EMMI Workshop and International Workshop XLIX on Gross Properties of Nuclei and Nuclear Excitations

"Effective Field Theories for Nuclei and Nuclear Matter"

Hirschegg, January 15-21 2023

Entanglement and quantum simulations of nuclear systems in effective model spaces

Caroline Robin

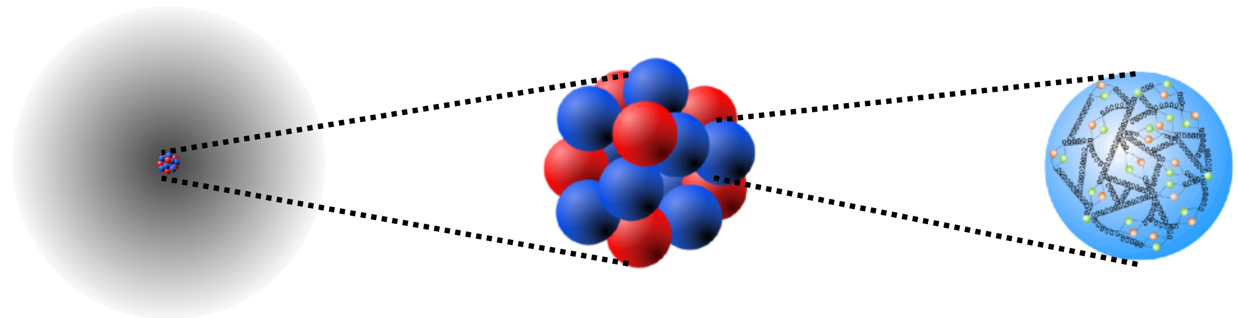
Fakultät für Physik, Universität Bielefeld, Germany
GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt, Germany

in collaboration with M. J. Savage, IQuS UW, Seattle

UNIVERSITÄT BIELEFELD

GSI

Entanglement and the nuclear many-body problem

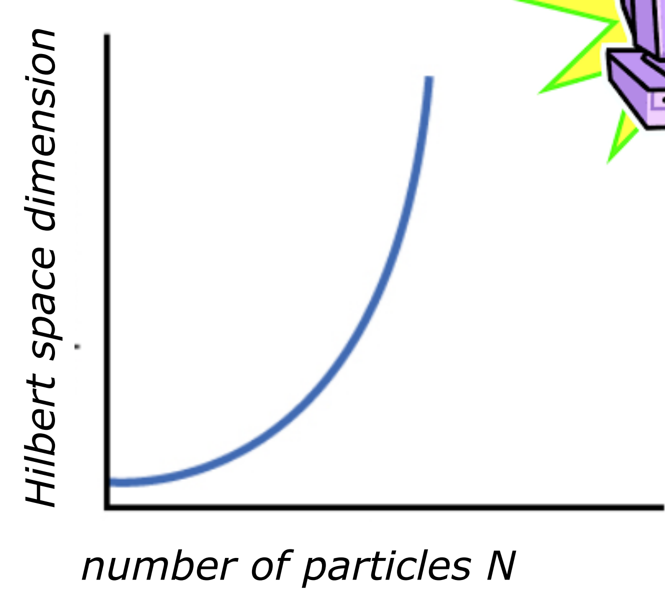


One of the goals of low-energy nuclear theory is to solve the nuclear many-body problem

- specific features: the nuclear force is not fully known, non-perturbative, two species of non-elementary particles…

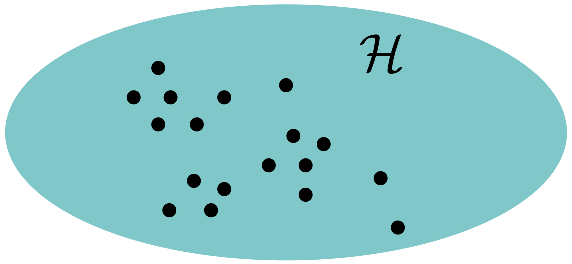
- one feature that is shared with other quantum many-body systems is ***entanglement***

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



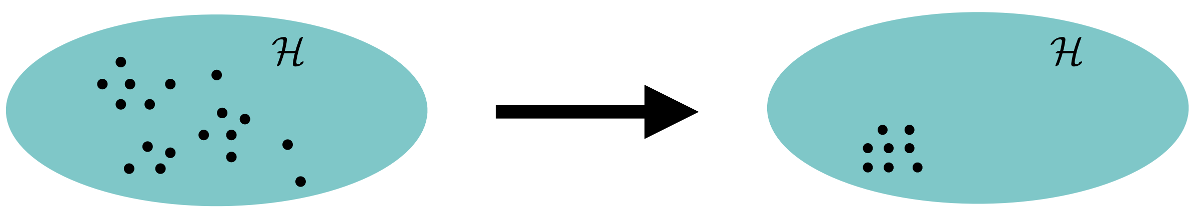
Entanglement and the nuclear many-body problem

But, typically not all configurations are important



☞ Understanding and manipulating entanglement can guide:

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



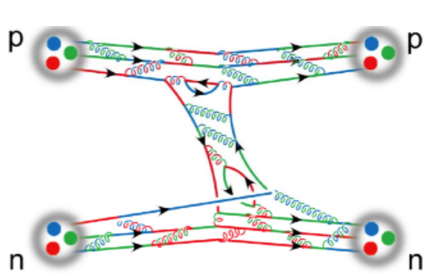
$$\Rightarrow \; |\Psi\rangle \approx \sum_{n}^{n_{trunc}} C_n |\Phi_n\rangle$$

density matrix renormalization group (DMRG), tensor networks…

- The development of quantum simulations of physical systems

  on current noisy intermediate scale quantum (NISQ) devices

- Our fundamental understanding of nature

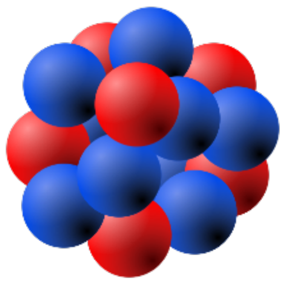


e.g. *"Entanglement Suppression and Emergent Symmetries of Strong Interactions"*
Beane, Kaplan, Klco, Savage, PRL122,102001 (2019).

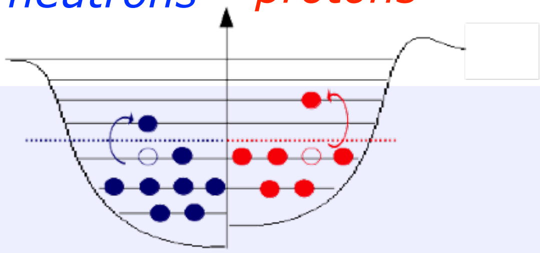
"Entanglement minimization in hadronic scattering with pions"
Beane, Farrell, Varma. Int. J. Mod. Phys. A 36,2150205 (2021).

…

Entanglement and the nuclear many-body problem



= Z protons + N neutrons



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

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

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

$$n_{\pi_1} + n_{\pi_2} \dots + n_{\nu_1} + n_{\nu_2} \dots = Z + N$$

Several types of entanglement are present in the nucleus:

✳ Entanglement between proton and neutron subsystems

see e.g. Papenbrock & Dean PRC 67, 051303(R) (2003), in the framework of DMRG;
Johnson & Gorton arXiv:2210.14338 (2022), in the traditional Shell Model.

✳ Entanglement of modes (single-particle 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 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+ arXiv:2203.12079 (2022), arXiv:2203.04843 (2022) entanglement and SRC

Outline

★ Entanglement in effective model space calculations of light nuclei: How does the entanglement structure evolve with the Hamiltonian transformation?

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

★ Using entanglement rearrangement to leverage current NISQ computers:

Hamiltonian-learning-VQE applied to the Lipkin-Meshkov-Glick model

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

Outline

★ Entanglement in effective model space calculations of light nuclei: How does the entanglement structure evolve with the Hamiltonian transformation?

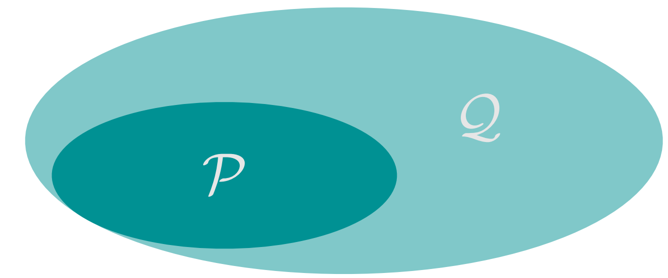
CR, M. J. Savage, N. Pillet, PRC 103, 034325 (2021)

★ Using entanglement rearrangement to leverage current NISQ computers:
Hamiltonian-learning-VQE applied to the Lipkin-Meshkov-Glick model

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

Nuclear structure calculations in effective model spaces

Nuclear structure calculations in effective model spaces:



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

full space Hamiltonian and wave function

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

effective model space and Hamiltonian

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

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

$$\left(\begin{array}{c|c} H(\boldsymbol{\beta})_{\mathcal{PP}} & H(\boldsymbol{\beta})_{\mathcal{QP}} \\ \hline H(\boldsymbol{\beta})_{\mathcal{PQ}} & H(\boldsymbol{\beta})_{\mathcal{QQ}} \end{array}\right)$$

Here we will consider $\quad U(\boldsymbol{\beta}) = e^{iT(\boldsymbol{\beta})}$

where $T(\boldsymbol{\beta})$ = one-body hermitian operator determined by a variational principle

→ corresponds to an orbital transformation

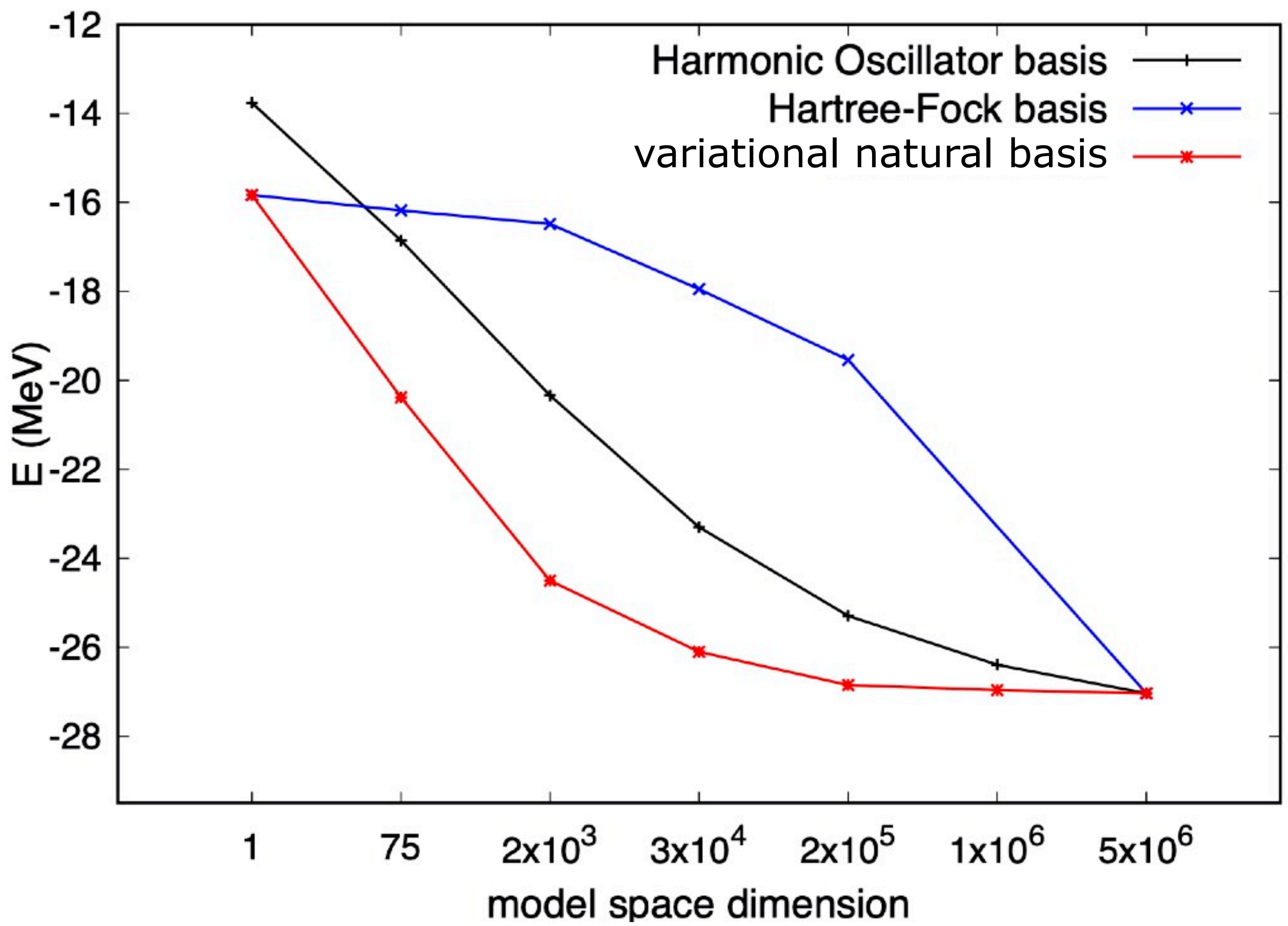
$\hat{H}$ *and* $\hat{H}(\beta)$ *are unitarily equivalent but the transformation will increase* $\langle\Psi|\Psi\rangle^{\mathcal{P}}$

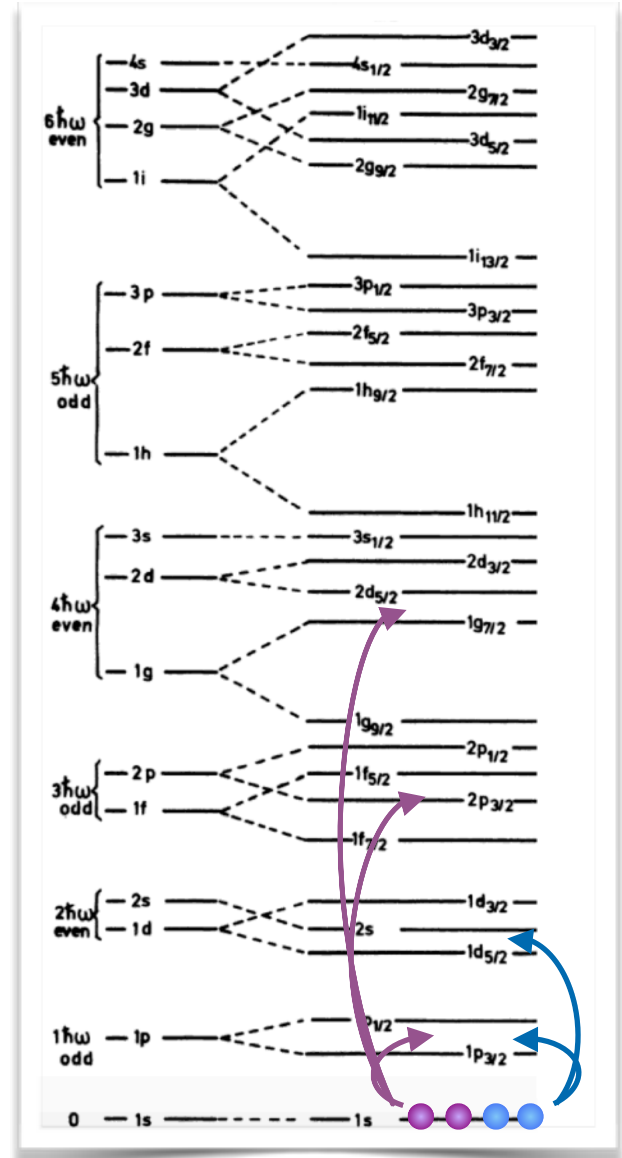
Nuclear structure calculations in effective model spaces

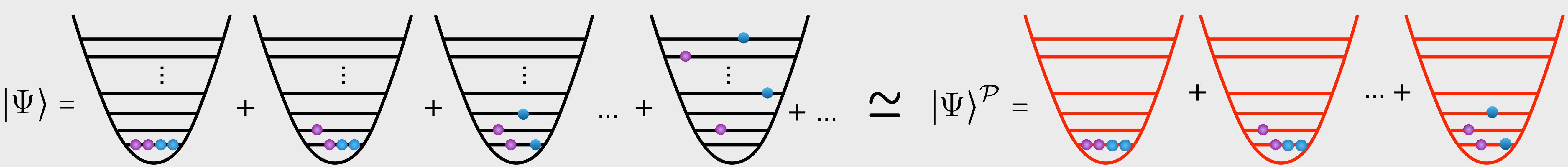
★ ***⁴He with a chiral interaction*** *(2-body force N2LO$_{opt}$ [Ekström+ PRL 110 192502 (2013)])*

single-particle bases expanded on 7 HO major shells

full diagonalization in active space with $N_{shell} \leq 7$



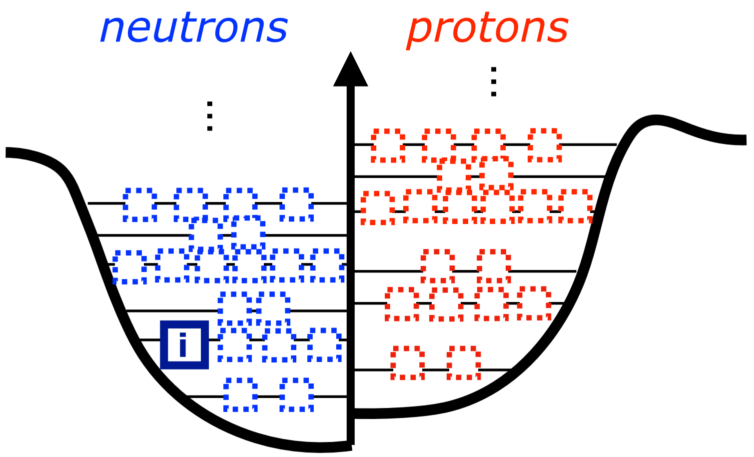




Single-orbital entanglement in ^{4}He

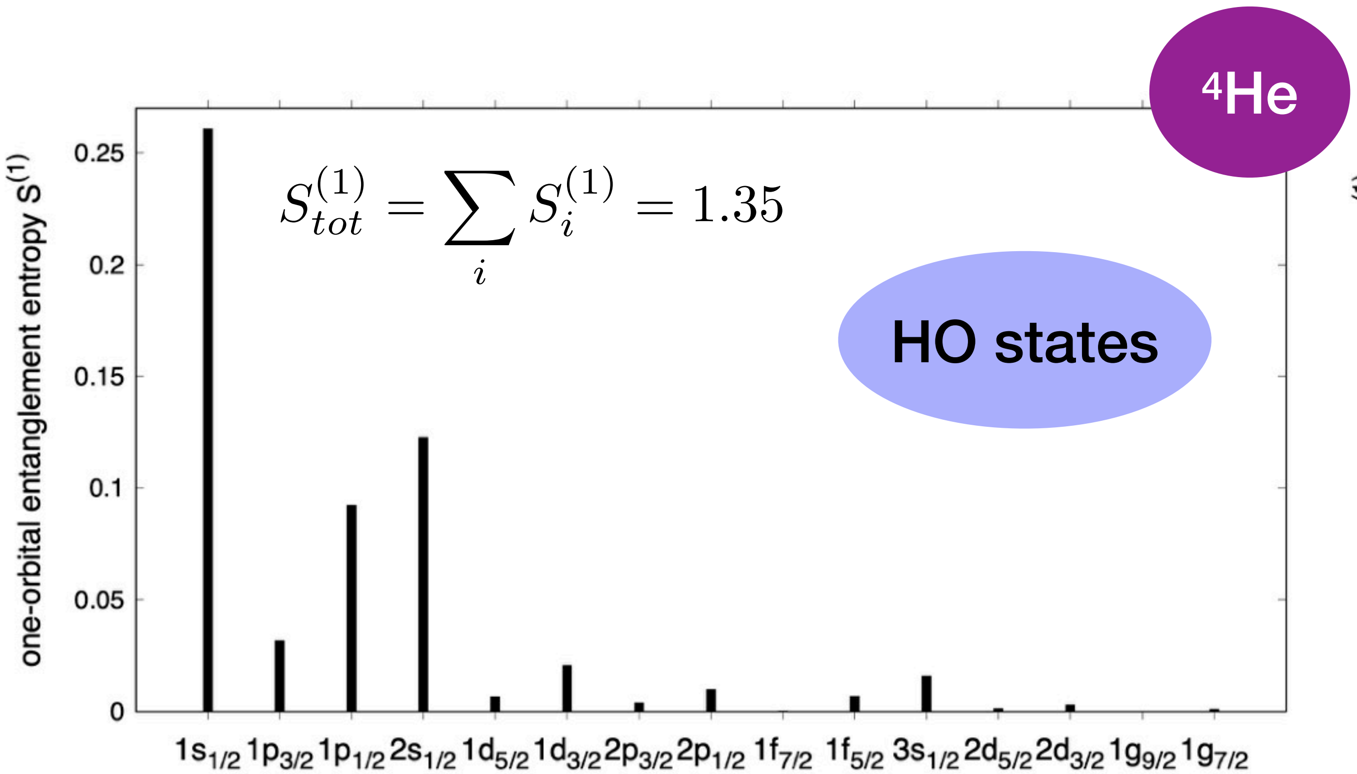
- Single-orbital Von Neumann entropy: $S^{(1)}_{(i)} = -\mathrm{Tr}\left[\rho^{(i)} \ln \rho^{(i)}\right]$

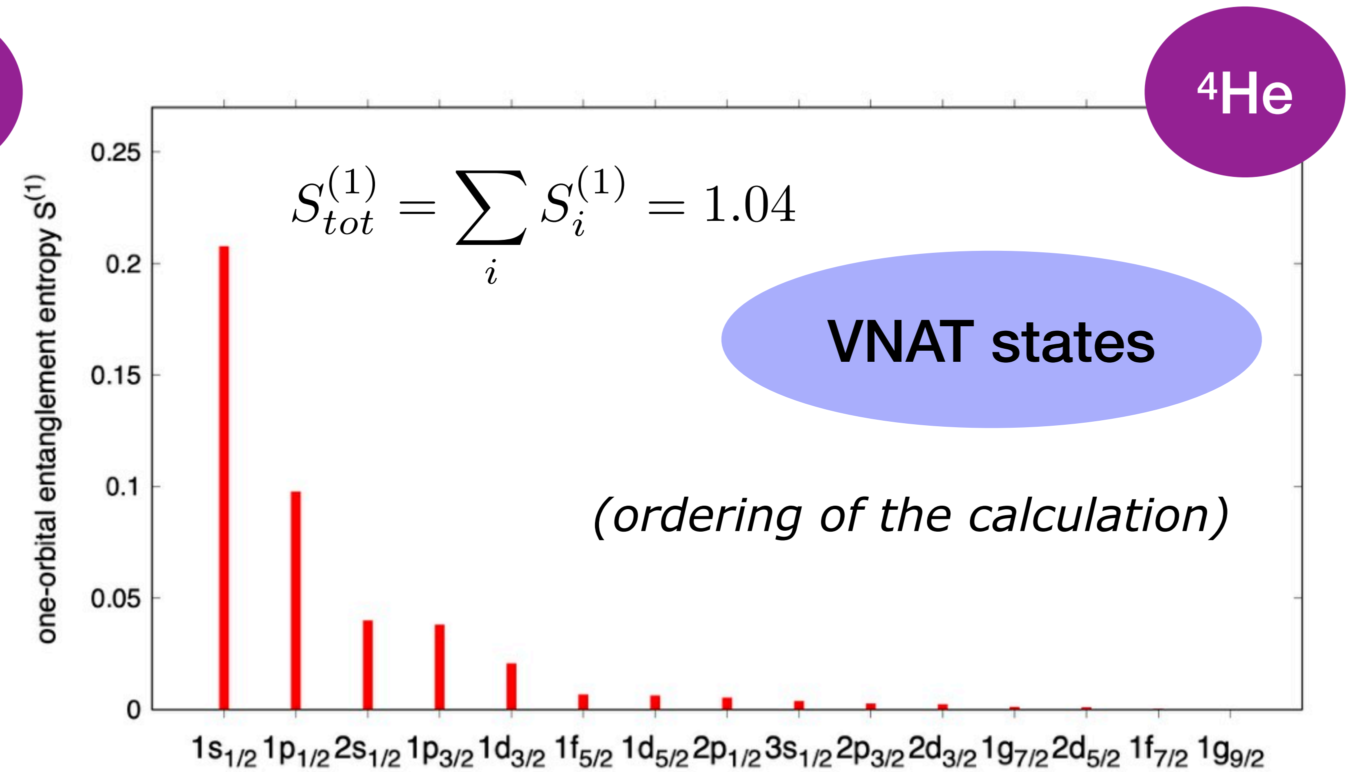
  = measure of entanglement of one orbital with the rest of the system



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

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



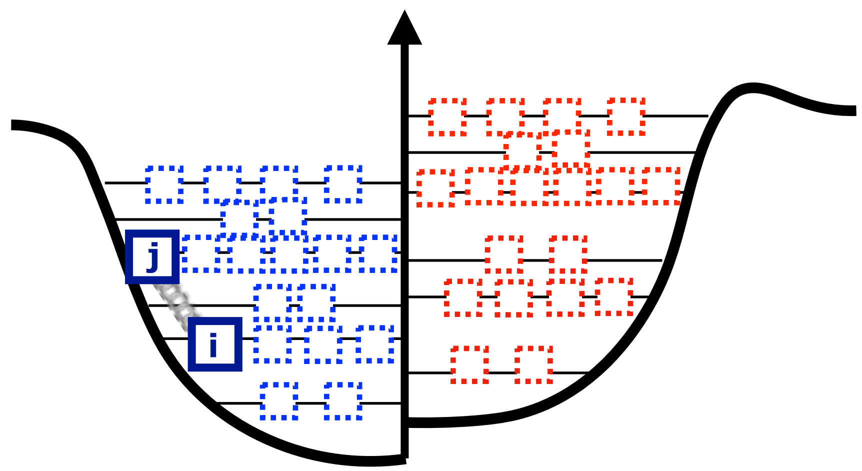


$N_{shell}=5 \quad \hbar\Omega = 30$ MeV

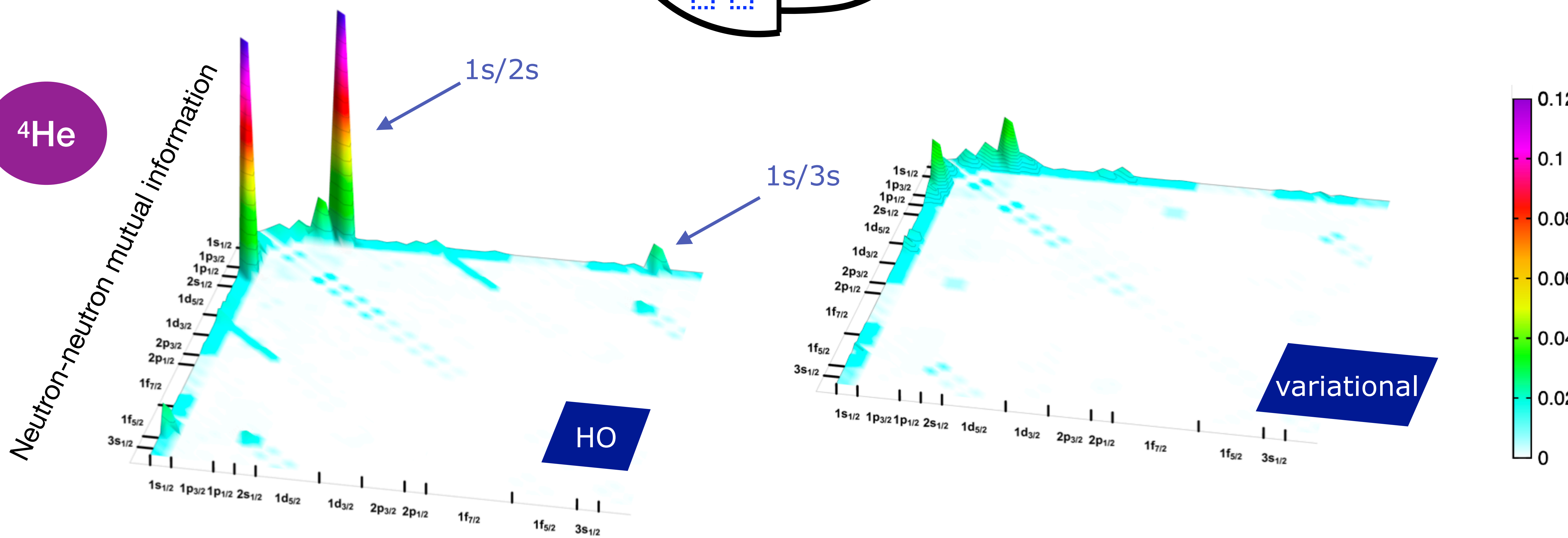
- *the VNAT basis is naturally ordered by decreasing entanglement entropy*
- *$S^{(1)}_{tot}$ is in fact minimized in the (V)NAT basis* *[Gigena and Rossignoli, PRA 92, 042326 (2015)]*

Two-orbital mutual information in ^{4}He

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



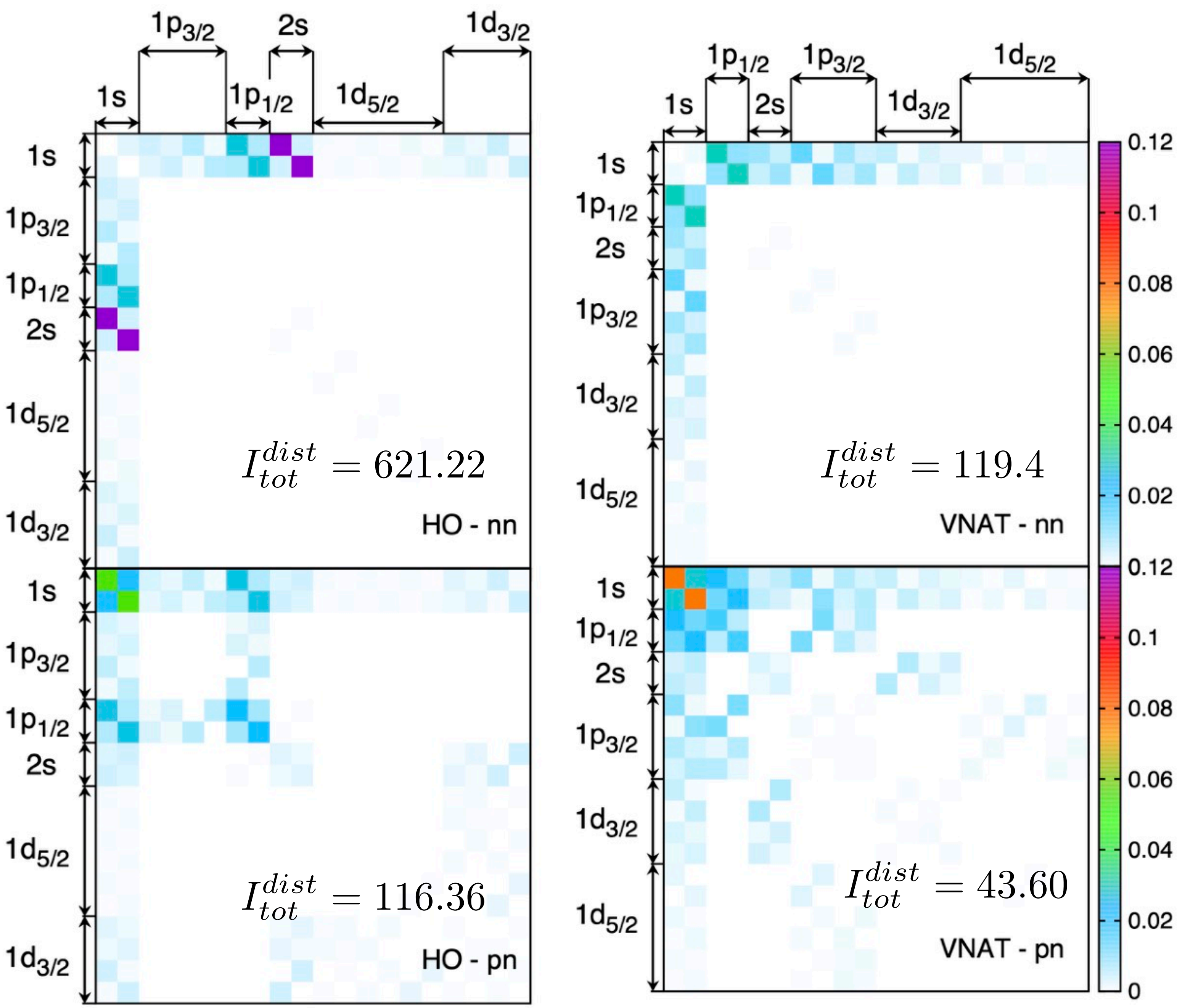
^{4}He



- *MI between s states is largely suppressed in the VNAT basis*
- *Correlations "localized" in the VNAT basis*

Two-orbital mutual information in ^4He

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



"Entanglement distance":

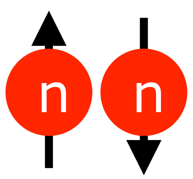
$$I_{ij}^{dist} = I_{ij} \times |i-j|^2$$

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

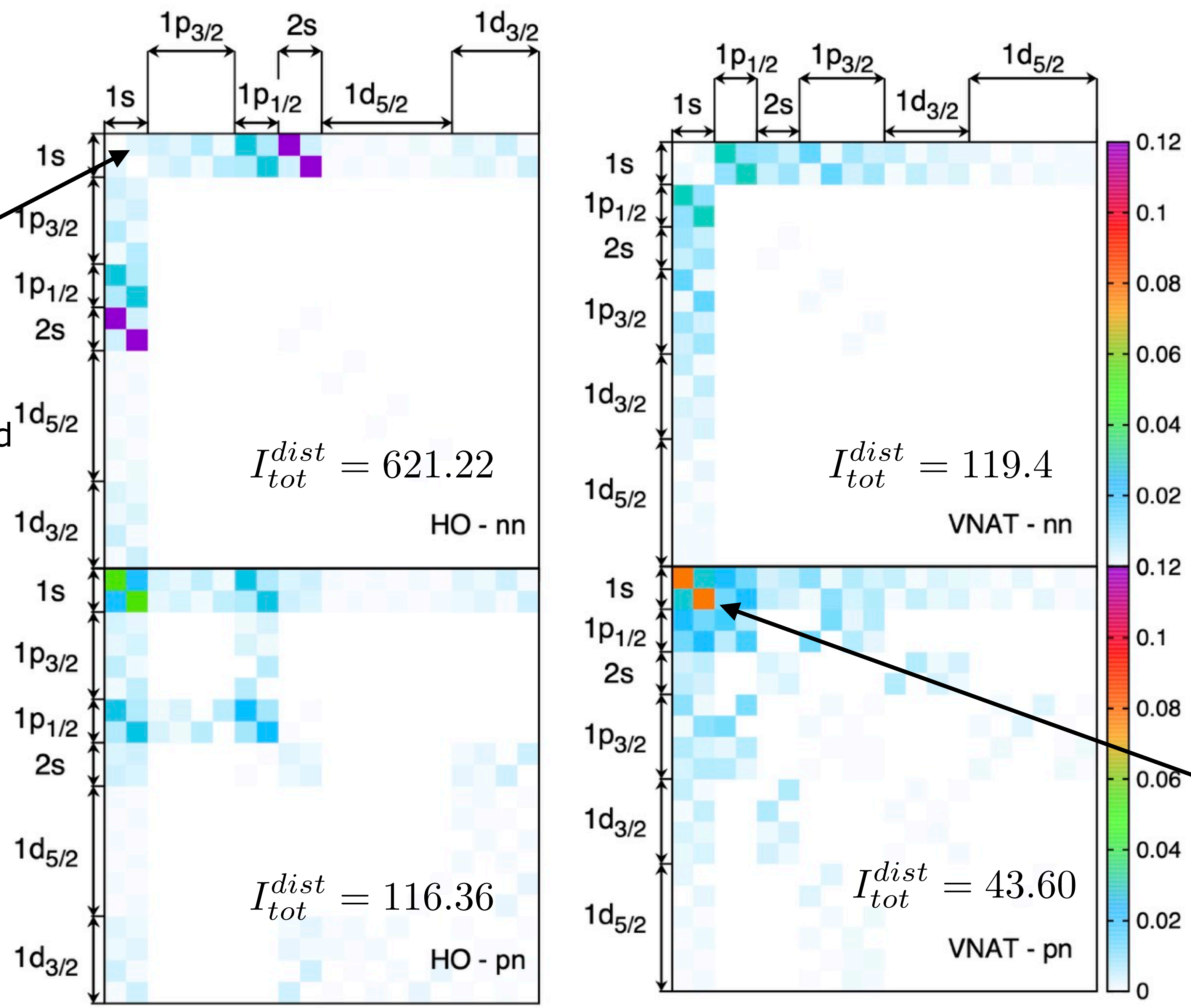
- In DMRG the entanglement distance is used to group the most interacting orbitals together, here such grouping occurs naturally

Two-orbital mutual information in ^{4}He

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



BCS pairing btw time-reversed states(?)

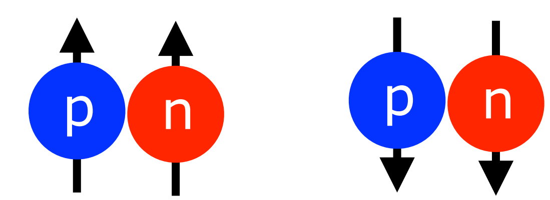


"Entanglement distance":

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

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

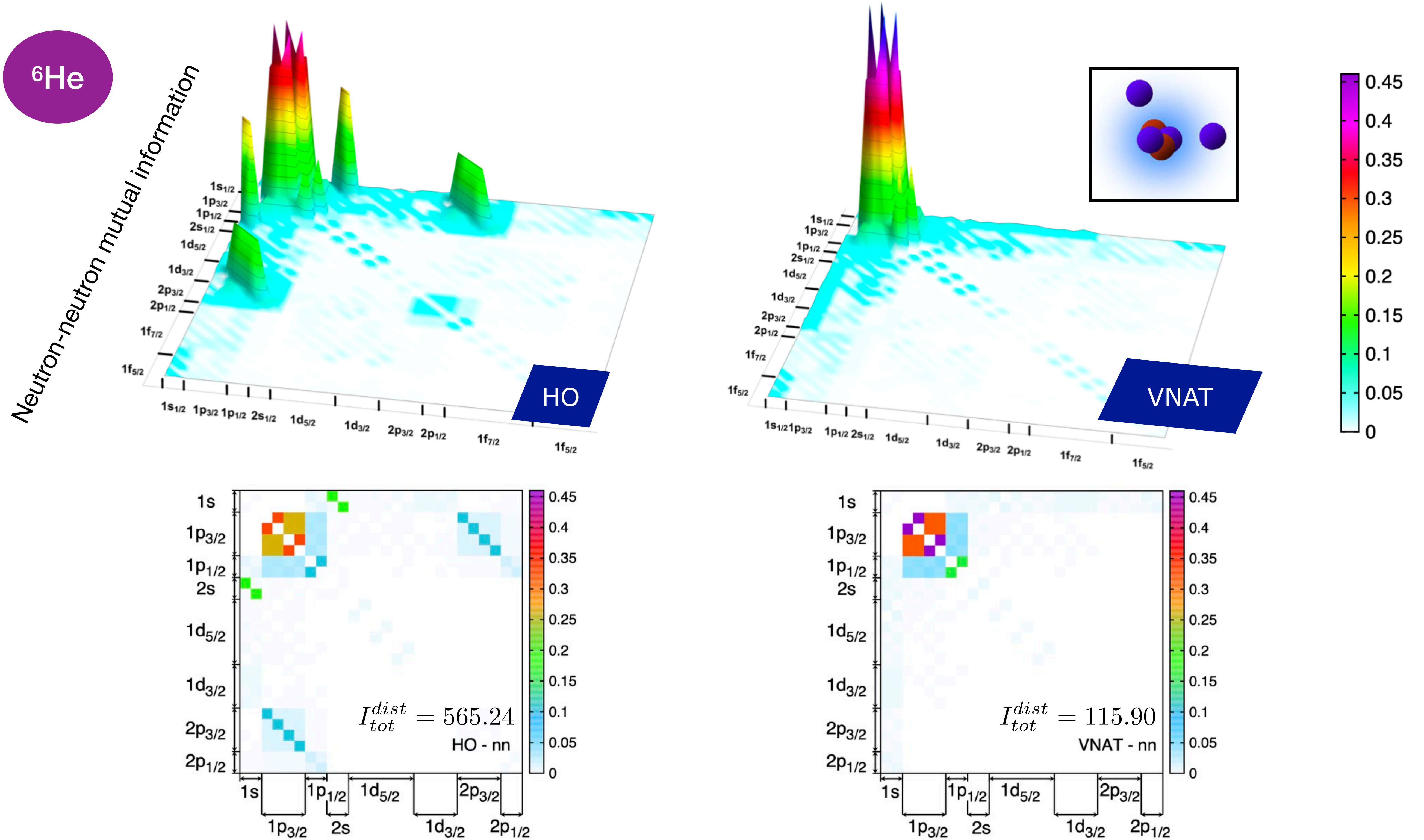
J=1, T=0 pairing (?)



- 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

^{6}He



- *HO orbitals: correlations distributed over the basis*
- *variational orbitals: decoupling of the 1p shell ⇒ clear emergence of ^{4}He-core + nn-valence structure*

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)

★ Using entanglement rearrangement to leverage current NISQ computers:
Hamiltonian-learning-VQE applied to the Lipkin-Meshkov-Glick model

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

The Lipkin-Meshkov-Glick Model

Several previous studies of the LMG 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)

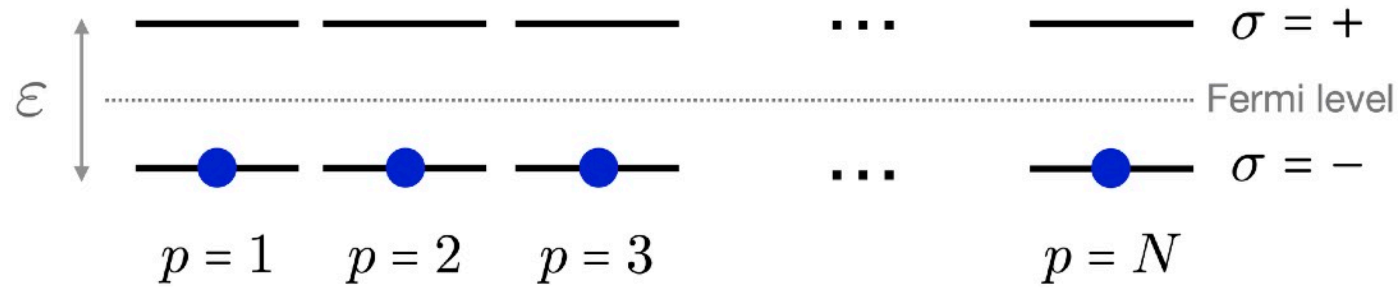
⇒ good benchmark for comparing different methods

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:



$$H = \frac{\varepsilon}{2}\sum_{\sigma p} \sigma c^\dagger_{p\sigma} c_{p\sigma} - \frac{V}{2}\sum_{pq\sigma} c^\dagger_{p\sigma} c^\dagger_{q\sigma} c_{q-\sigma} c_{p-\sigma}$$
$$= \varepsilon J_z - \frac{V}{2}\left(J_+^2 + J_-^2\right)$$

$$J_z = \frac{1}{2}\sum_{p\sigma} \sigma c^\dagger_{p\sigma} c_{p\sigma}$$
$$J_+ = \sum_p \sigma c^\dagger_{p+} c_{p-} \,, \qquad J_- = (J_+)^\dagger$$

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

np-nh excitation
n=J+M

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

⇒ the ground state (J=N/2) only contains even n

The Lipkin-Meshkov-Glick Model in effective model space

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

$\Lambda =$ cut-off on the np-nh excitations

$\beta =$ 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:

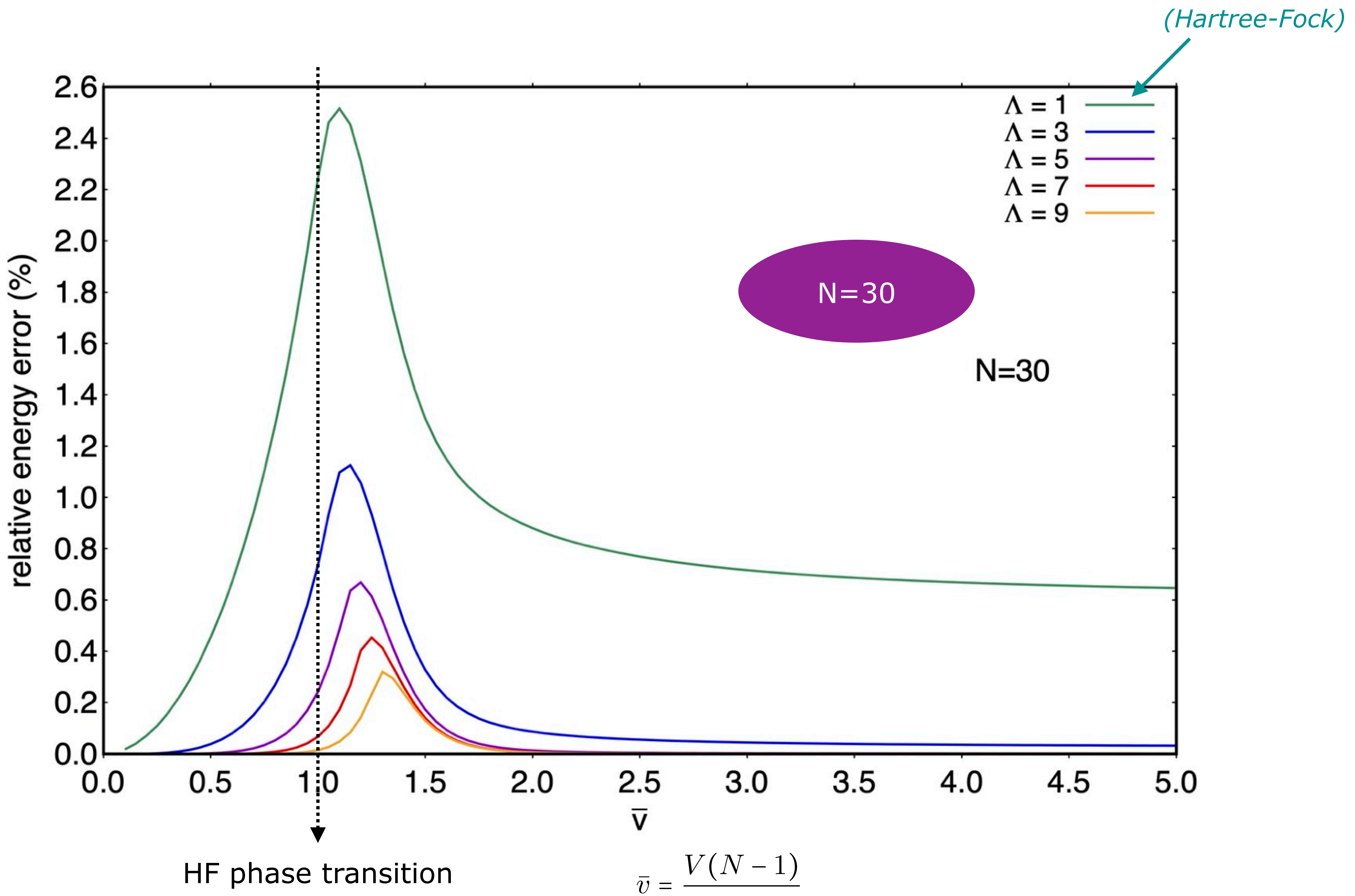
$$\begin{aligned} H(\beta) =& \varepsilon\Big[\cos\beta J_z(\beta) + \frac{1}{2}\sin\beta\big(J_+(\beta) + J_-(\beta)\big)\Big] \\ & - \frac{V}{4}\Big[\sin^2\beta\big(4J_z(\beta)^2 - \{J_+(\beta), J_-(\beta)\}\big) + (1+\cos^2\beta)\big(J_+(\beta)^2 + J_-(\beta)^2\big) \\ & - 2\sin\beta\cos\beta\big(\{J_z(\beta),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

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

The Lipkin-Meshkov-Glick Model in effective model space

★***Energy***

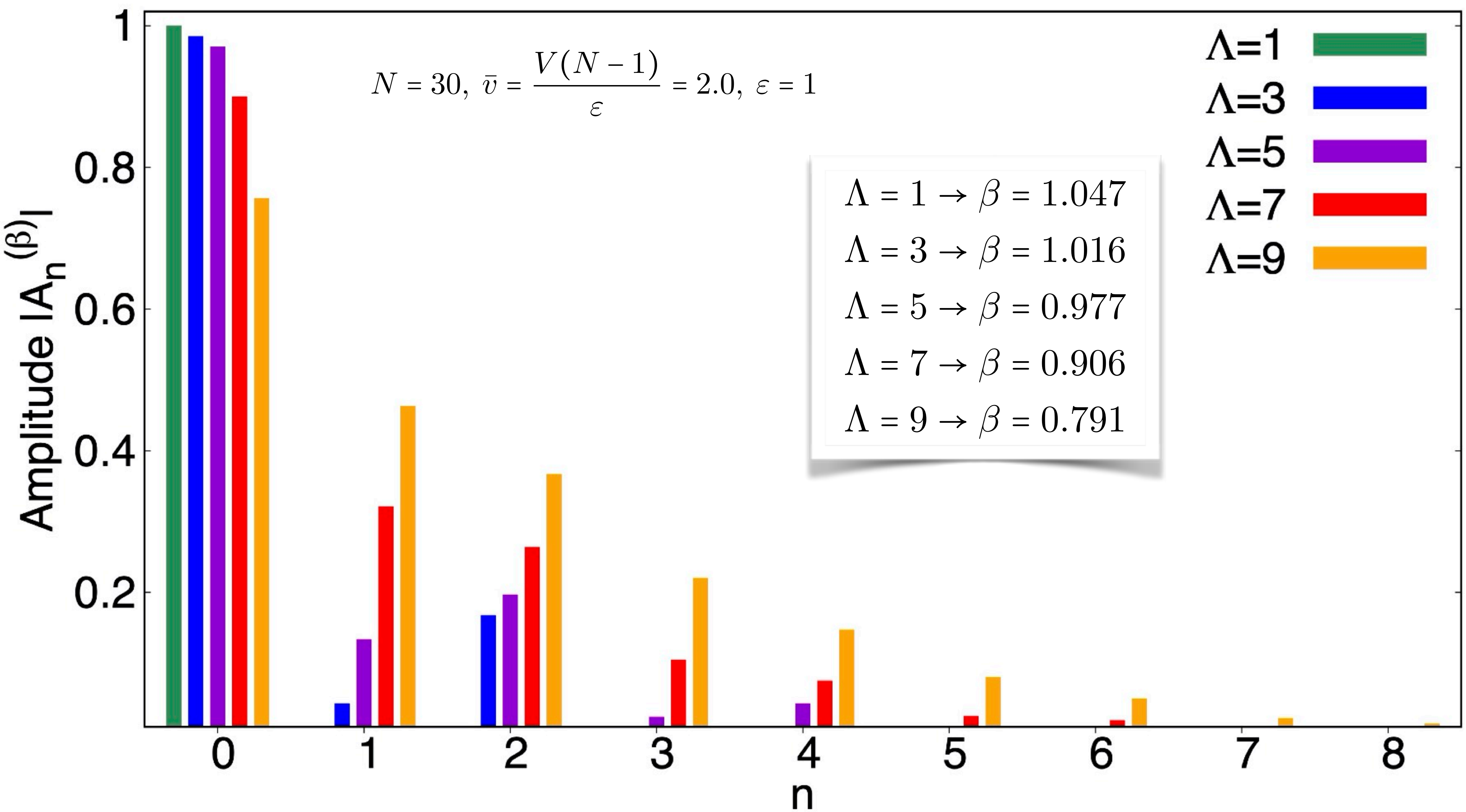
$$\frac{|E_{ex} - E|}{|E_{ex}|}$$



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

The Lipkin-Meshkov-Glick Model in effective model space

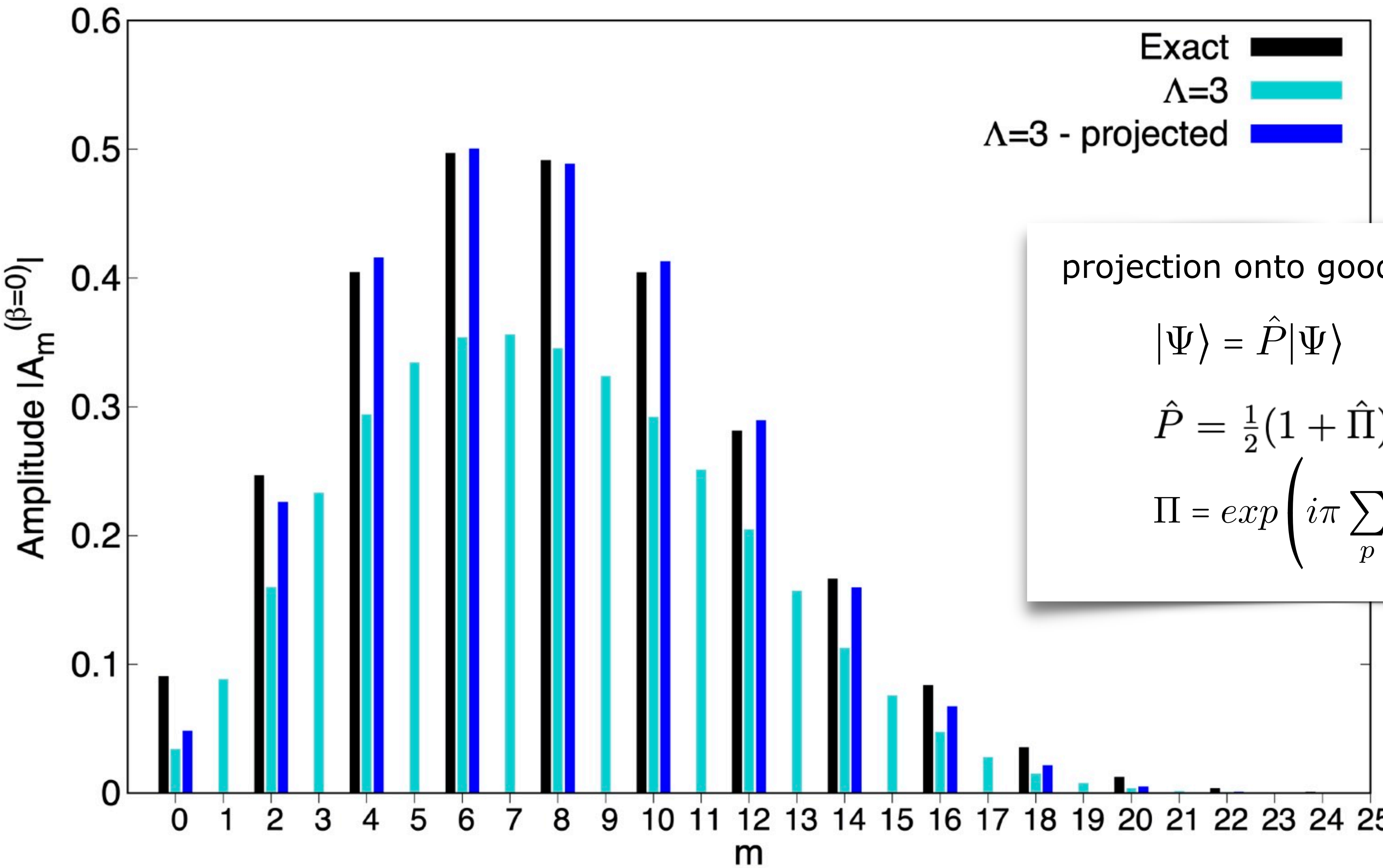
★ ***Wave function in the optimized (rotated) basis:***



- 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 effective model space

★ ***Wave function in the original basis (β=0):***



projection onto good parity state:

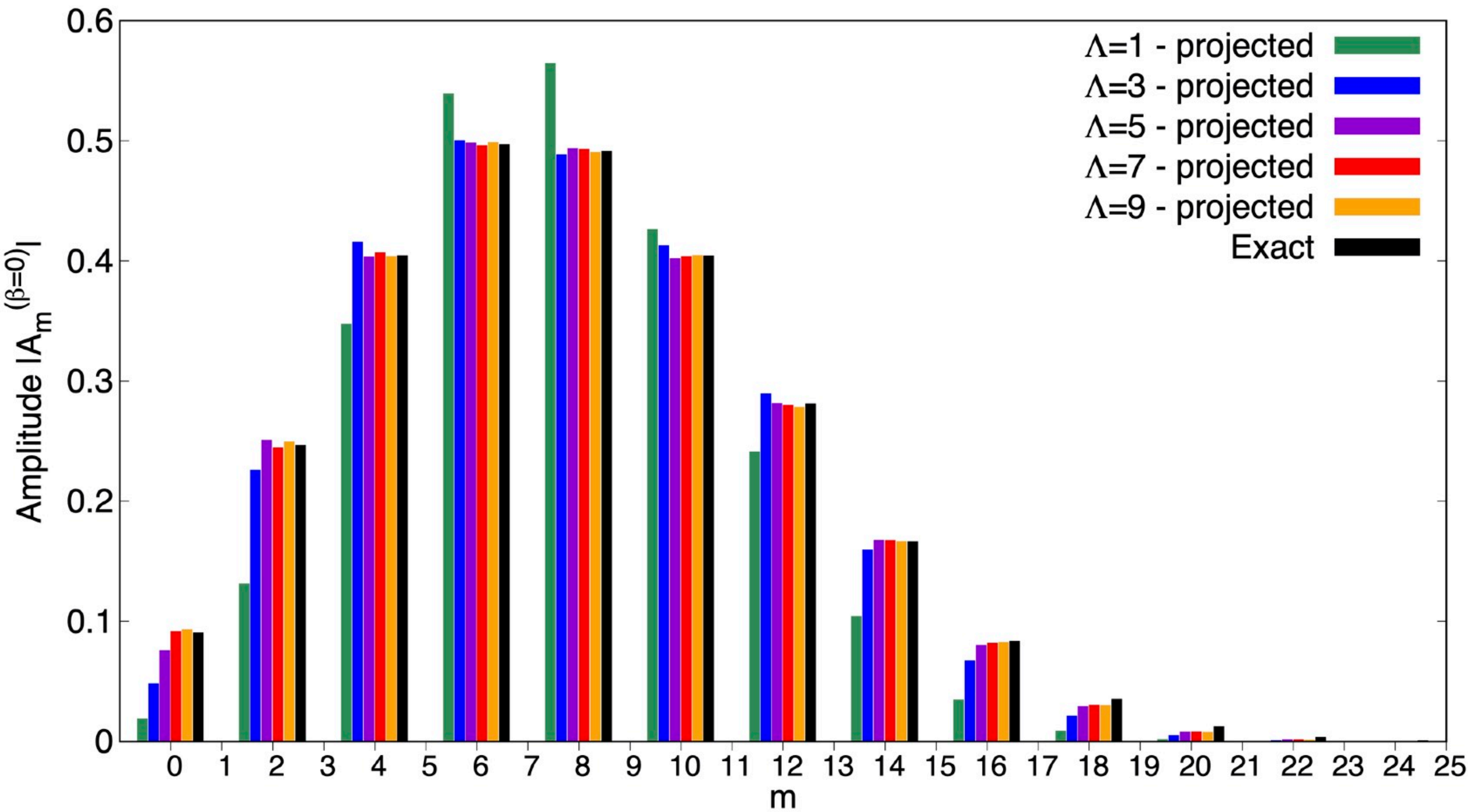
$$|\Psi\rangle = \hat{P}|\Psi\rangle$$

$$\hat{P} = \frac{1}{2}(1+\hat{\Pi})$$

$$\Pi = exp\left(i\pi \sum_p c^\dagger_{p+}c_{p+}\right)$$

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

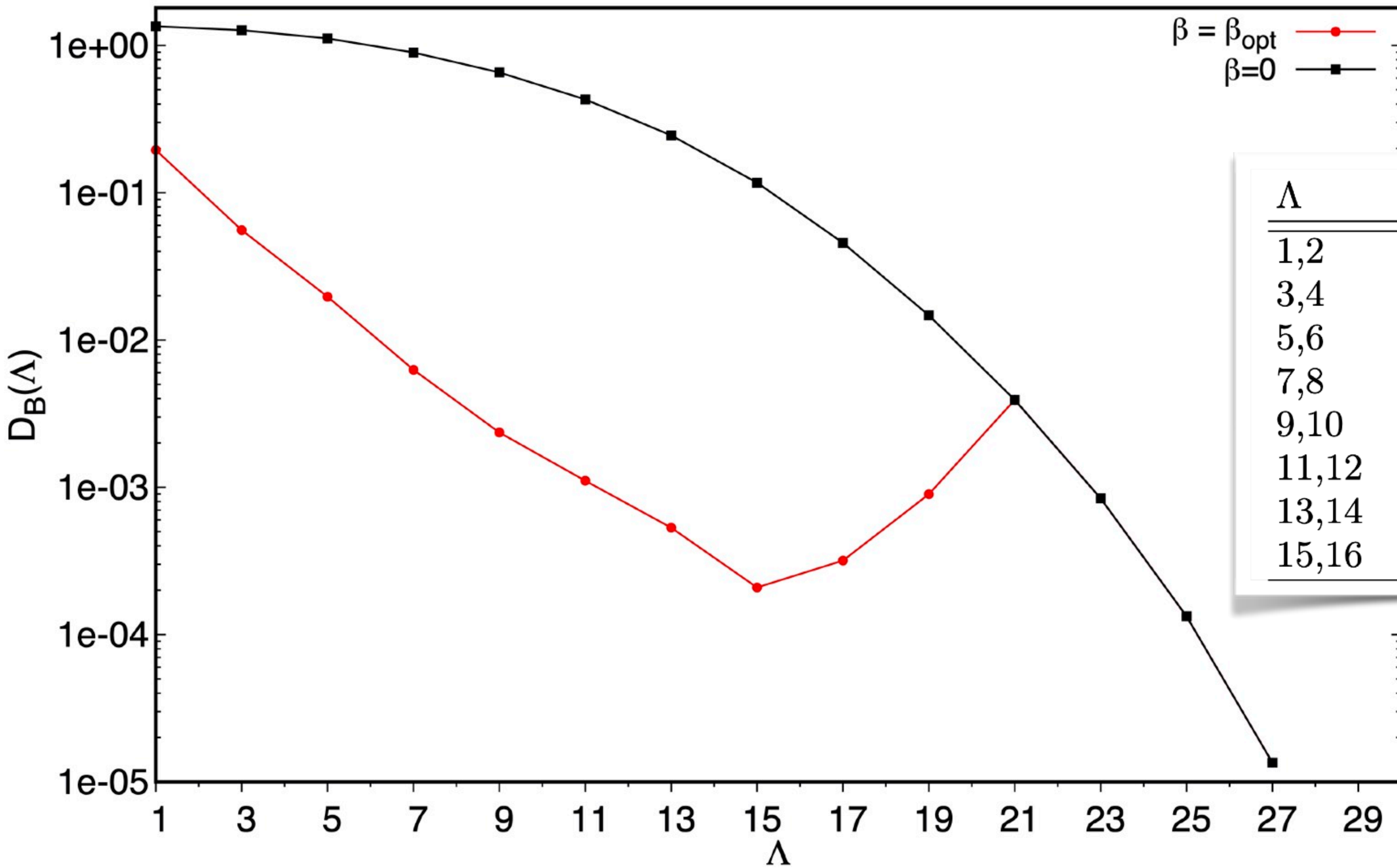
★ ***Wave function in the original basis (β=0) - convergence:***



The Lipkin-Meshkov-Glick Model in effective model space

★***Bures distance****

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

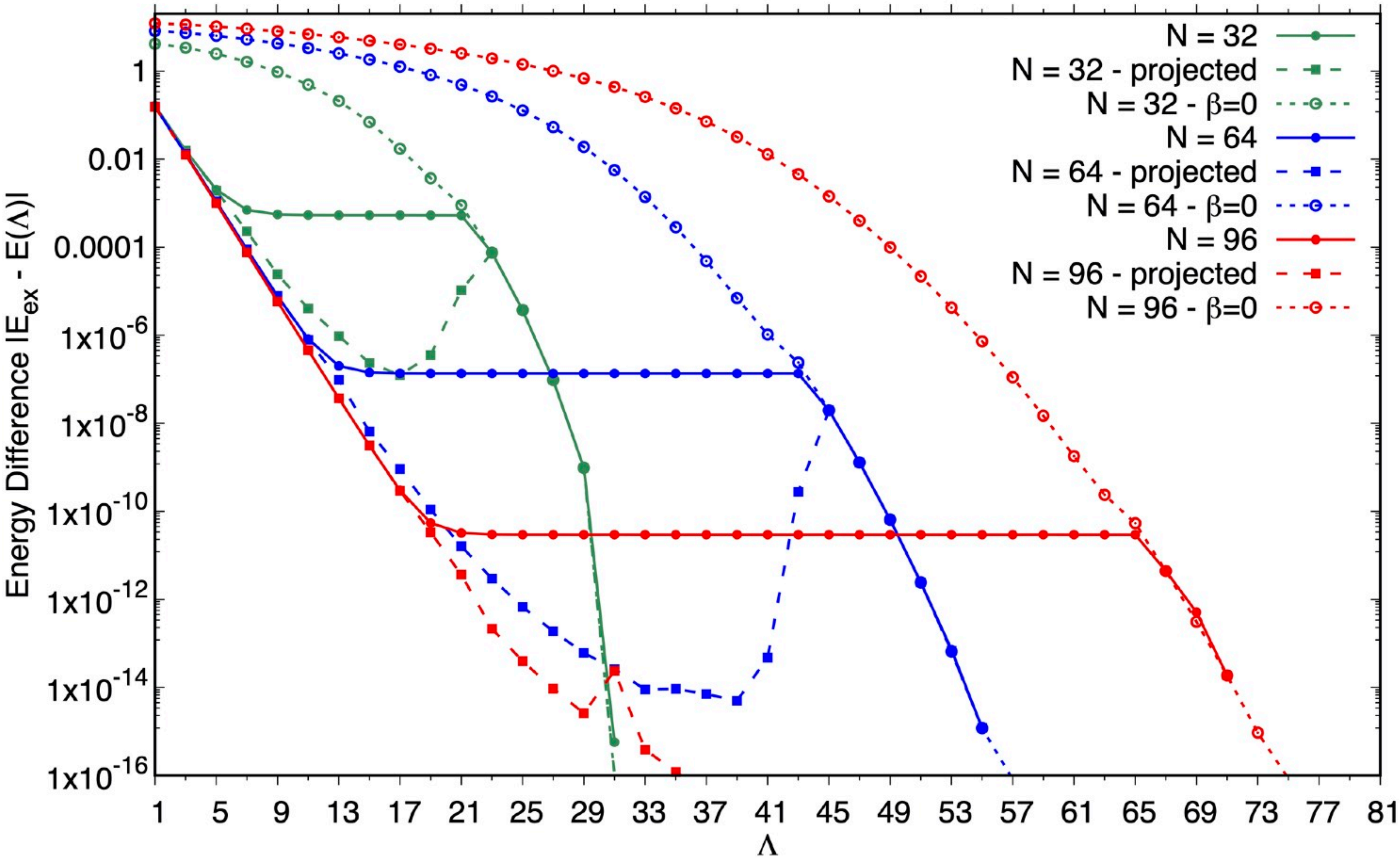


Λ	β	Λ	β
1,2	1.047	17,18	0.289
3,4	1.016	19,20	0.150
5,6	0.977	21,22	0.0
7,8	0.906	23,24	0.0
9,10	0.791	25,26	0.0
11,12	0.664	27,28	0.0
13,14	0.538	29,30	0.0
15,16	0.415	31	0.0

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

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

★ ***Implementation on a digital quantum computer:***

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

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

✳ 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 Λ-1 angles and can be implemented by unitary operators

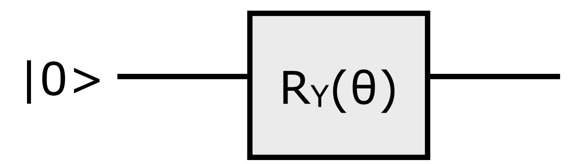
* see e.g. Klco and Savage *PRA* 99, 052335 (2019); *PRA* 102, 012612 (2020), …

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

Examples:

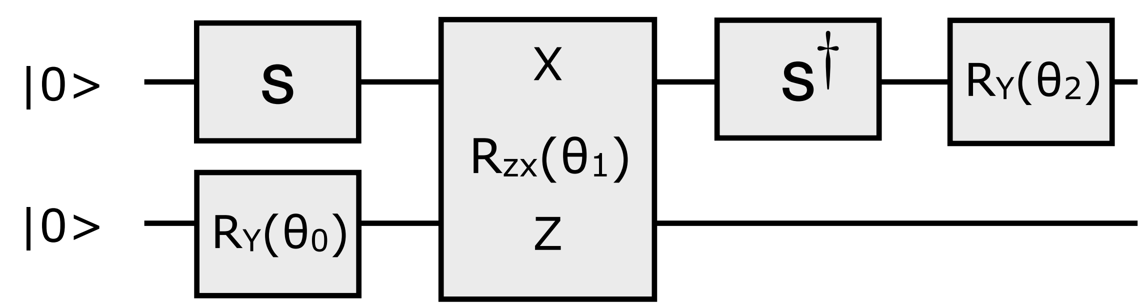
✳ 1 qubit ($\Lambda = 2$):

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



✳ 2 qubits ($\Lambda = 4$):

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



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

native IBM gate

→ replaces at least 3 CNOTs

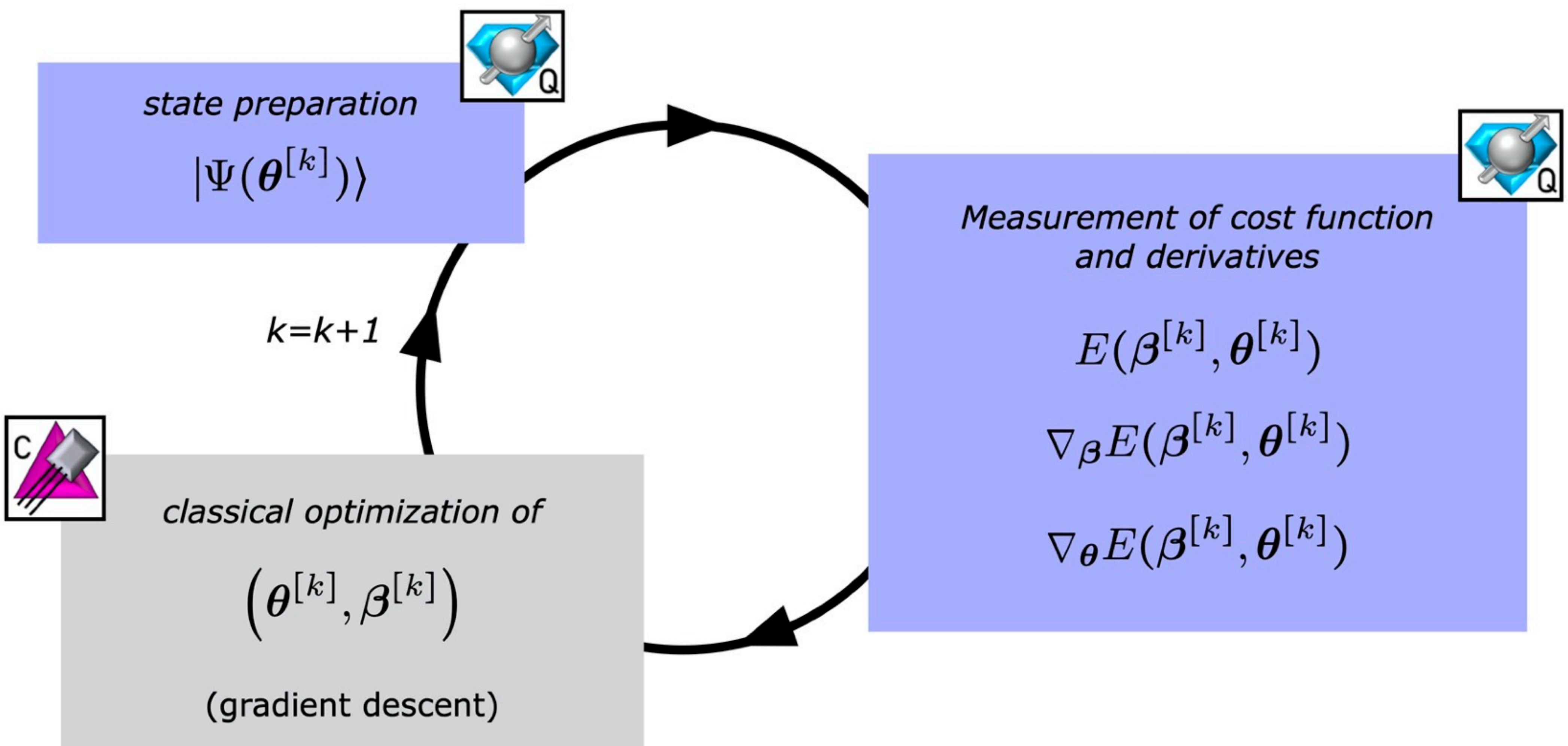
The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

★***Hamiltonian-Learning-VQE:***

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

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

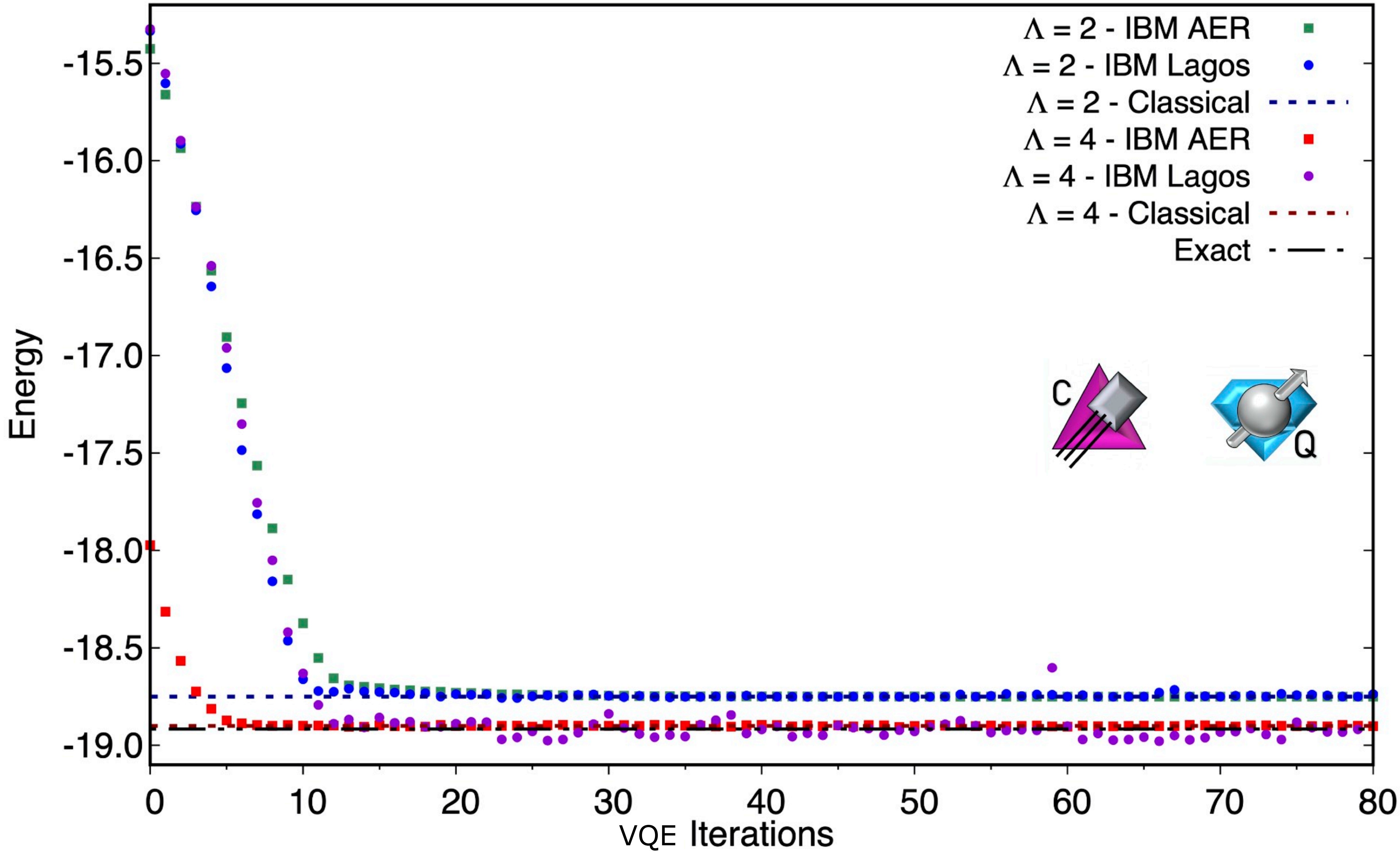
$$= \sum_{i_1,\ldots,i_{n_q}} h_{i_i,\ldots,i_{n_q}}(\beta) \, \langle \Psi(\boldsymbol{\theta}) | \overline{\sigma}_{i_1} \otimes \ \ldots \otimes \overline{\sigma}_{i_{n_q}} | \Psi(\boldsymbol{\theta}) \rangle$$



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

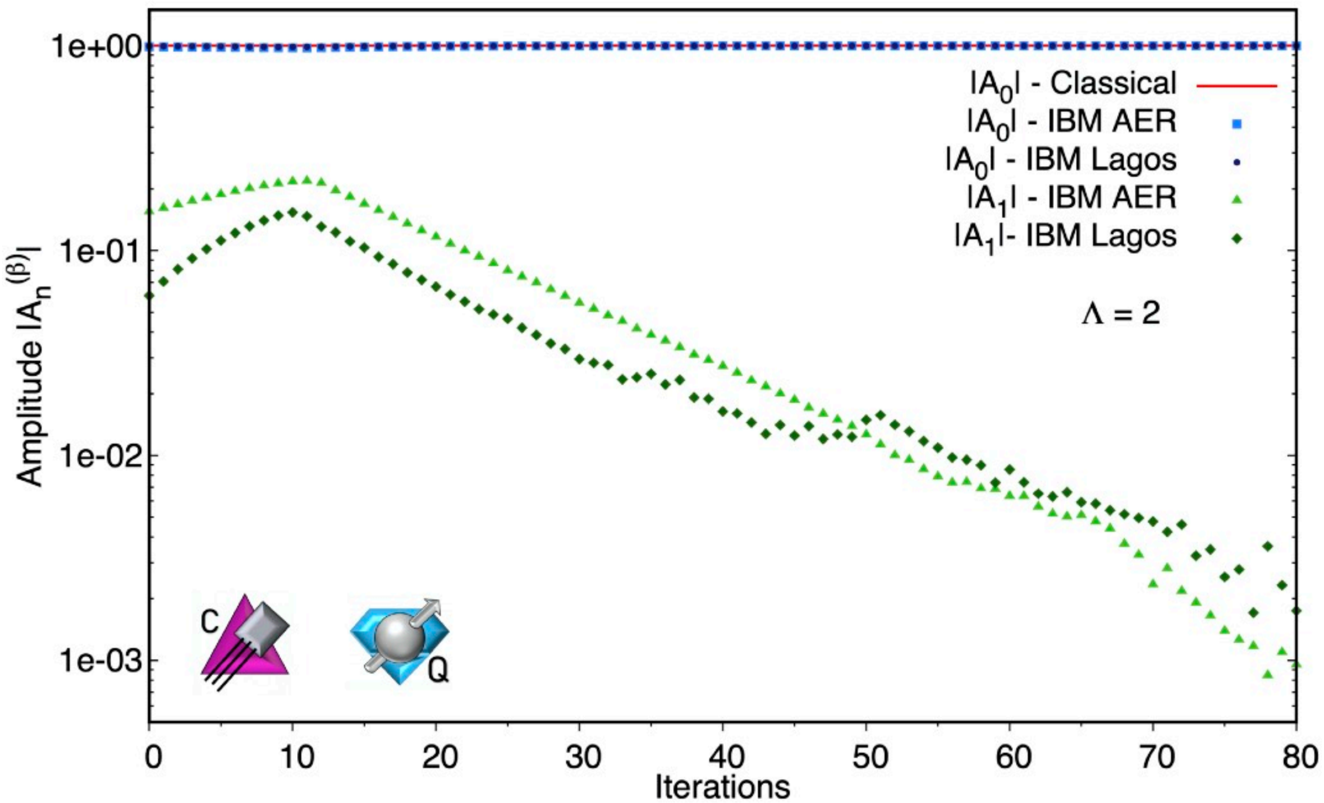
The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

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



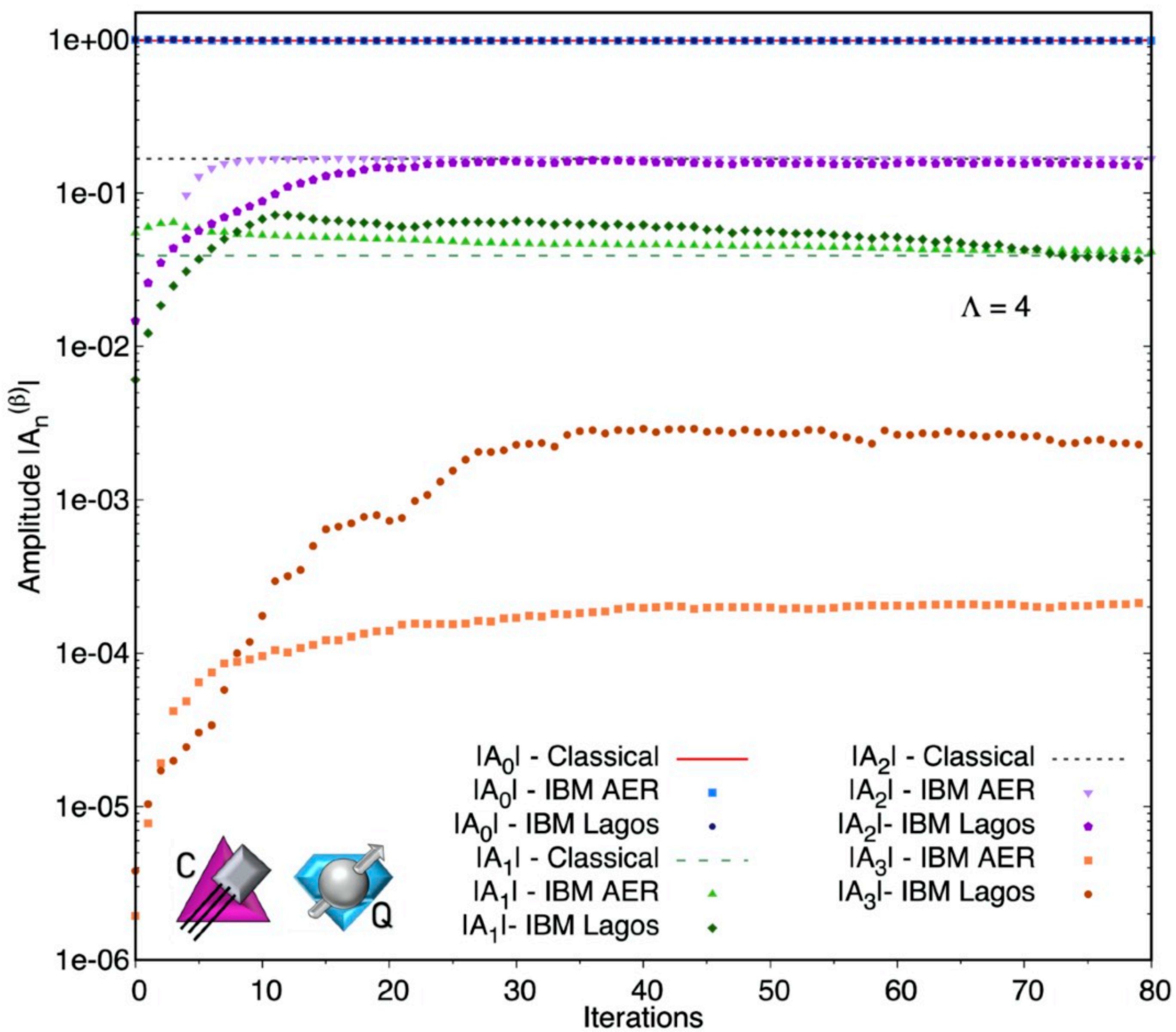
The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

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



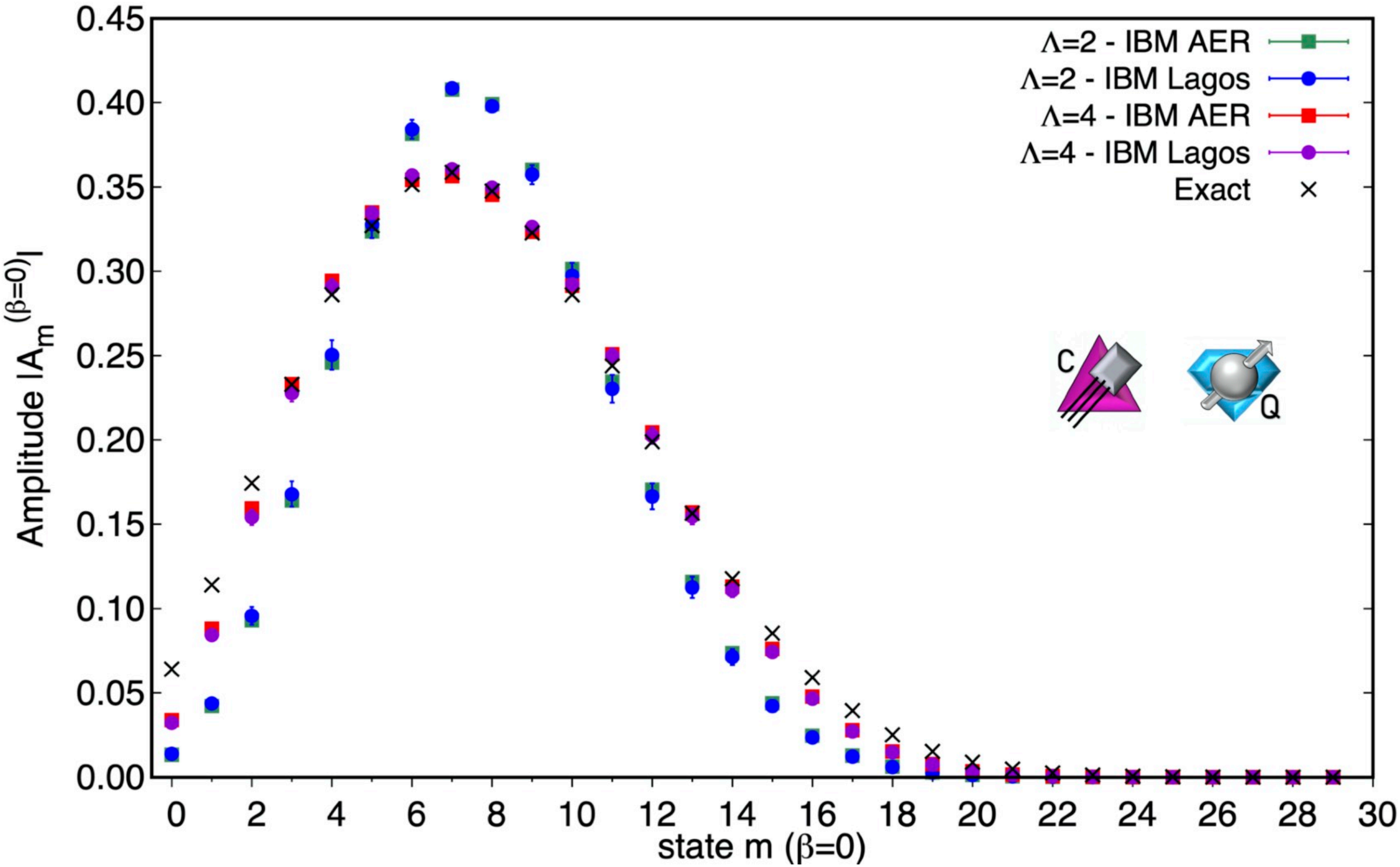
$$|\Psi\rangle = A_0|0\rangle + A_1|1\rangle$$

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



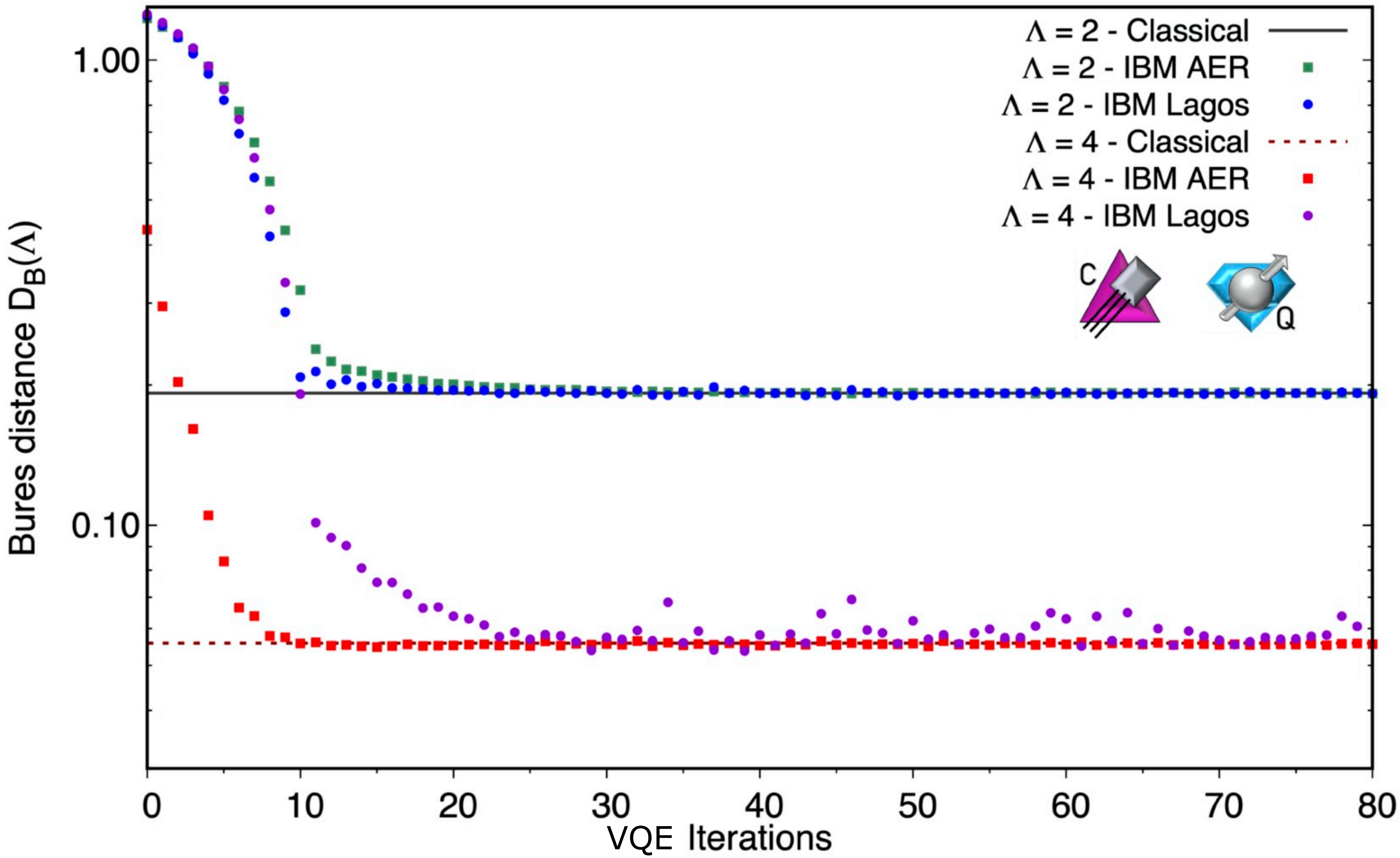
The Lipkin-Meshkov-Glick Model in effective space: Quantum Simulations

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



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

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



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 in the Hilbert space 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

UNIVERSITÄT BIELEFELD

GSI

European Research Council
Established by the European Commission

IQuS

UNIVERSITY of WASHINGTON

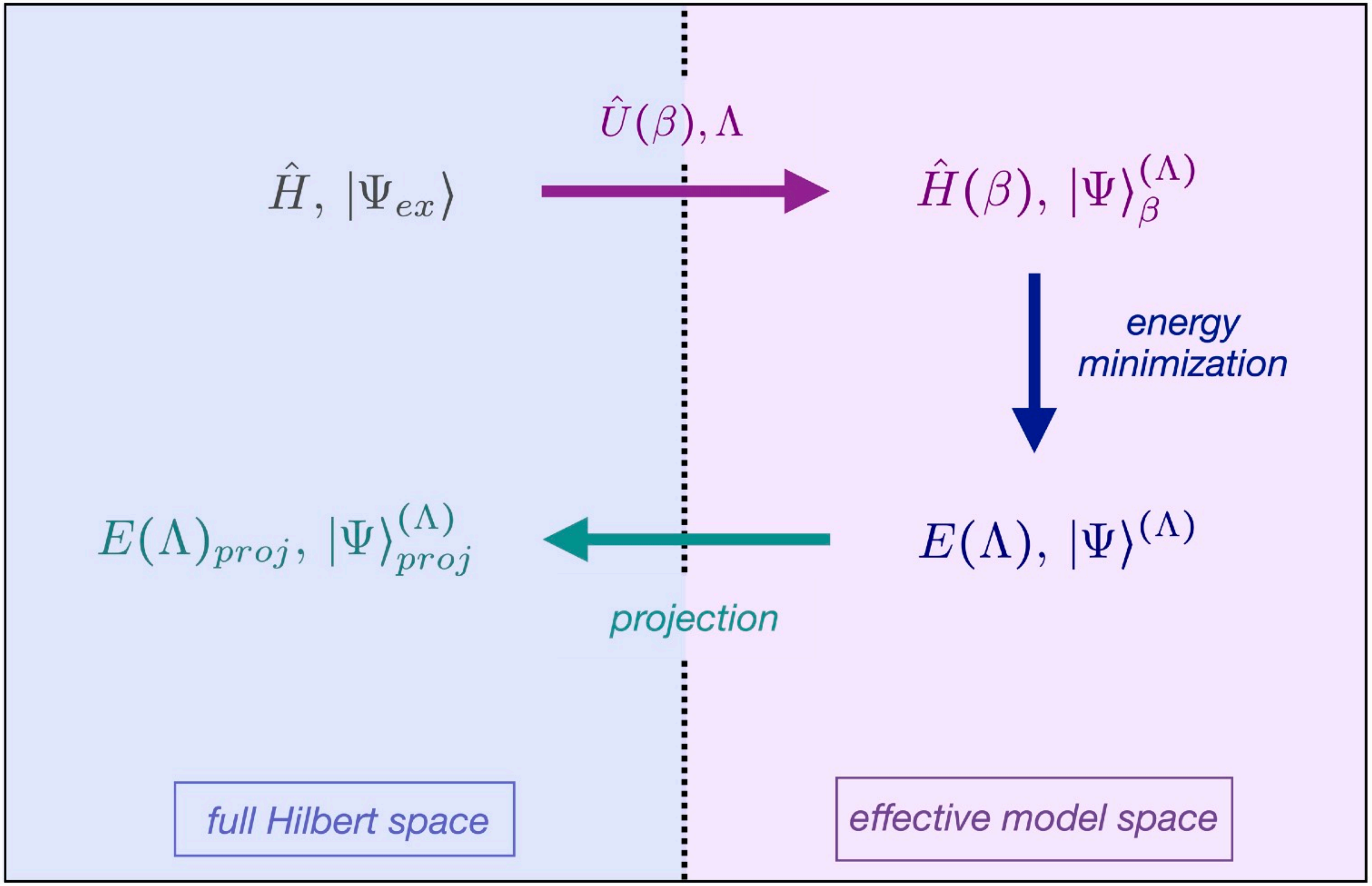
IBM Quantum

researcher program

for support

Backups

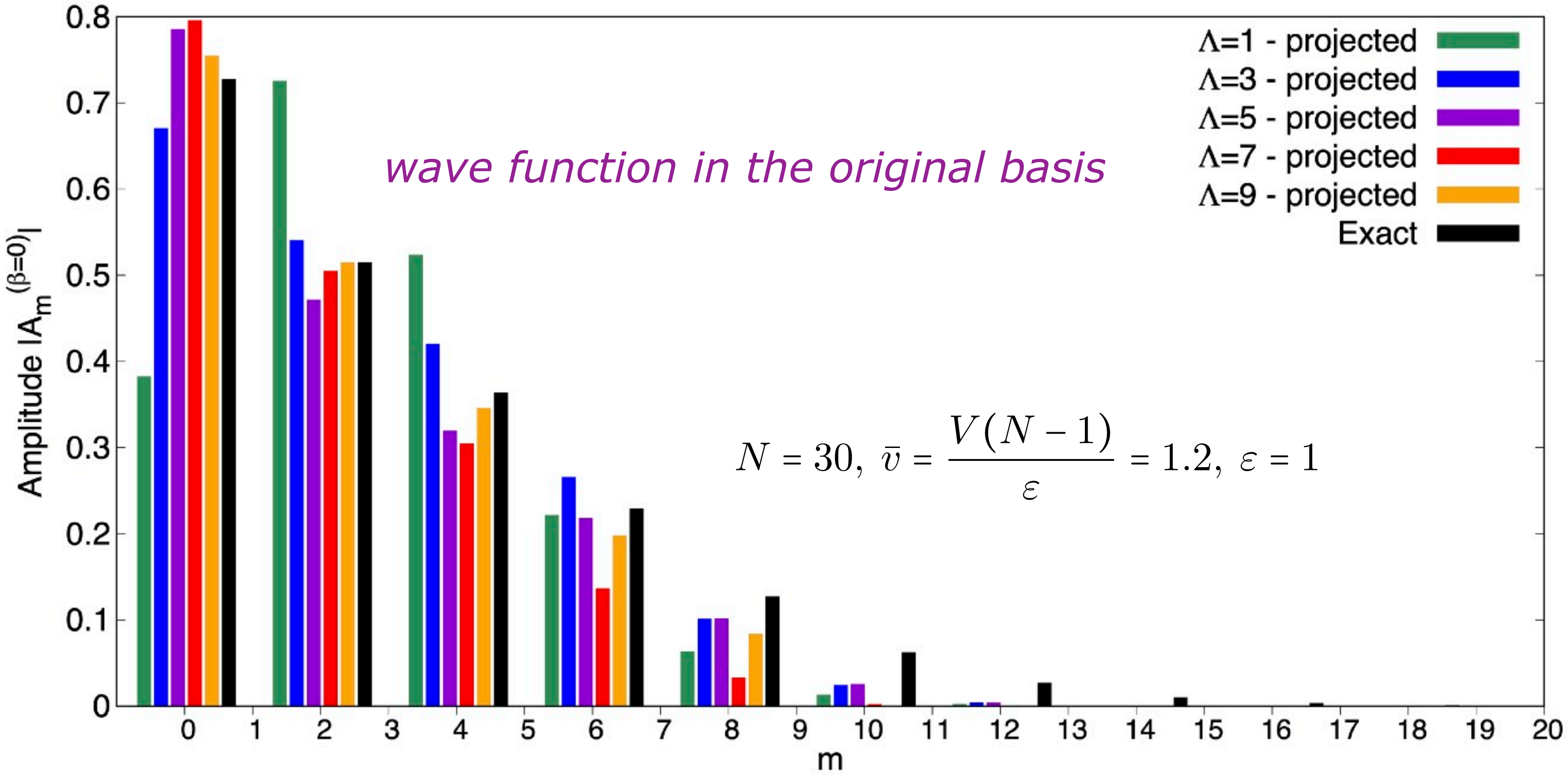
The Lipkin-Meshkov-Glick Model in effective model space



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

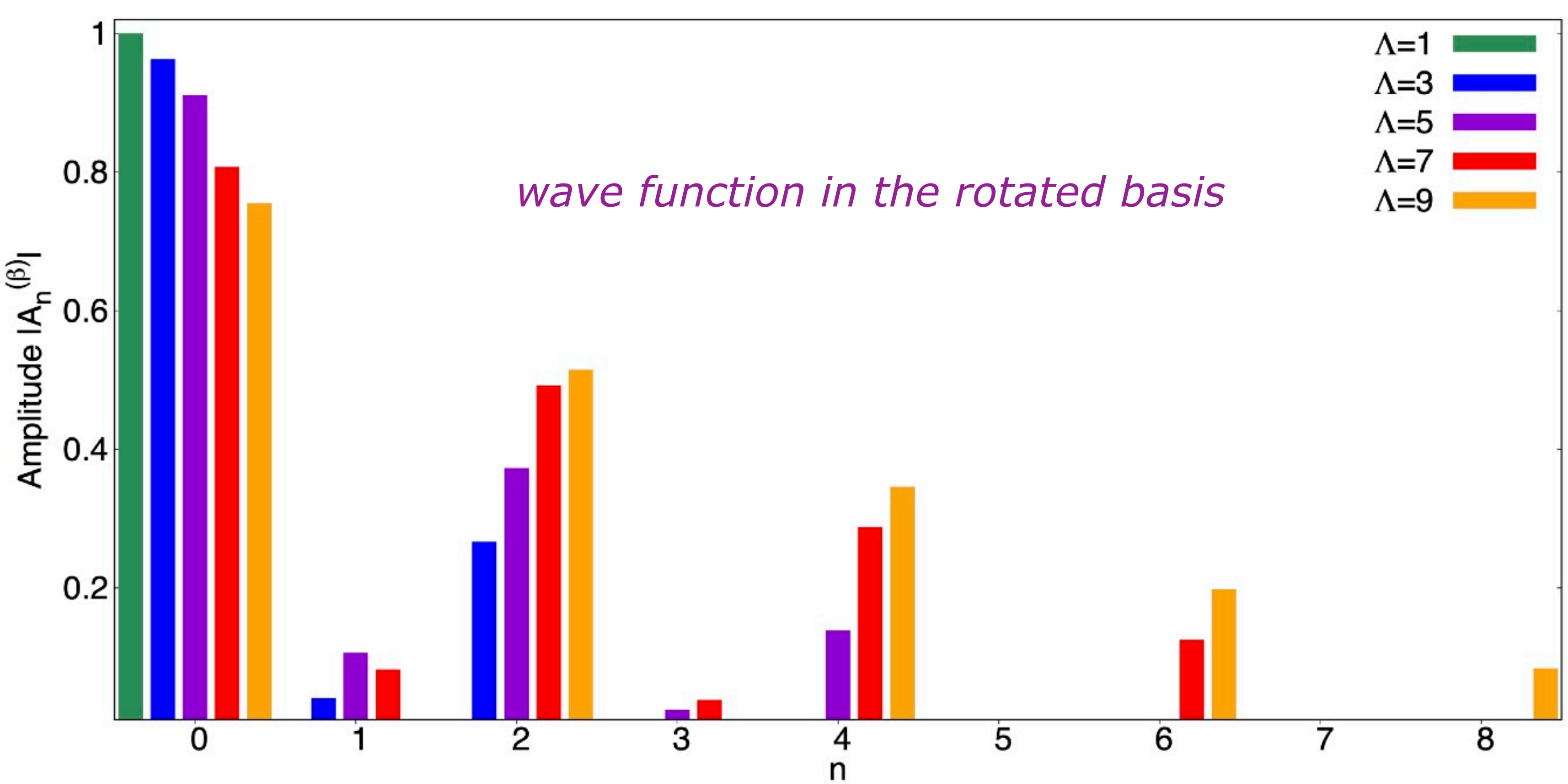
The Lipkin-Meshkov-Glick Model in effective model space

★***Near the phase transition:***



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

→ no "scale separation"



$$\Lambda = 1 \rightarrow \beta = 0.586$$
$$\Lambda = 3 \rightarrow \beta = 0.496$$
$$\Lambda = 5 \rightarrow \beta = 0.371$$
$$\Lambda = 7 \rightarrow \beta = 0.113$$
$$\Lambda = 9 \rightarrow \beta = 0.000$$

Multi-configuration self-consistent field method

$$|\Psi\rangle = \sum_{n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots} C_{n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots} |n_{\pi_1} n_{\pi_2} \ldots n_{\nu_1} n_{\nu_2} \ldots\rangle$$ **- truncated!**

Variational principle determines:

★ The expansion coefficients:

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

Large-scale diagonalization

to introduce explicit correlations in the truncated configuration space

★ The single-particle states:

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

Generalized mean-field equation

general mean field
(→ single-particle energies)

Source term
σ = two-body correlation matrix

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

One-nucleon density

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

(→ single-particle states)

⇒ "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:*

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

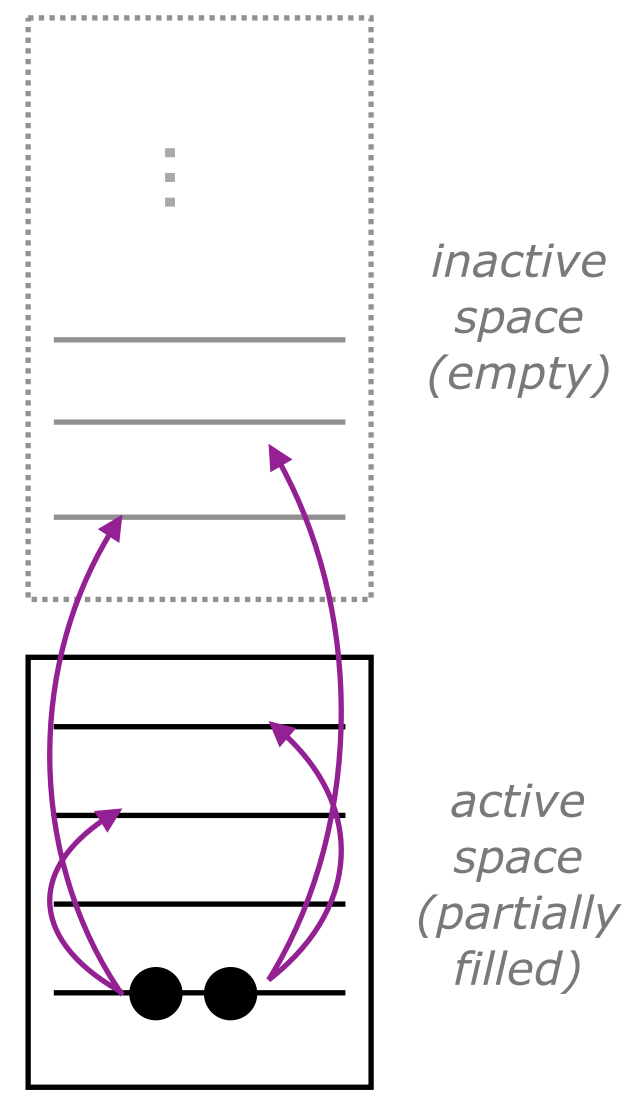
✳ *With variational orbital equation:*

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

Single-particle energies

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

∈ whole basis ∈ active space



⇒ coupling between active and inactive spaces

⇒ the density operator is modified

Multi-configuration self-consistent field method

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

starting point:
Harmonic Oscillator

Solve the 1st equation

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

⇒ Mixing coefficients $\{C_{\pi\nu}\}$

Calculation of the densities
and source term

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

$\Rightarrow G(\sigma)$

Solve the 2nd equation

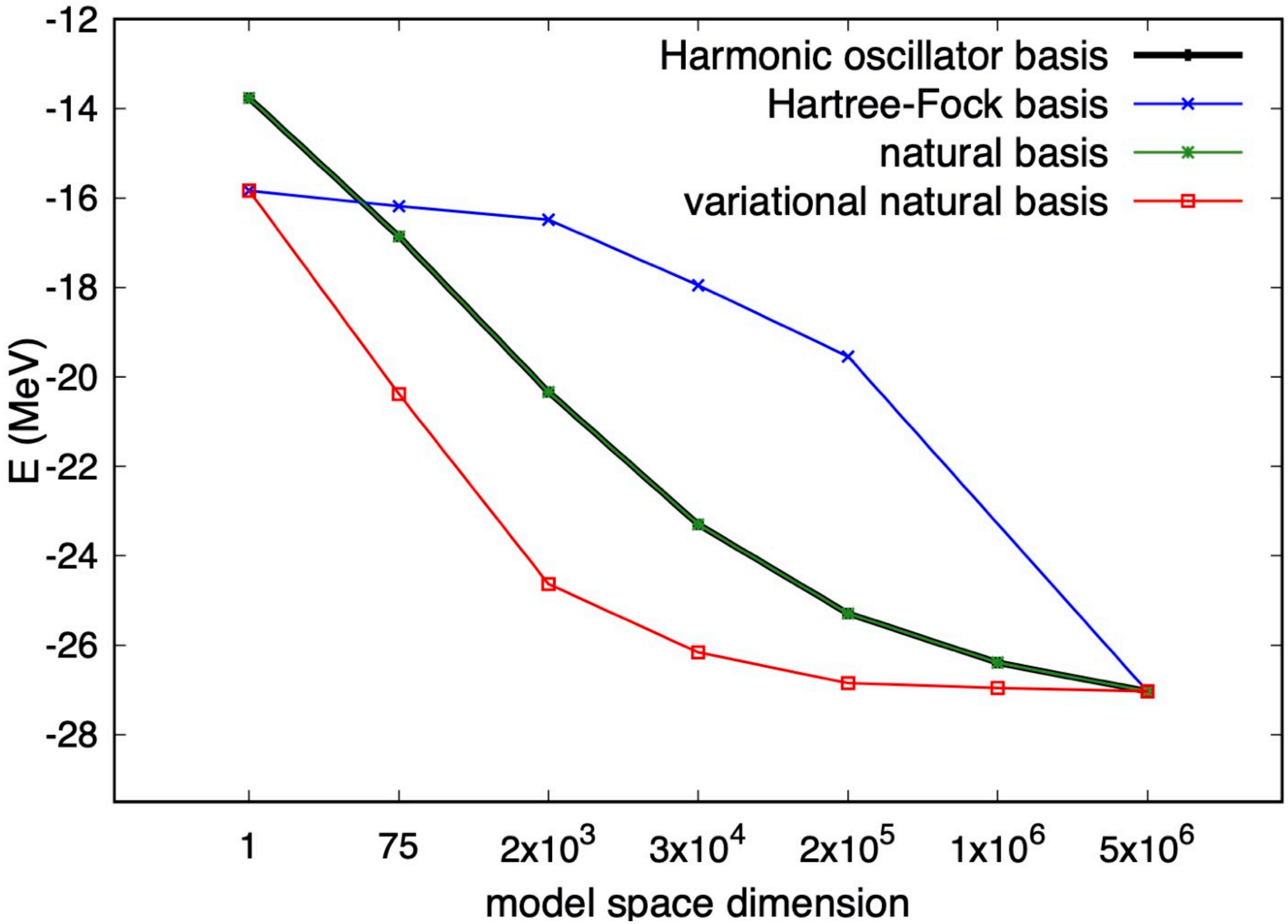
$$\left[\hat{h}(\gamma), \hat{\gamma}\right] = \hat{G}(\sigma)$$

⇒ single-particle orbitals $\{\varphi_i\}$

… until convergence

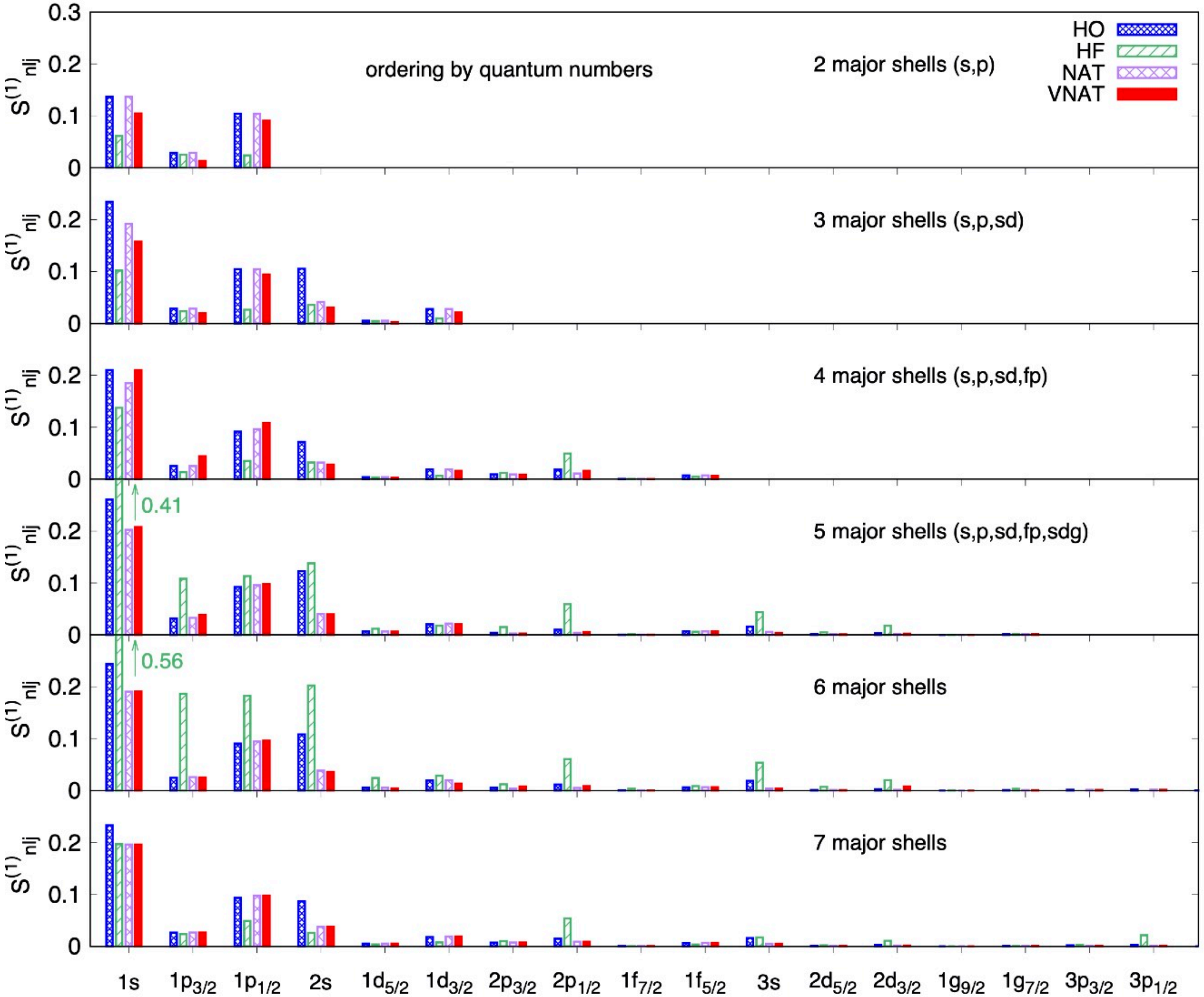
C.R., N. Pillet, D. Peña Arteaga & J.-F. Berger, PRC 93, 024302 (2016).

binding energy in ^{4}He



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*

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

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

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

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

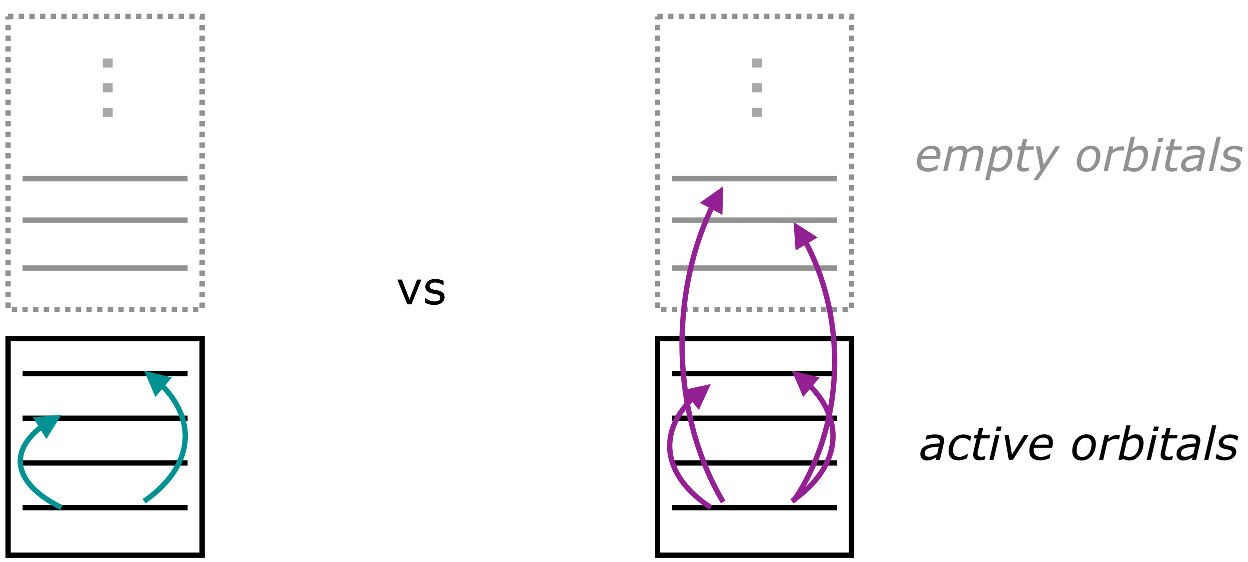
✳ *NAT & VNAT typically have similar entanglement patterns*

Two-orbital mutual information in ^{6}He

✳ ***Comparison NAT and VNAT bases:***

so far, similar entanglement patterns but different convergence of energy

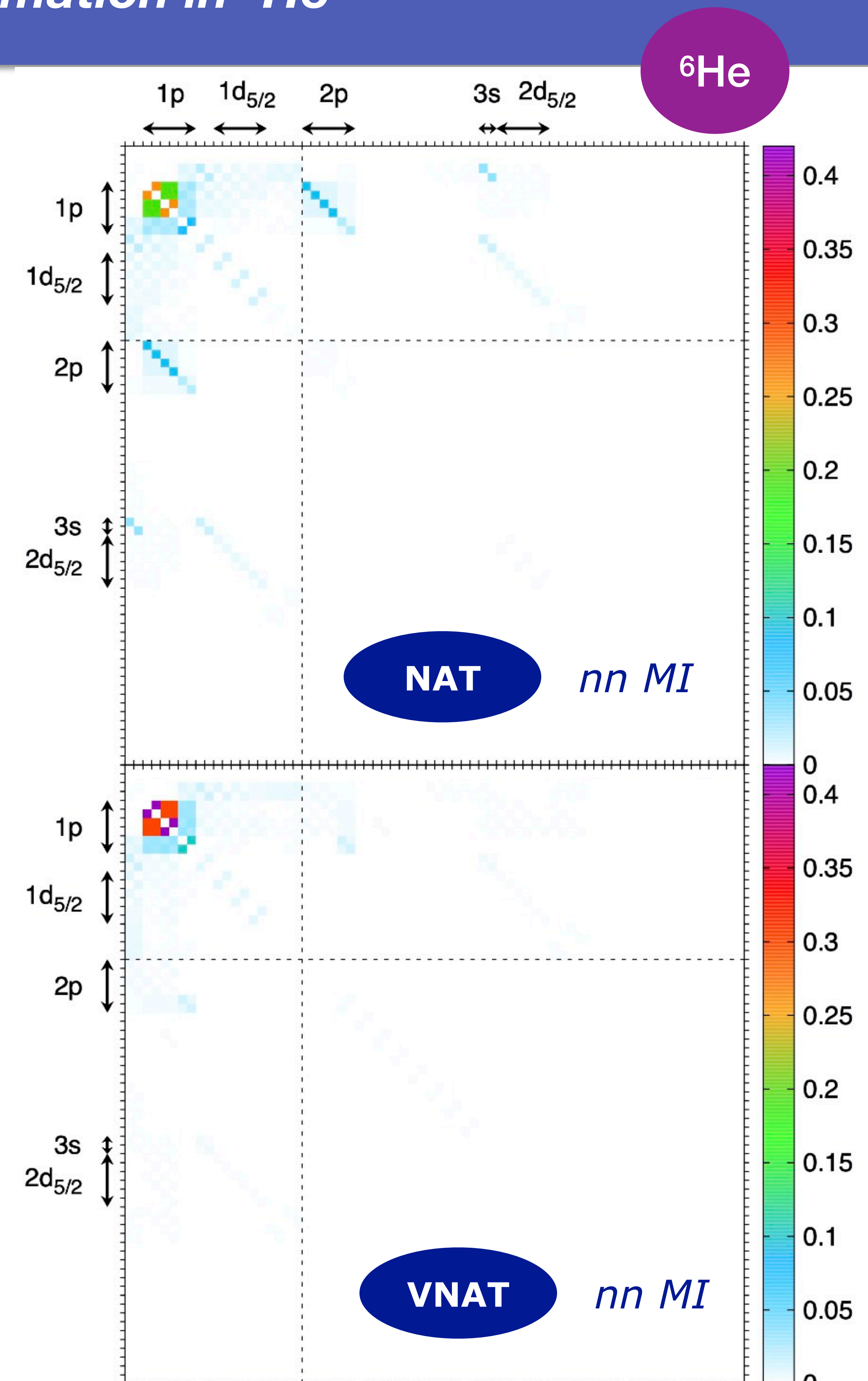
NAT basis mixes *active* HO states only
while
VNAT basis mixes the full basis



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

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

‣ *VNAT decouples inactive and active spaces*

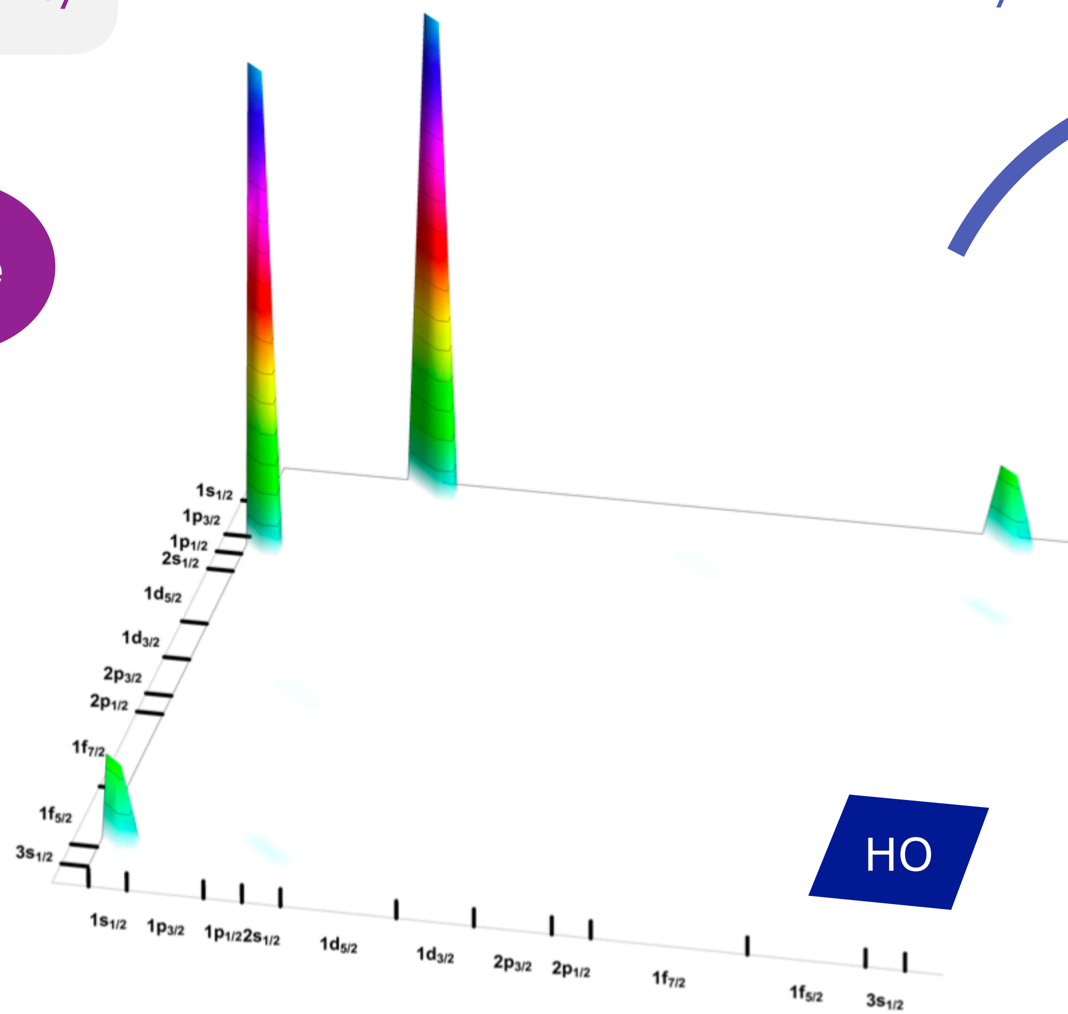


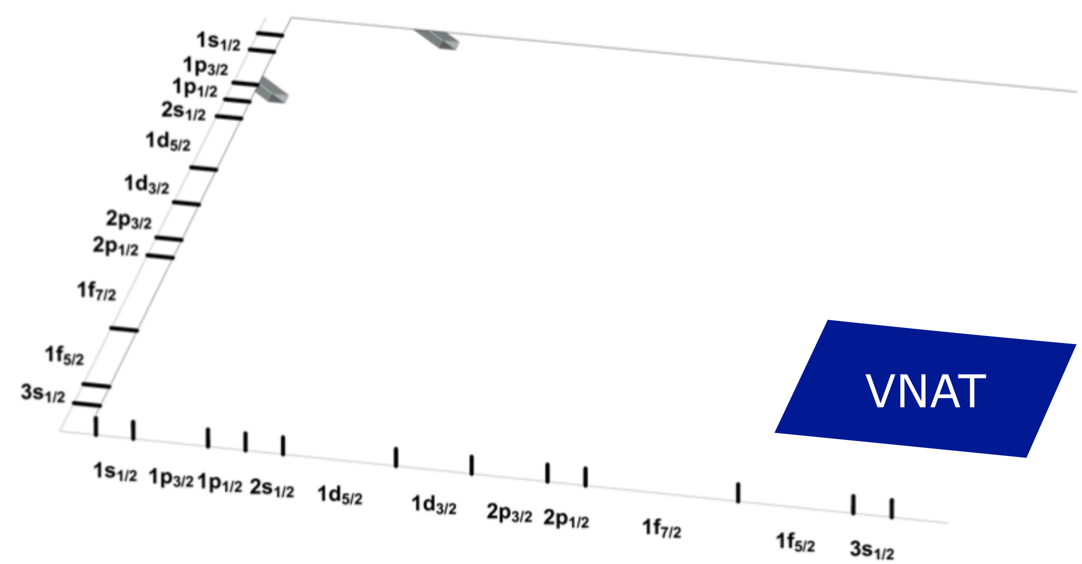
Two-orbital negativity in ^{4}He

- Negativity:

^{4}He

unitary transformations of modes





- *Negativity identically cancels in the (V)NAT basis because γ diagonal ➙ 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