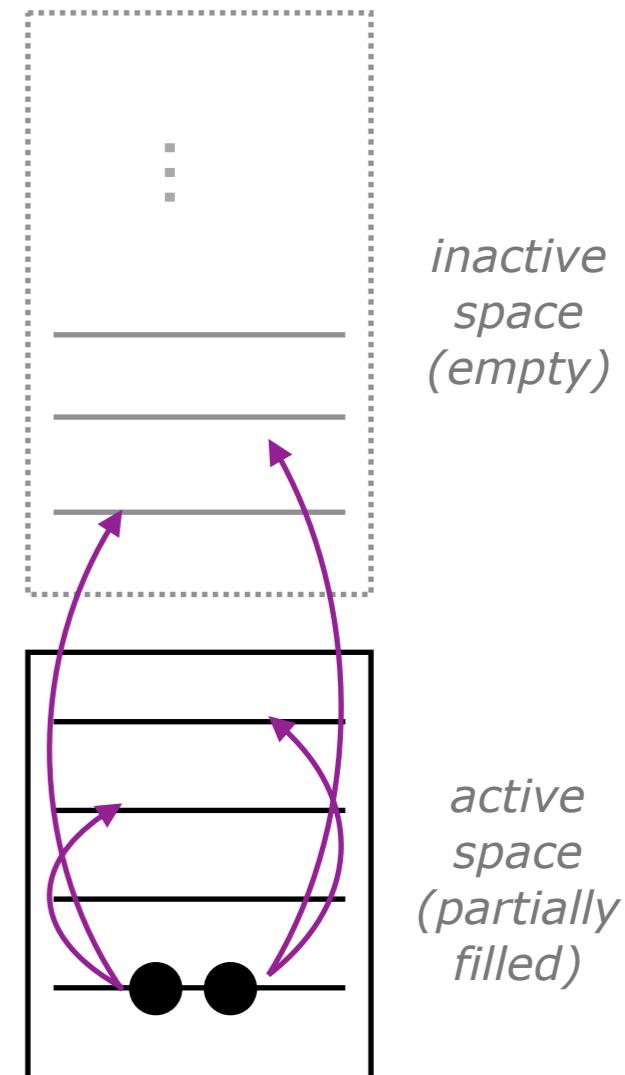
to partly compensate for the truncations made on the nuclear state

Application to Helium isotopes

★ Role of the variational orbital equation:

* Without variational orbital equation:

$$\gamma_{ij} = \langle \Psi | a_j^\dagger a_i | \Psi \rangle \begin{cases} \in [0, 1] & \text{if } i, j \text{ active} \\ = 0 & \text{if } i, j \text{ inactive} \end{cases}$$



* With variational orbital equation:

$$[\hat{h}(\gamma), \hat{\gamma}] = \hat{G}(\sigma) \Rightarrow \gamma_{ij} = \frac{G_{ij}[\sigma]}{\varepsilon_i - \varepsilon_j}$$

$$G_{ij}[\sigma] = \frac{1}{2} \sum_{klm} \tilde{V}_{kmjl} \sigma_{ki,ml} - \frac{1}{2} \sum_{klm} \tilde{V}_{kiml} \sigma_{jl,km}$$

Single-particle energies

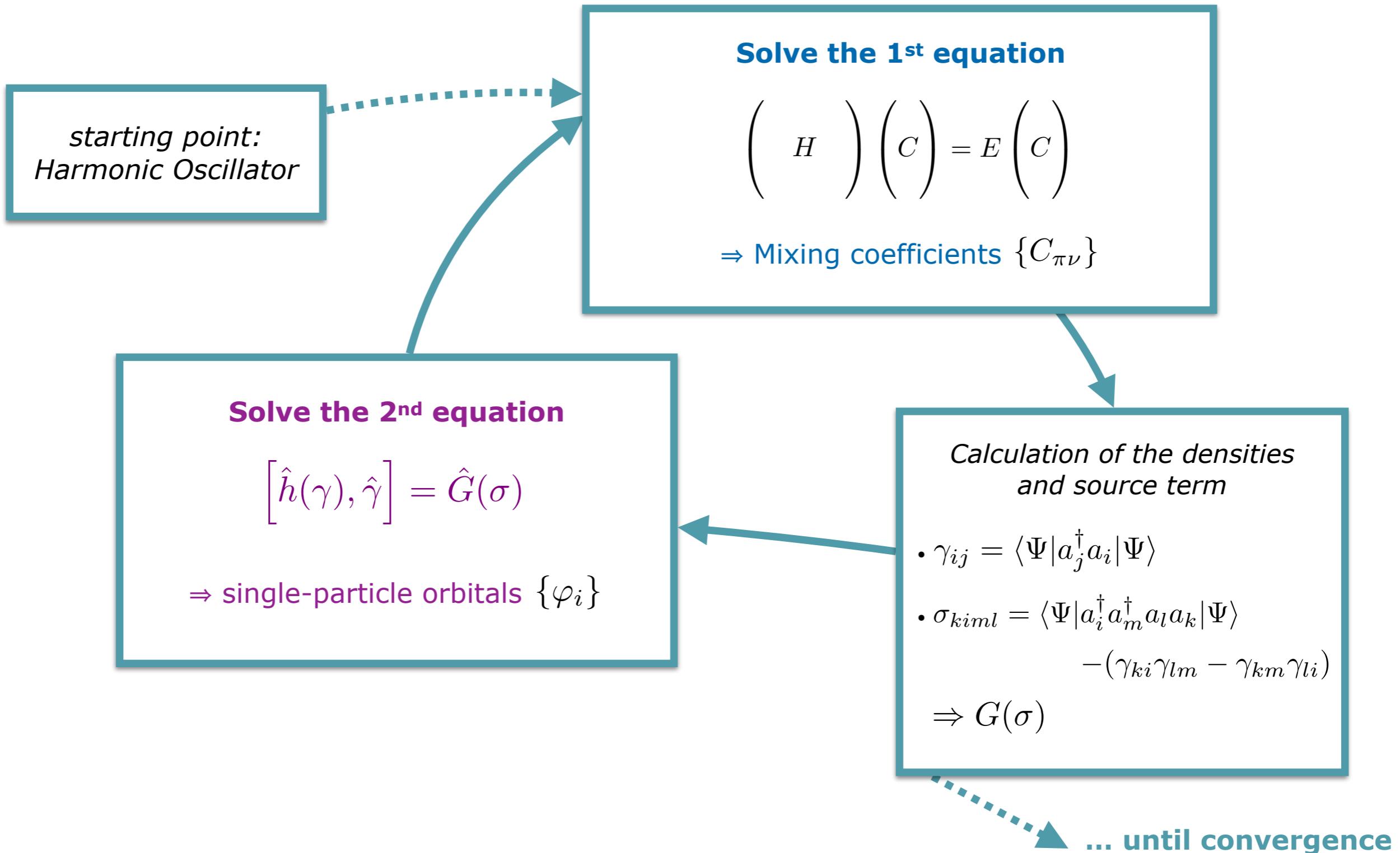
\in whole basis \in active space

\Rightarrow coupling between active and inactive spaces

\Rightarrow the density operator is modified

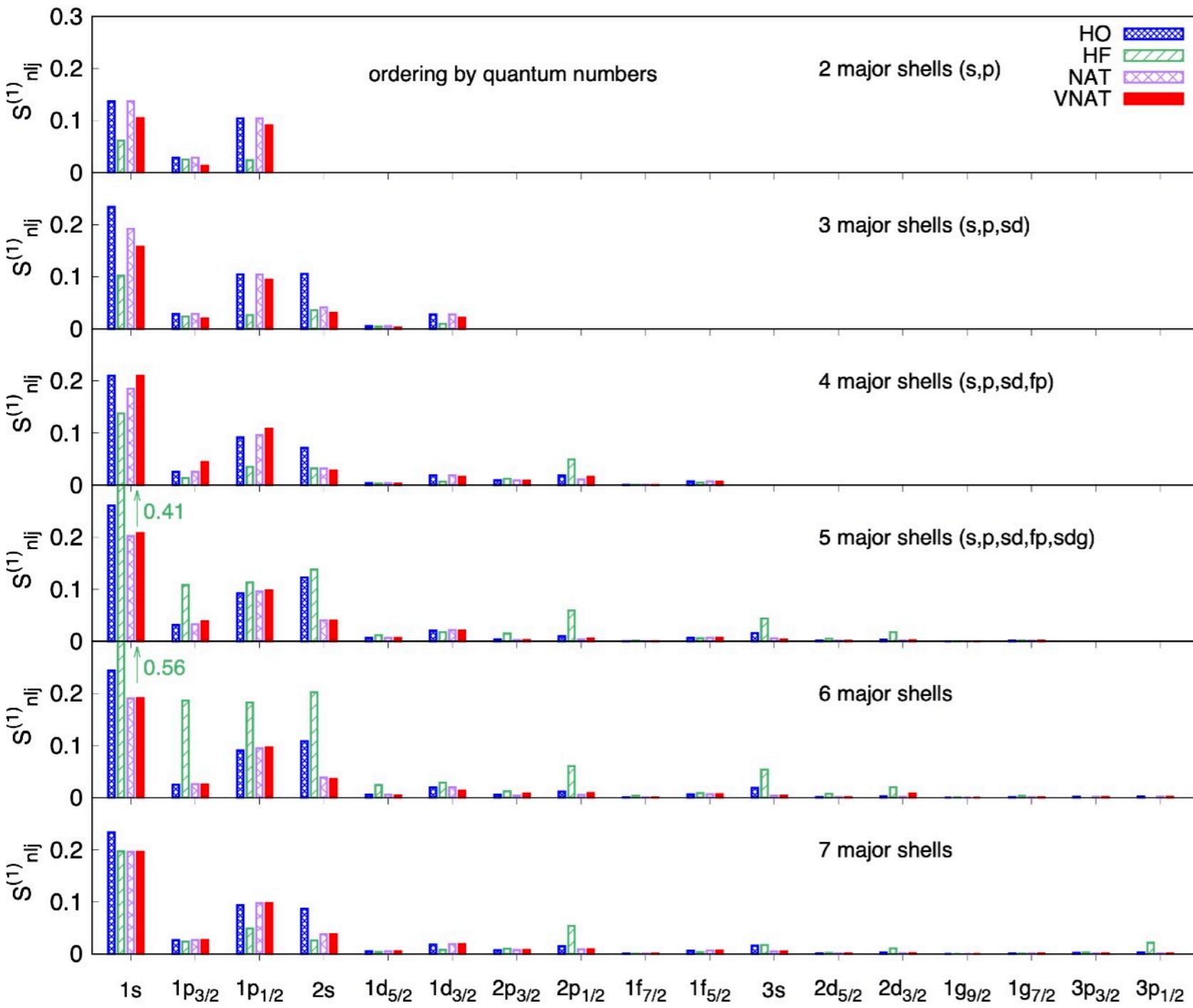
Multi-configuration self-consistent field method

→ The full solution is obtained via a doubly-iterative algorithm:



Single-orbital entanglement in ^4He

- Convergence of the single-orbital Von Neumann entropy:



$$S_{tot}^{(1)} = \sum_i S_i^{(1)}$$

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

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

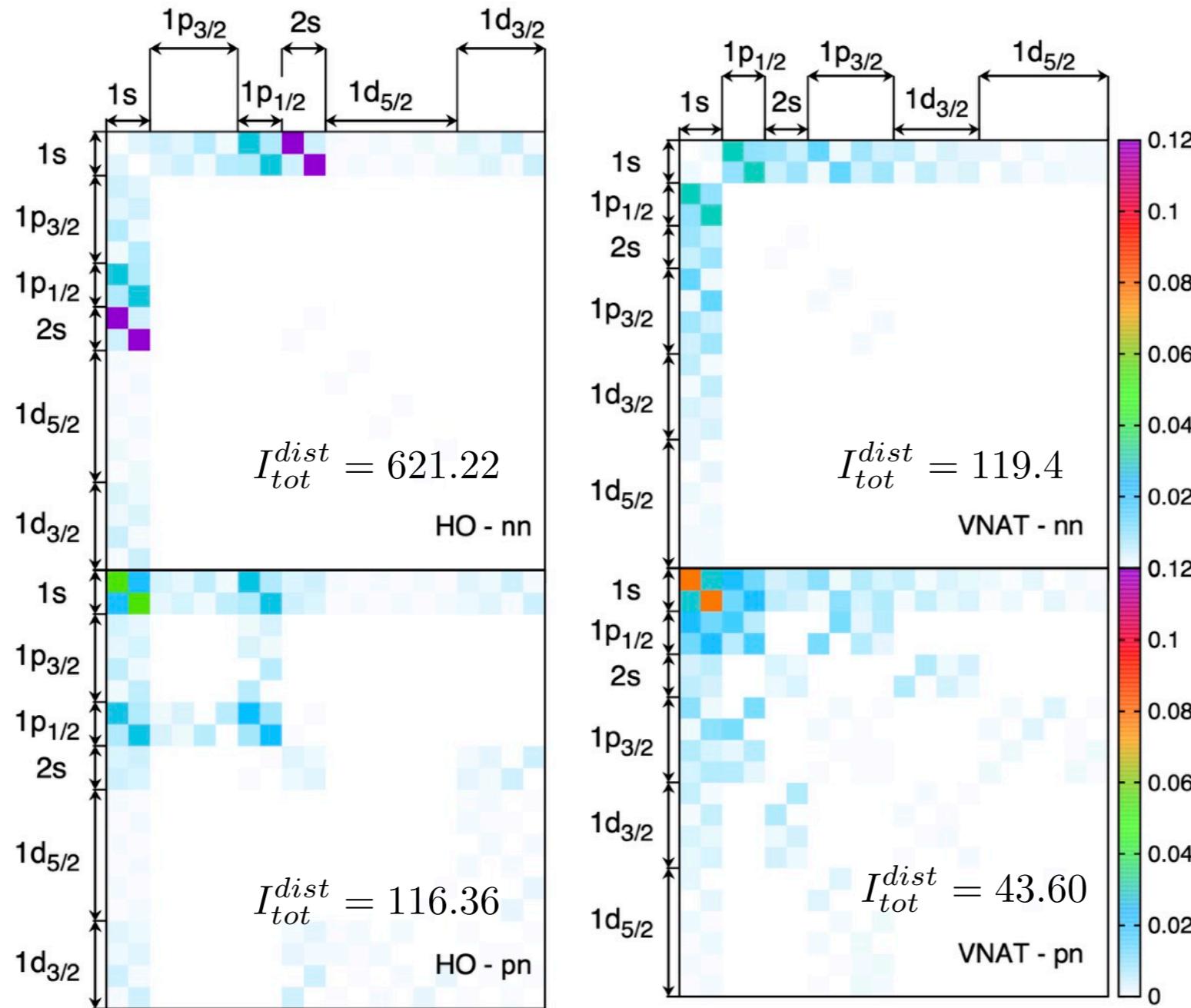
6 shells : $|\Psi_{HF}\rangle \simeq 56\% \text{ SD}$

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

* NAT & VNAT typically have similar entanglement patterns

Two-orbital mutual information in ^4He

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



"Entanglement distance":

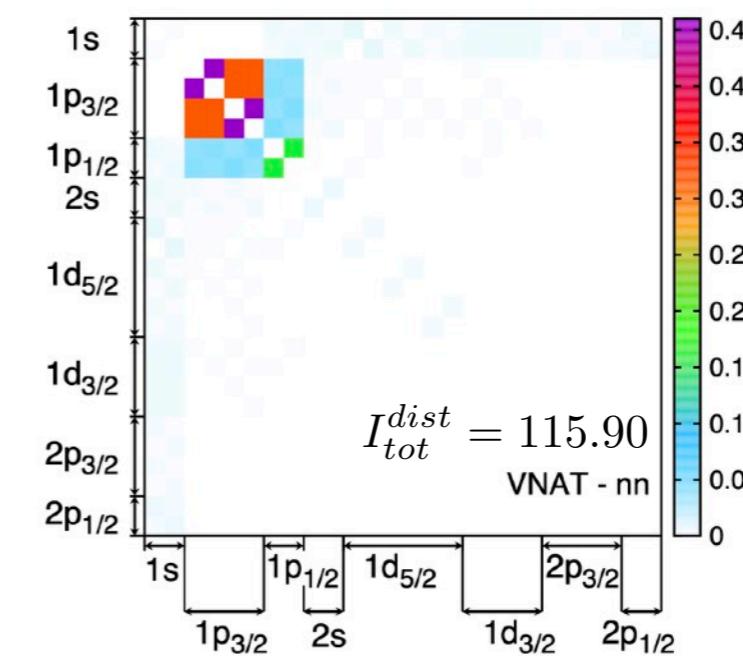
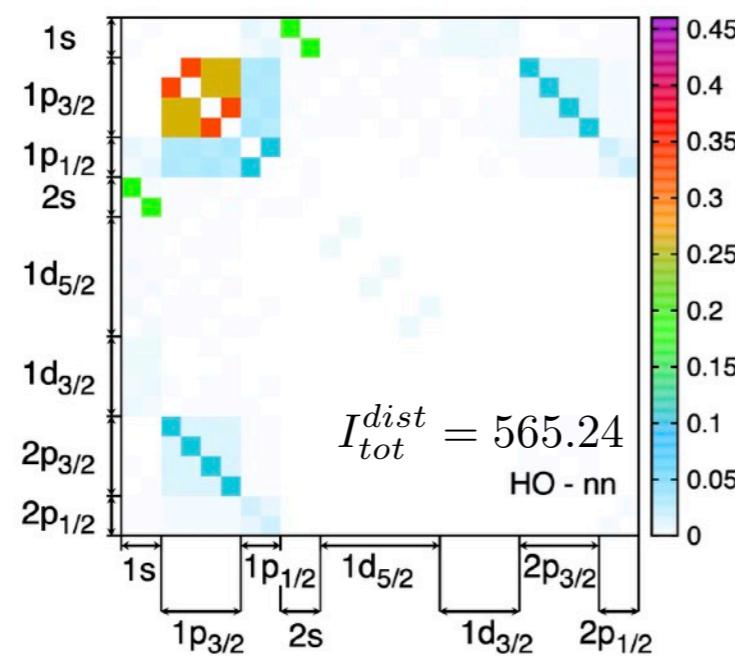
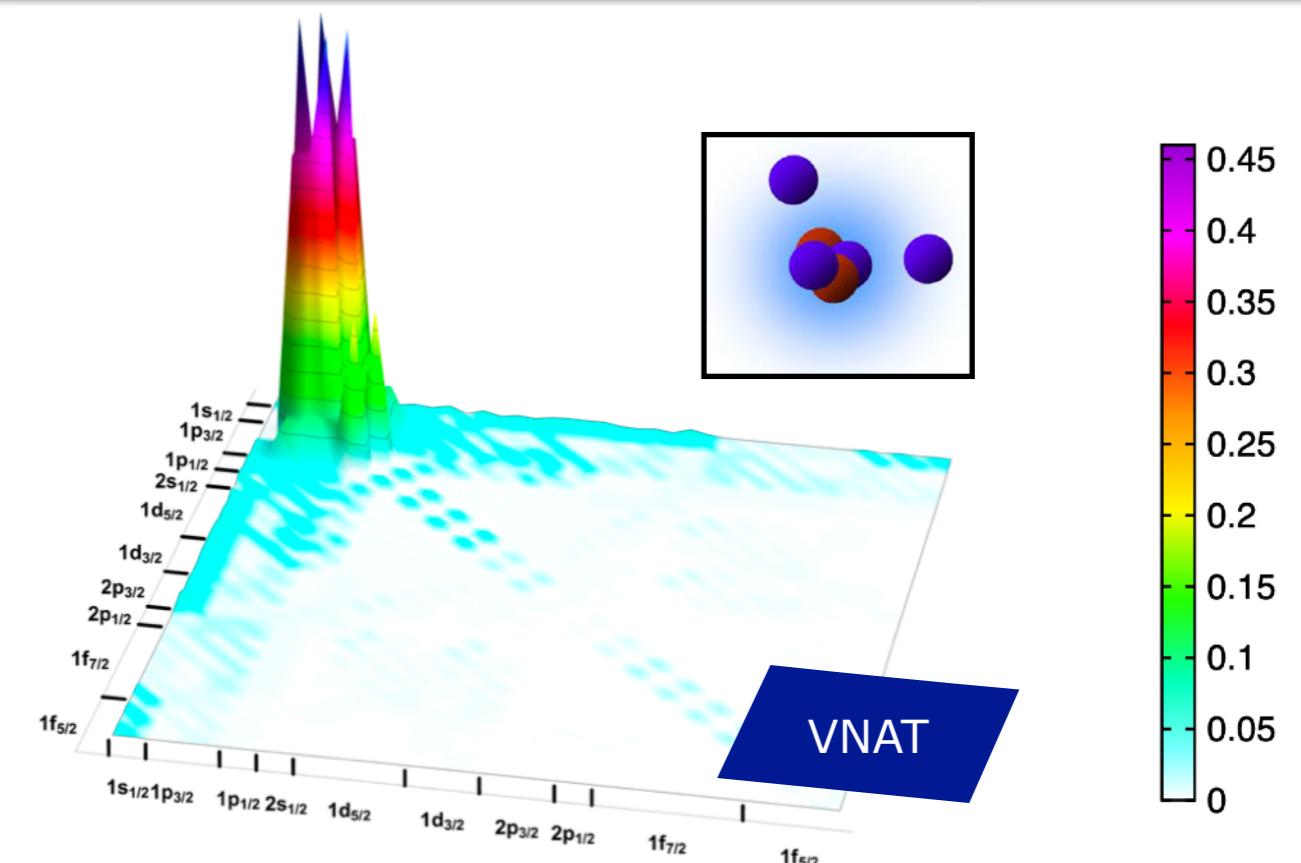
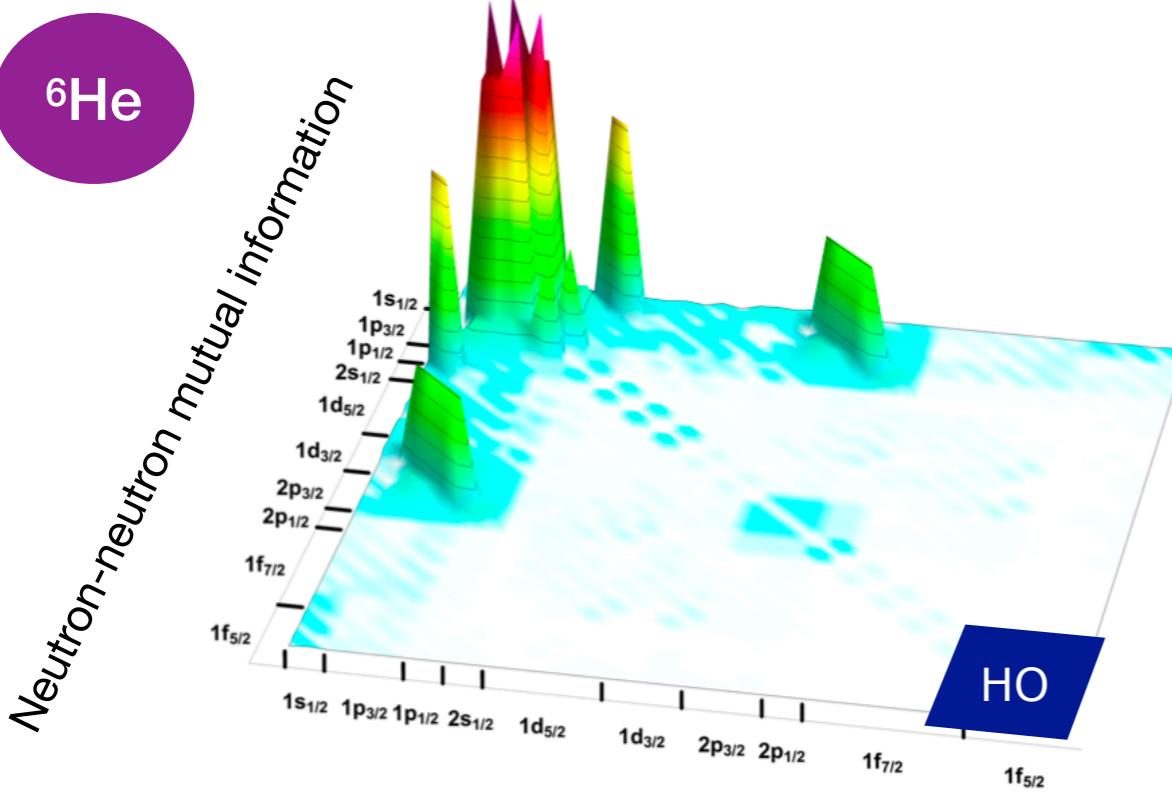
$$I_{ij}^{dist} = I_{ij} \times |i - j|^2$$

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

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

Two-orbital mutual information in ${}^6\text{He}$

${}^6\text{He}$



- ▶ HO orbitals: correlations distributed over the basis
- ▶ variational orbitals: decoupling of the 1p shell \Rightarrow clear emergence of ${}^4\text{He}$ -core + nn-valence structure

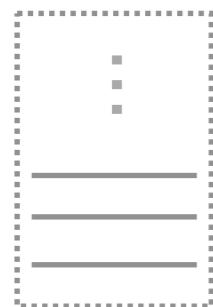
Two-orbital mutual information in ${}^6\text{He}$

${}^6\text{He}$

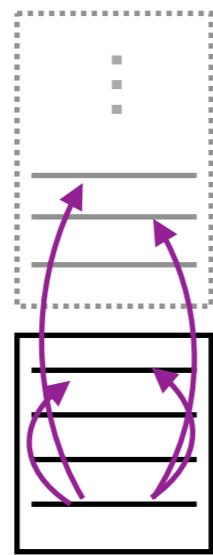
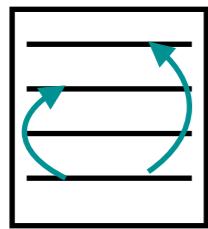
* Comparison NAT and VNAT bases:

so far, similar entanglement patterns but different convergence of energy

NAT basis mixes *active* HO states only while
VNAT basis mixes the full basis



vs



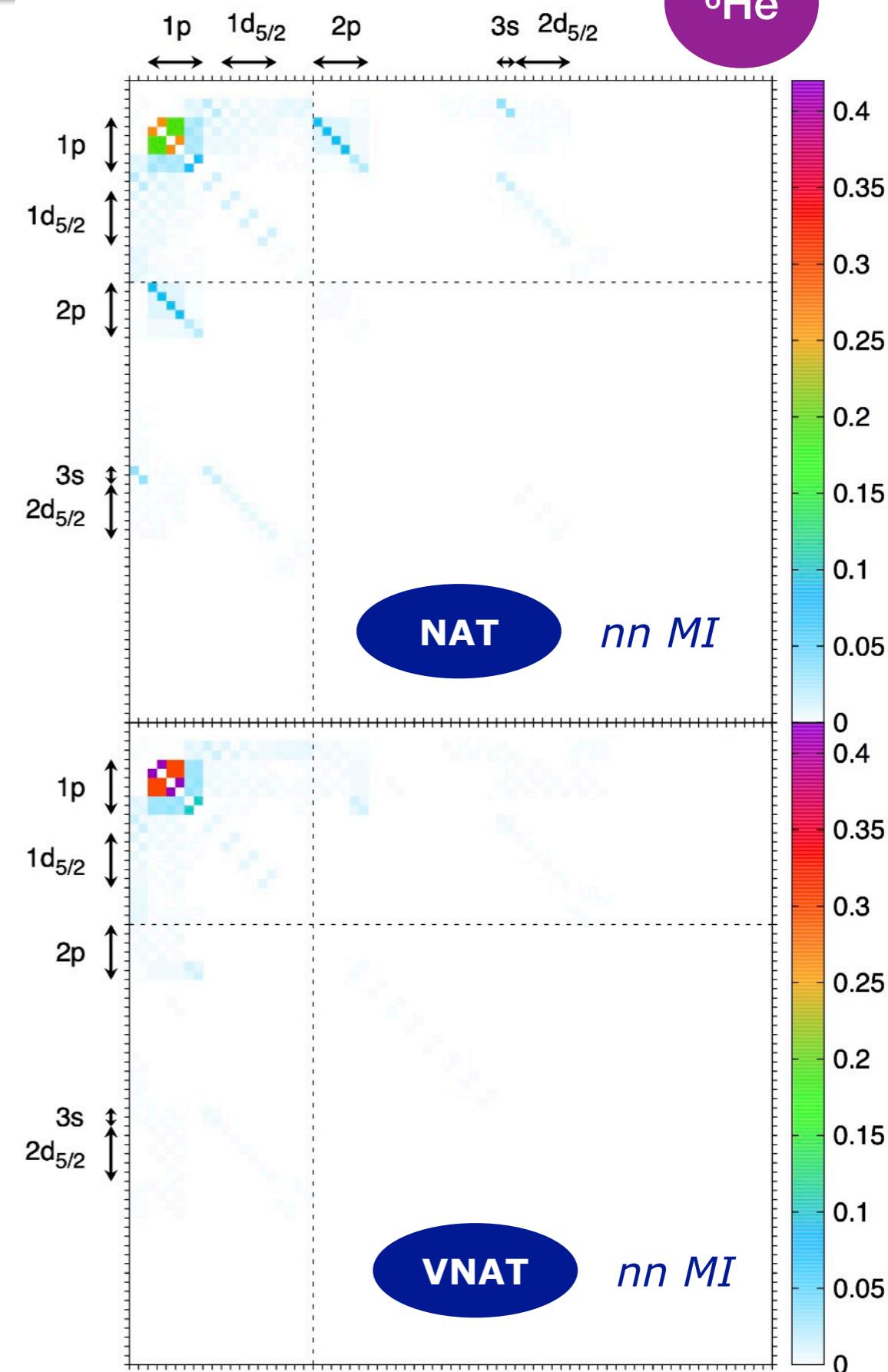
empty orbitals

active orbitals

→ How to differentiate them from the point of view of entanglement/correlations?

→ Test: Use NAT and VNAT basis obtained for $N_{\text{tot}}=3$ to perform calculation with $N'_{\text{tot}}=5 > N_{\text{tot}}$

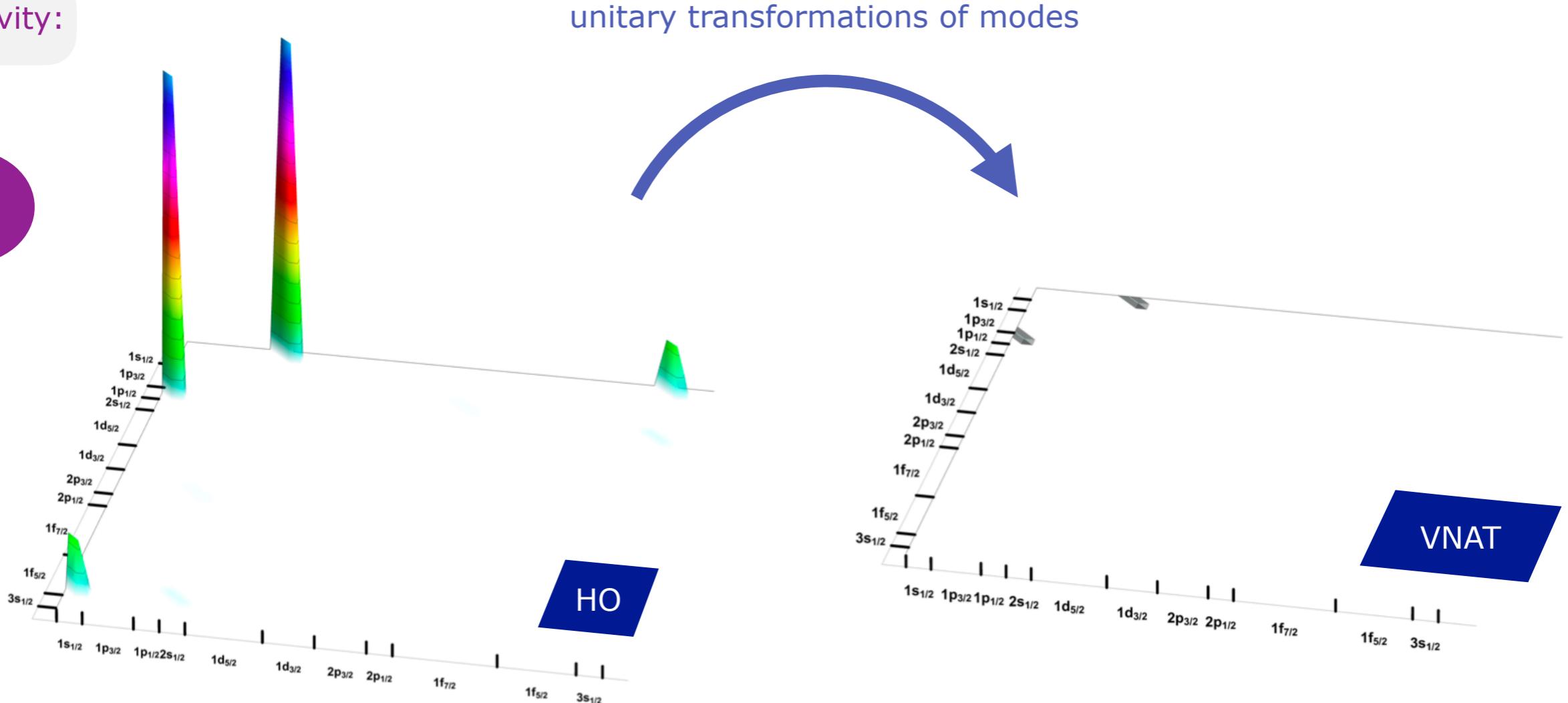
▶ VNAT decouples inactive and active spaces



Two-orbital negativity in ^4He

Negativity:

^4He



- Negativity identically cancels in the (V)NAT basis because γ diagonal \rightarrow true for all nuclei

\Rightarrow no distillable entanglement

- Would be useful to have a measure of bound entanglement, difficult

Faba, Martín, Robledo, PRA 103, 032426 (2021) "Two-orbital quantum discord in fermion systems"

\Rightarrow no bound entanglement in (V)NAT basis