Progress in Ab Initio Techniques in Nuclear Physics
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Self-consistent multiparticle-multihole configuration mixing method: first application to light nuclei with a chiral interaction

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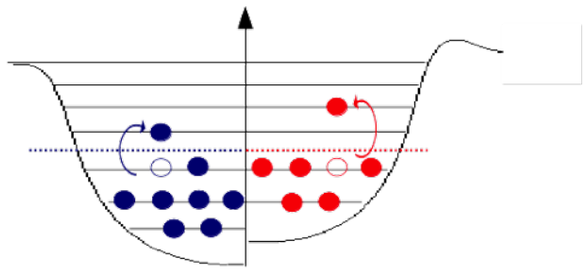
Introduction

Self-consistent Multiparticle-Multihole Configuration Mixing Method (SCMPMH):

★ Method already applied in atomic physics and quantum chemistry:

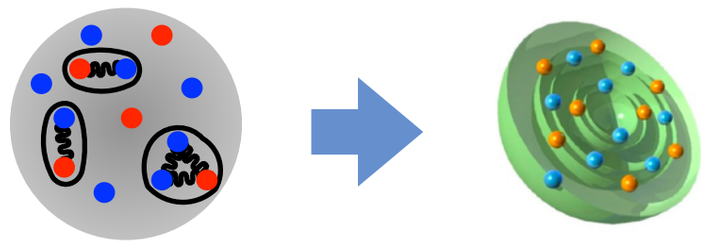
↠ Multi-Configuration Hartree-Fock (MCHF), Multi-Configuration Self-Consistent Field (MCSCF)

★ Based on the determination of a Configuration Interaction (CI) wave function ➡ allows:



- explicit symmetry preservations
  (particle number, spherical symmetry, Pauli principle),
- indiscriminate treatment of long-range correlations,
- treatment of ground and excited states in even-even, odd-even & odd-odd nuclei on the same footing.

★ The underlying mean-field and the single-particle states evolve with the correlations of the system



➡ **fully self-consistent approach**

Outline

- Formalism of the SCMPMH method

  → *role and interpretation of the orbital optimization*

- Numerical algorithm

- Previous applications with the Gogny force

  → *brief review*

- *Applications with interactions derived from chiral effective field theory*

  → *preliminary study of ^{4}He*

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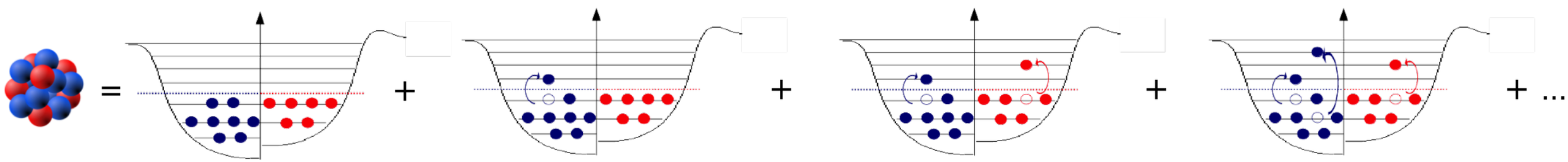
SCMPMH method: Formalism

✱ ***Trial wave function $|\Psi\rangle$ = superposition of Slater determinants***

$$|\Psi\rangle = A_{0p0h}|\Phi_{0p0h}\rangle + \sum_{1p1h} A_{1p1h}|\Phi_{1p1h}\rangle + \sum_{2p2h} A_{2p2h}|\Phi_{2p2h}\rangle + \sum_{3p3h} A_{3p3h}|\Phi_{3p3h}\rangle + \ldots$$



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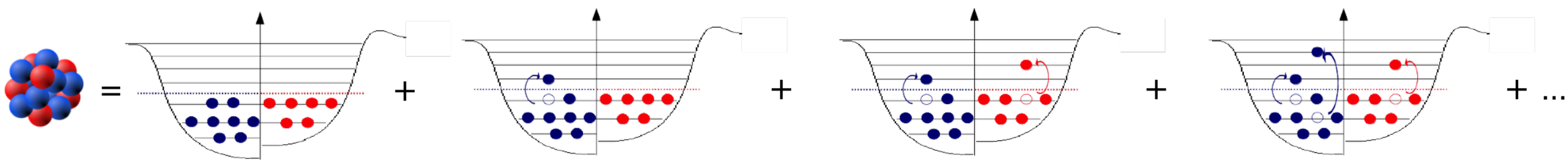

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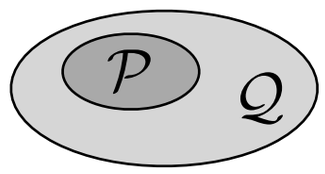
Factorial growth of the number of configurations $\Longrightarrow$ select the most relevant ones

Possible truncation schemes:

- *Core + Valence space*
- *Excitation order (Np-Nh)*
- *Excitation energy*
- *etc (symmetry-constrained)*

→ *defines subspace* $\mathcal{P}$ *of Hilbert space*

$\mathcal{H} =$ 

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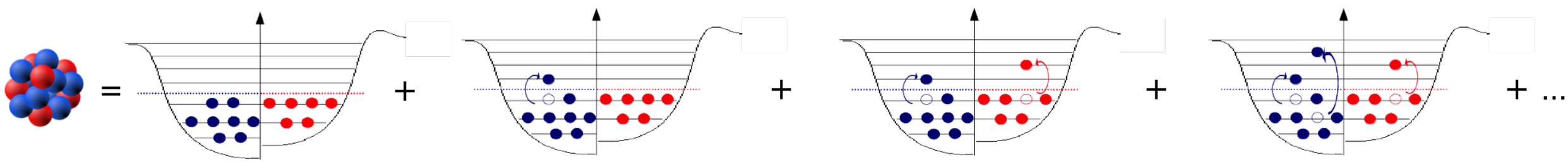

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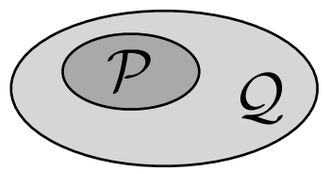
$\mathcal{H} =$ 

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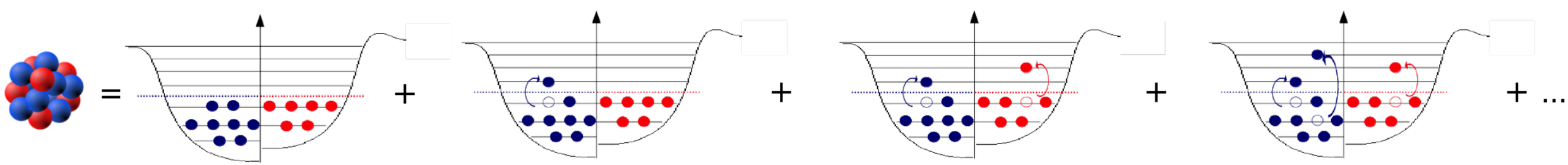

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Unknowns? $\left\{ \right.$ The mixing coefficients $\{A_\alpha\}$

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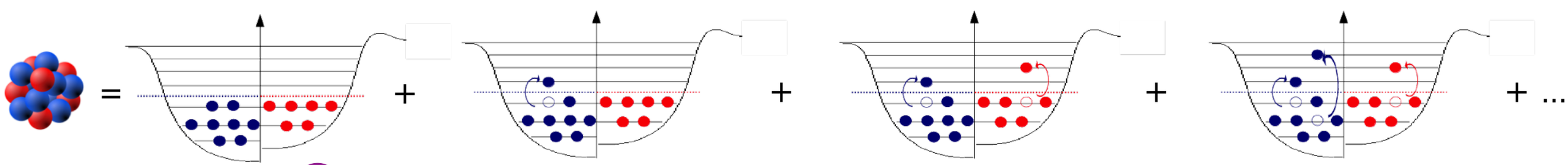

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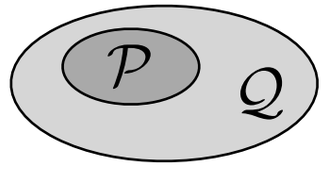
$\mathcal{H} =$ 

Unknowns? $\begin{cases} \text{The mixing coefficients } \{A_\alpha\} \\ \text{The single-particle states } \{\varphi_i\} \end{cases}$

SCMPMH method: Formalism

✱ ***Variational principle applied to the energy of the system:*** $\mathcal{E}[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle = 0$

➡ Two *coupled* equations to solve:

$$\begin{cases} \delta\mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \\ \\ \delta\mathcal{E}[\Psi]_{/\{\varphi^*_i\}} = 0 \end{cases}$$

Note: formalism shown here for a 2-body Hamiltonian

derivations for 2-body density-dependent or 3-body interaction available in *C.R., N. Pillet, D. Peña Arteaga & J.-F. Berger, PRC 93, 024302 (2016).*

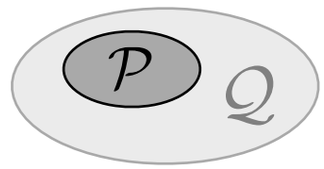
SCMPMH method: Formalism

Usual CI diagonalization

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

★ 1st variational equation: The mixing coefficients

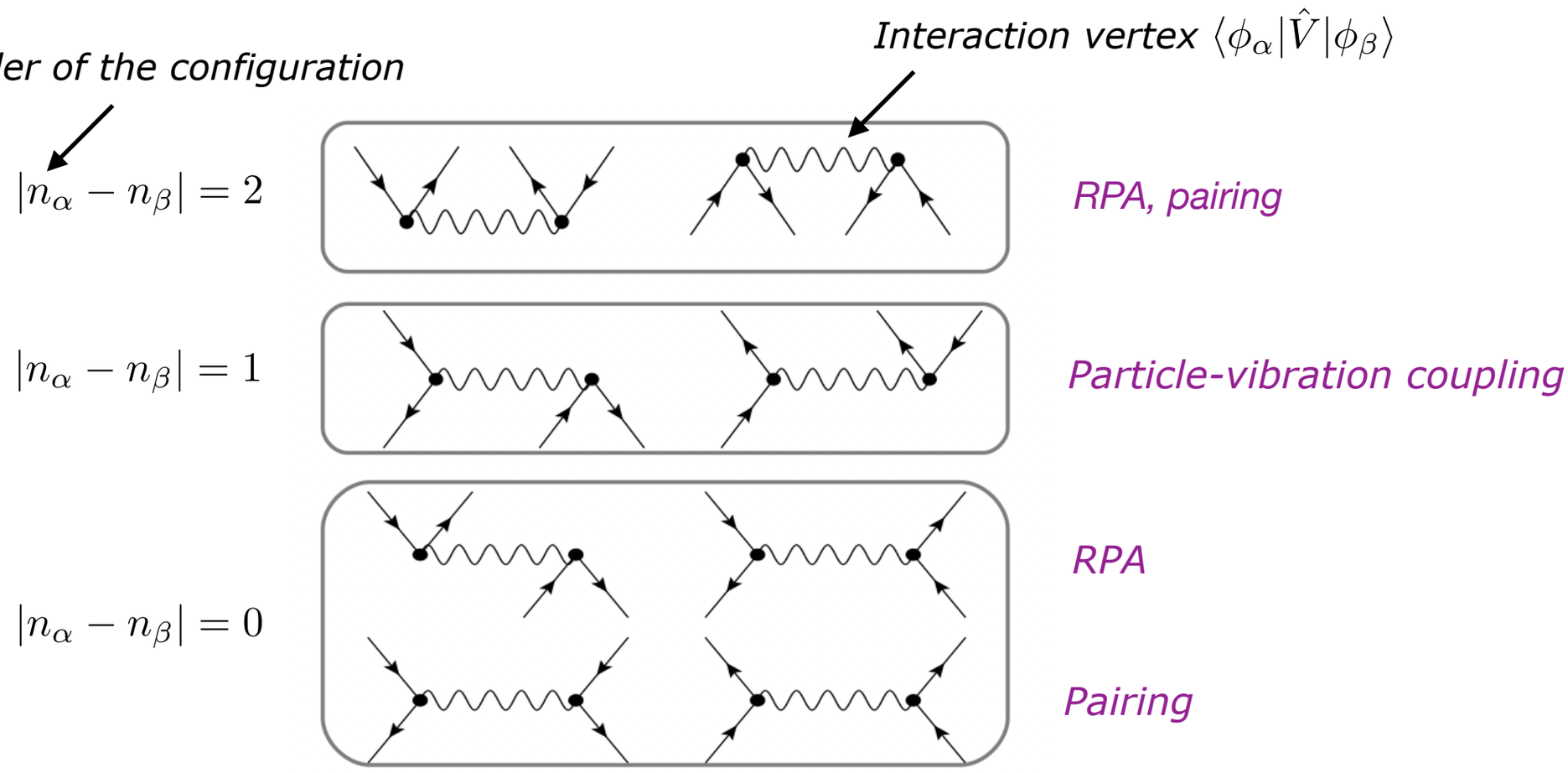
$$\delta \mathcal{E}[\Psi]_{/\{A^*_\alpha\}} = 0 \quad \Rightarrow \quad \sum_\beta A_\beta \langle \phi_\alpha | \hat{H} | \phi_\beta \rangle = E A_\alpha$$



➡ introduces explicit correlations in restricted configuration space $\mathcal{P}$
All types of long-range correlations are treated at the same time:

Excitation order of the configuration

Interaction vertex $\langle \phi_\alpha | \hat{V} | \phi_\beta \rangle$



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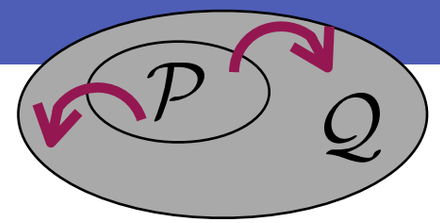

★ 2nd variational equation: The single-particle states

✦ variation of the single-particle states:

$$a_i^\dagger \to e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}} \quad \Rightarrow \delta a_i^\dagger = i\left[\hat{T}, a_i^\dagger\right]$$

T = hermitian 1-body operator

✦ 1st order variation of the many-body wave function:

$$\begin{aligned} |\delta\Psi\rangle &= i\hat{T}|\Psi\rangle_{\mathcal{P}} \\ &= |\delta\Psi\rangle_{\mathcal{P}} + |\delta\Psi\rangle_{\mathcal{Q}} \end{aligned}$$

↠ *Note:* $\delta\mathcal{E}[\Psi]_{/\{\varphi_i^*\}} = {}_{\mathcal{P}}\langle\Psi|H|\delta\Psi\rangle + \langle\delta\Psi|H|\Psi\rangle_{\mathcal{P}}$

$$= {}_{\mathcal{P}}\langle\Psi|\hat{P}\hat{H}\hat{P}|\delta\Psi\rangle_{\mathcal{P}} + {}_{\mathcal{P}}\langle\delta\Psi|\hat{P}\hat{H}\hat{P}|\Psi\rangle_{\mathcal{P}} + {}_{\mathcal{P}}\langle\Psi|\hat{P}\hat{H}\hat{Q}|\delta\Psi\rangle_{\mathcal{Q}} + {}_{\mathcal{Q}}\langle\delta\Psi|\hat{Q}\hat{H}\hat{P}|\Psi\rangle_{\mathcal{P}}$$

↠ the orbital optimization takes into account the coupling H_{PQ}/H_{QP} between P and Q spaces (however not H_{QQ})

$$\delta\mathcal{E}[\Psi]_{/\{\varphi_i^*\}} = \langle\Psi|\left[\hat{H}, \hat{T}\right]|\Psi\rangle = 0 \quad \Leftrightarrow \quad \left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma)$$

"Generalized Brillouin equation"

Generalized mean-field equation

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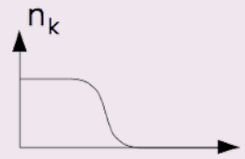
correlated one-body density

$$\rho_{ki} = \langle \Psi | a_i^\dagger a_k | \Psi \rangle$$

➡ "natural" basis

➡ occupation numbers



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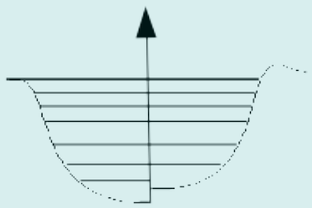
$$h_{ij}(\rho) = K_{ij} + \sum_{kl} \langle ik|\widetilde{V}|jl\rangle \rho_{lk}$$

contribution from particles & holes

➡ "canonical basis"

➡ single-particle energies



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= centroid of one-nucleon separation energies
= "most unambiguous definition of single-particle energies"

(Baranger (1970), Duguet & Hagen (2012)…)

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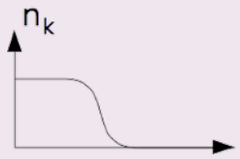

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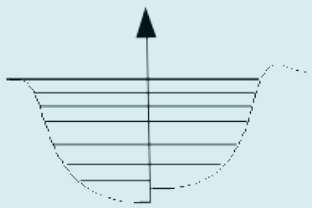

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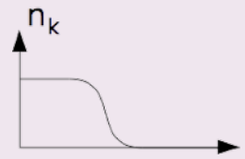

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$$G_{ij}(\sigma) = \frac{1}{2} \sum_{klm} \left(\widetilde{V}_{kmjl}\sigma_{kiml} - \widetilde{V}_{kiml}\sigma_{jlkm} \right)$$

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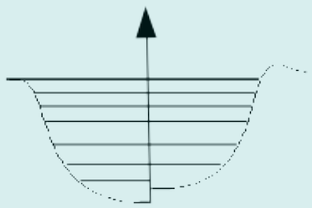

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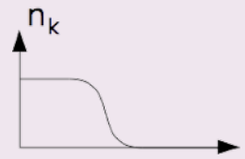

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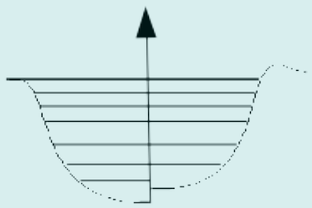

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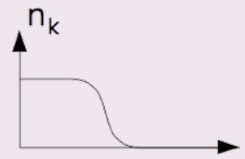

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the mean field h(ρ) is related to the energy while the density ρ contains information on the wave function
➡ choose eigenfunctions of ρ that satisfies the general mean field equation = "variational natural orbitals"

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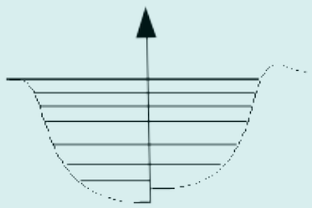

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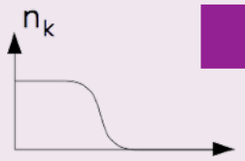

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$$\sigma_{kiml} = \langle \Psi|a_k^\dagger a_m^\dagger a_l a_i|\Psi\rangle - (\rho_{ik}\rho_{lm} - \rho_{im}\rho_{lk})$$

variational natural orbitals

Note: Because of the source term ➡ no common eigenbasis for h(ρ) and ρ ➡ which basis do we choose ?

the mean field h(ρ) is related to the energy while the density ρ contains information on the wave function
➡ choose eigenfunctions of ρ that satisfies the general mean field equation = "variational natural orbitals"

MPMH method: Formalism

★ ***Role of the orbital equation:***

I) Consistency between correlations and single-particle picture

General equation in physics:

Equation of motion for the one-body Green's function (at equal times)

$\Rightarrow$ $\boxed{[h(\rho), \rho] = G(\sigma)}$ $\Rightarrow$

1-body GF $\mathcal{G}^{(1)}$ — Connected 2-body GF $\mathcal{G}^{(2)}_C$

Dressing of the one-body propagator

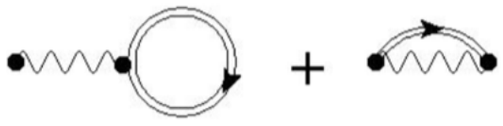
—

equivalent to solving a Dyson equation

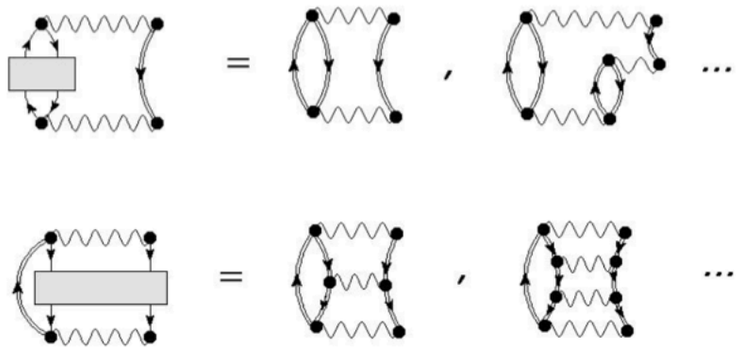
Self-energy: $\Sigma(t_1 - t_2) = \Sigma^{(0)}\delta(t_1 - t_2) + \Sigma^{(dyn)}(t_1 - t_2)$

Static part — Dynamical part

- $\Gamma_{ij}(\rho) = \sum_{kl} \langle ik|\widetilde{V}|jl\rangle \rho_{kl} = \Sigma^{(0)}_{ij}$



- $G(\sigma) = \lim_{t_2 \to t_1^+} \int dt \left[\mathcal{G}^{(1)}(t - t_2), \Sigma^{(dyn)}(t_1 - t)\right]$



➡ full consistency between mean-field and correlations, which is important to have a fully variational theory

(see e.g. "*Quantum Theory of Finite systems*" by Blaizot and Ripka)

SCMPMH method: Formalism

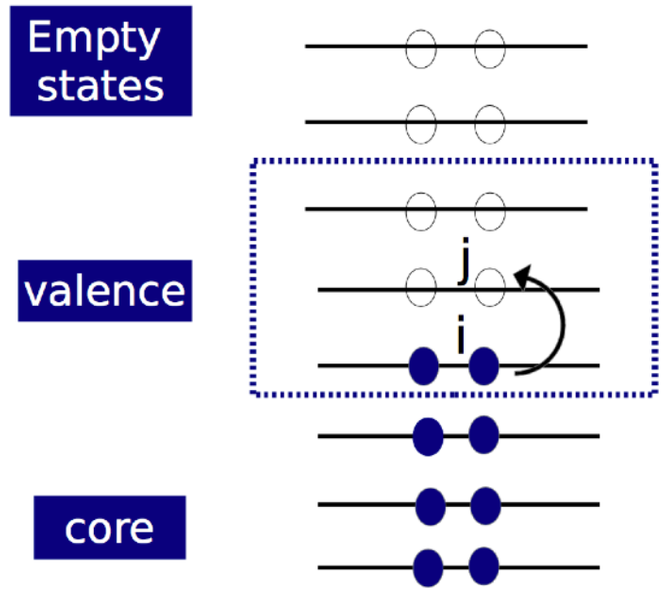
★ ***Role of the orbital equation:***

II) Partial compensation of the truncation P/Q

- Ex: truncation core/valence space

→ Without orbital equation:

$$\rho_{ij} \begin{cases} = \delta_{ij} \text{ if } i,j \in \text{core} \\ \in [0,1] \text{ if } i,j \in \text{valence} \\ = 0 \text{ otherwise} \end{cases}$$



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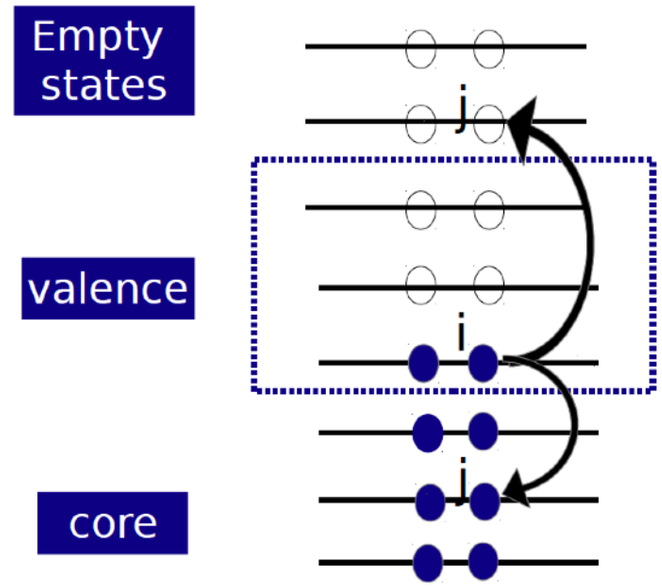


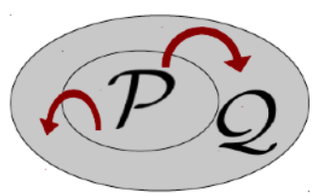
→ With orbital equation:

$$\left[h[\rho], \rho\right] = G[\sigma] \Rightarrow \rho_{ij} = \frac{G_{ij}[\sigma]}{\varepsilon_i - \varepsilon_j}$$

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 ∈ valence



⇒ coupling between valence space and rest of the basis.

Outline

- ✦ Formalism of the MPMH method

  → *role and interpretation of the orbital optimization*

- ✦ Numerical algorithm

- ✦ Previous applications with the Gogny force

  → *brief review*

- ✦ *Applications with interactions derived from chiral effective field theory*

  → *preliminary study of ^{4}He*

SCMPMH method: Numerical algorithm

The full solution requires a doubly-iterative algorithm:

starting point:
Harmonic Oscillator
or
Hartree-Fock
orbitals

Solve the 1st equation

$$\begin{pmatrix} & H & \end{pmatrix} \begin{pmatrix} A \end{pmatrix} = \lambda \begin{pmatrix} A \end{pmatrix}$$

$\Rightarrow$ Mixing coefficients $\{A_\alpha\}$

Calculation of the densities and source term

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

$\Rightarrow G(\sigma)$

Solve the 2nd equation

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

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

... until convergence

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

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The full solution requires a doubly-iterative algorithm:

Solve the 2nd equation:

$$\left[\hat{h}(\rho), \hat{\rho}\right] = \hat{G}(\sigma) \Leftrightarrow \left[\hat{h}(\rho) - \hat{Q}(\rho, \sigma), \hat{\rho}\right] = 0$$

New "correlation field"

In the natural basis $\hat{\rho}|\mu\rangle = n_\mu|\mu\rangle$

$$\begin{cases} Q_{\mu\nu}(\rho,\sigma) = \dfrac{G_{\mu\nu}(\sigma)}{n_\mu - n_\nu} \text{ , if } n_\mu \neq n_\nu \\ Q_{\mu\nu}(\rho,\sigma) = 0 \text{ , otherwise.} \end{cases}$$

⇒ self-consistent single-particle states $\{\varphi_i\}$ = eigenfunctions of h-Q and ρ

⇒ *non-linear problem ⇒ iterative solution:*

orbitals $\{\varphi^{(0)}\}$ density $\rho^{(0)}$ *(from 1st eq.)* → $h(\rho^{(0)}) - Q(\rho^{(0)}, \sigma)$ → orbitals $\{\varphi^{(1)}\}$ density $\rho^{(1)}$ → $h(\rho^{(1)}) - Q(\rho^{(1)}, \sigma)$ → ...

→ *until convergence* → *Back to the 1st equation…*

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

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$\Rightarrow G(\sigma)$

Solve the 2nd equation

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

$h(\rho) - Q(\rho, \sigma)$ $\quad\leftrightarrow\quad$ $\rho, \{\varphi_i\}$

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

... until convergence

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

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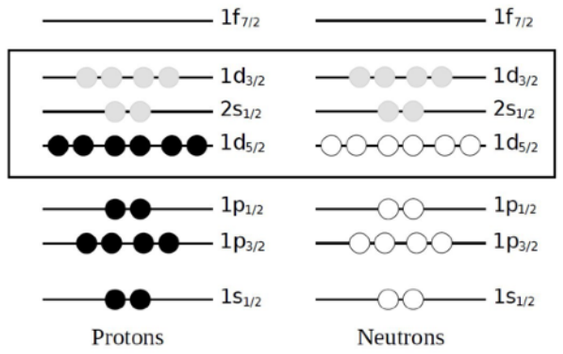
Previous applications with the Gogny force

- *Even-even sd-shell nuclei*

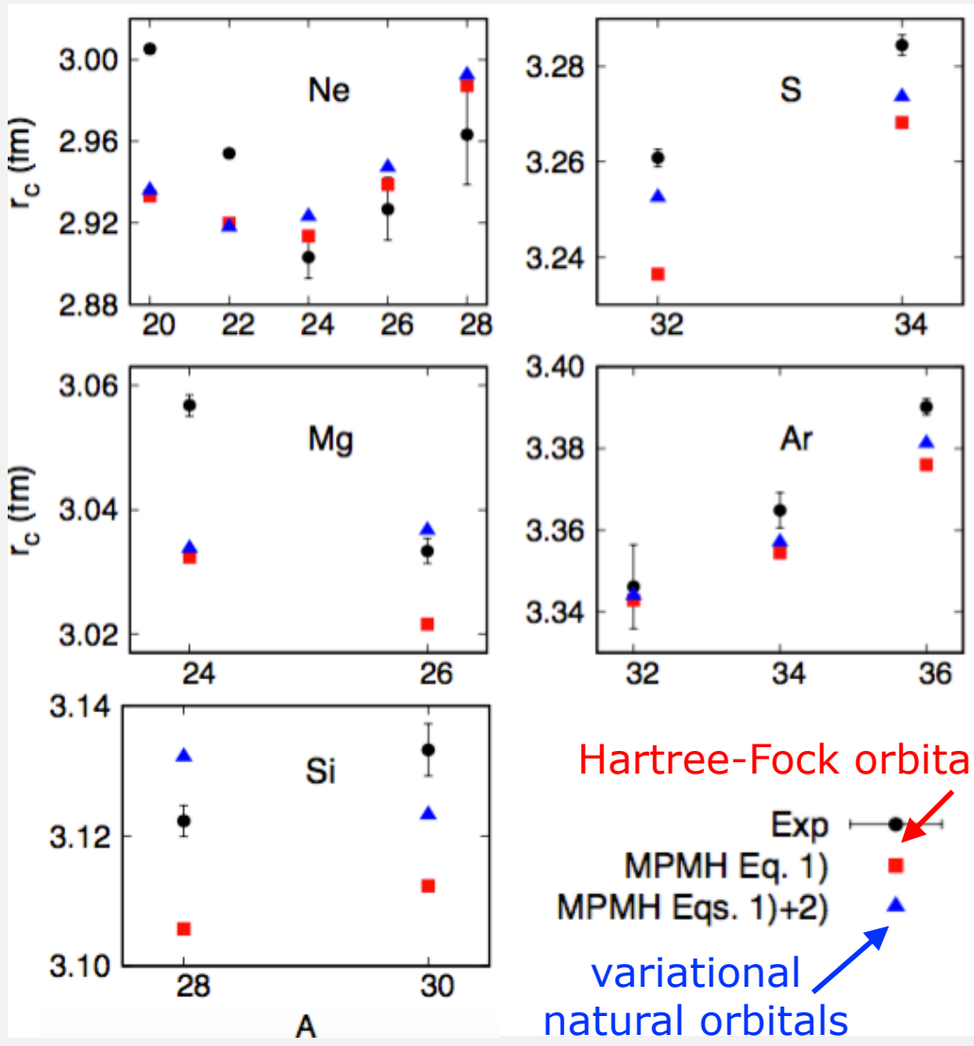
$$10 \leqslant (Z, N) \leqslant 18$$

- *truncation scheme:*
core of ^{16}O + valence space



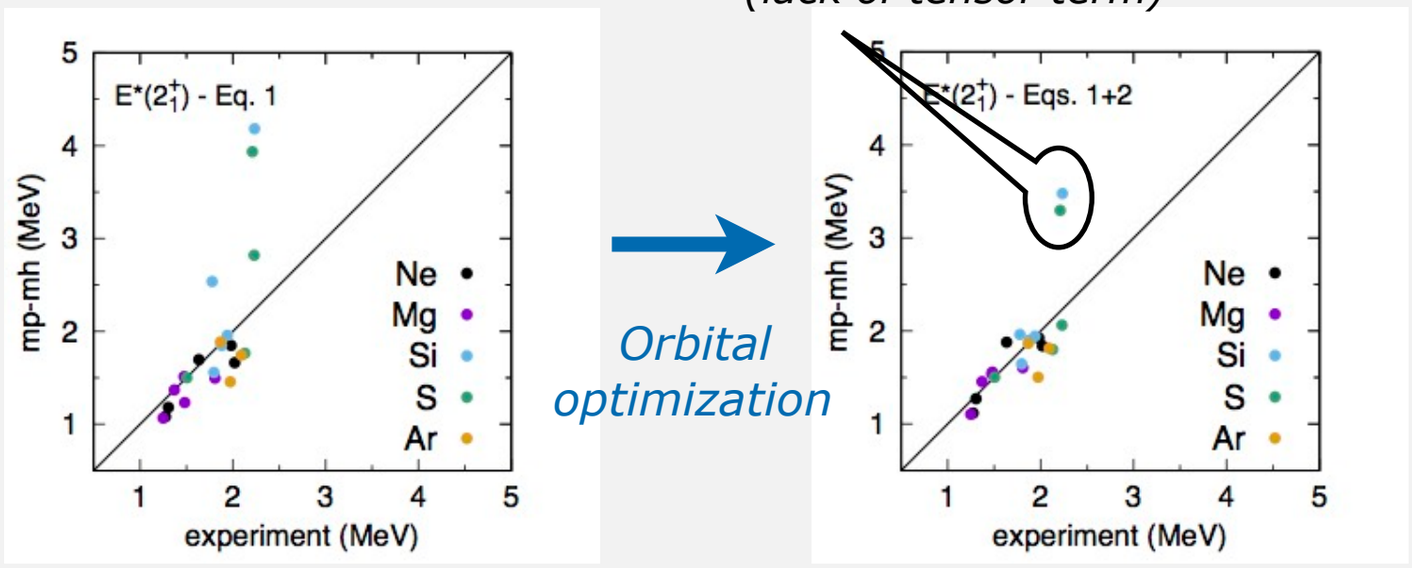
Calculation of many observables
→ How are they impacted by the optimization of orbitals?

✳ Charge radii



✳ Excitation energies

T=0 component of the Gogny force
(lack of tensor term)



Orbital optimization

$$\left.\begin{aligned}\langle \Delta E^* \rangle &= 226 \text{ keV} \\ \sigma(\Delta E^*) &= 214 \text{ keV}\end{aligned}\right\}$$

^{30}S & ^{30}Si excluded

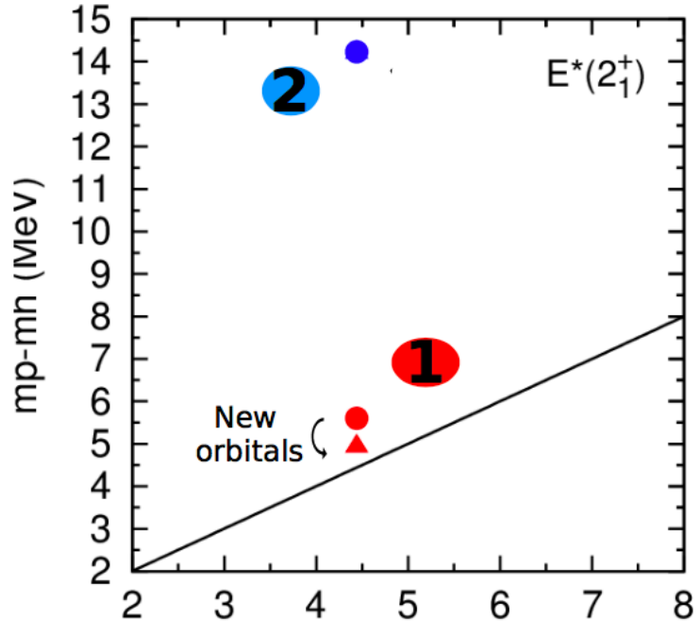
$$\left\{\begin{aligned}\langle \Delta E^* \rangle &= 142 \text{ keV} \\ \sigma(\Delta E^*) &= 122 \text{ keV}\end{aligned}\right.$$

*C.R. et al. Phys. Rev. C, **93**, 024302 (2016) and Phys. Rev. C **95**, 044315 (2017)*

Previous applications with the Gogny force

✱ Encouraging results… but:

- ✦ The D1S Gogny interaction is in principle not adapted (double counting of correlations…), and
- ✦ can lead to divergent behaviors when enlarging the valence space due to the zero-range spin-orbit and ρ-dependent terms.



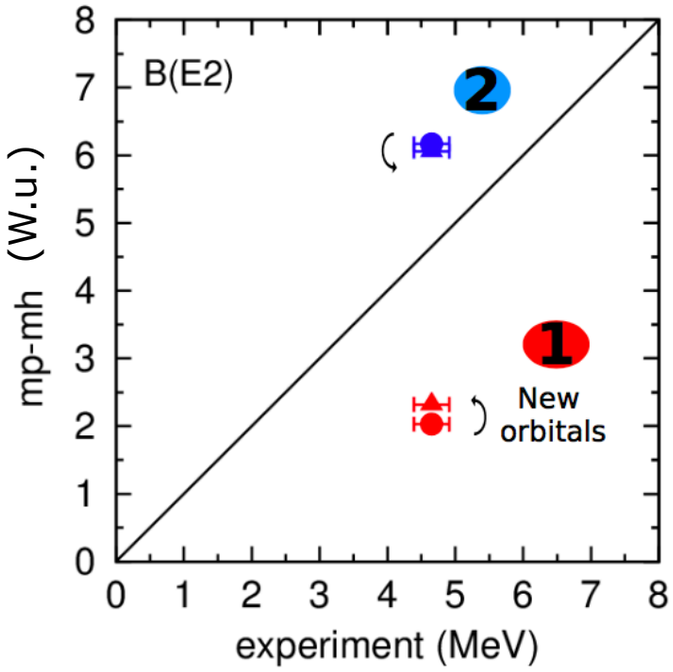
See e.g. study of ^{12}C:

1 0ħω space

collectivity ✗,excitation energies ✓, overbinding ~ 6 MeV

2 Nħω space (no core, up to 4p-4h)

collectivity ✓, excitation energies ✗, overbinding ~ 60 MeV!



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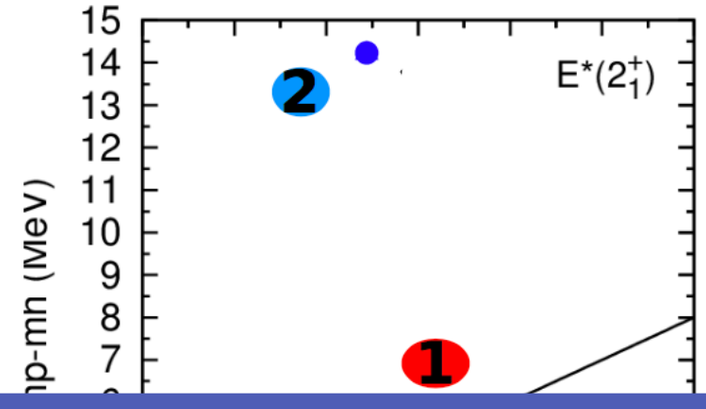


➡ ***Need a better suited interaction***

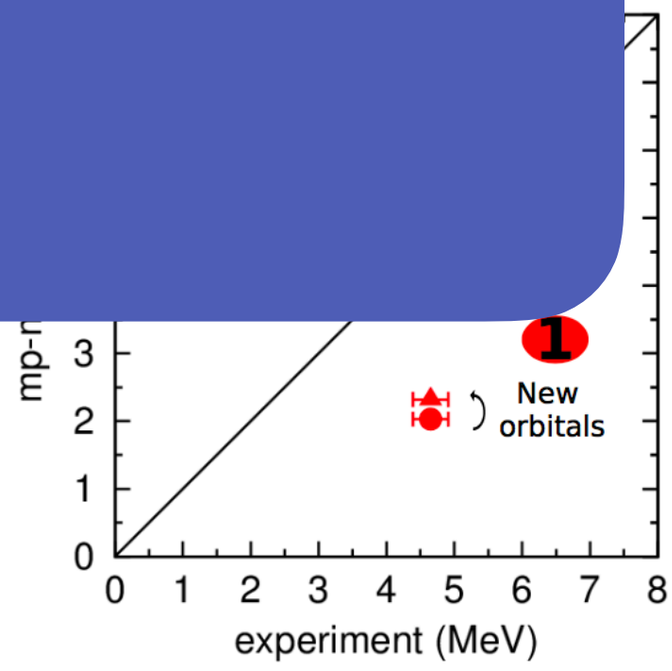
- ***Generalized Gogny interaction: fully finite-range, with tensor, better constrained*** (see e.g. Chappert, Pillet, Girod, Berger PRC 91, 034312 (2015) for D2 interaction with finite-range density dependence)

or

- ***interaction derived from chiral EFT (here)***

2 Nħω space (no core, up to 4p-4h)

collectivity ✓, excitation energies ✗, overbinding ~ 60 MeV!



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Test application to ^{4}He with a chiral interaction

✱ ***Binding energy: convergence with respect to the model space***

N2LO$_{OPT}$ interaction (2-body only)

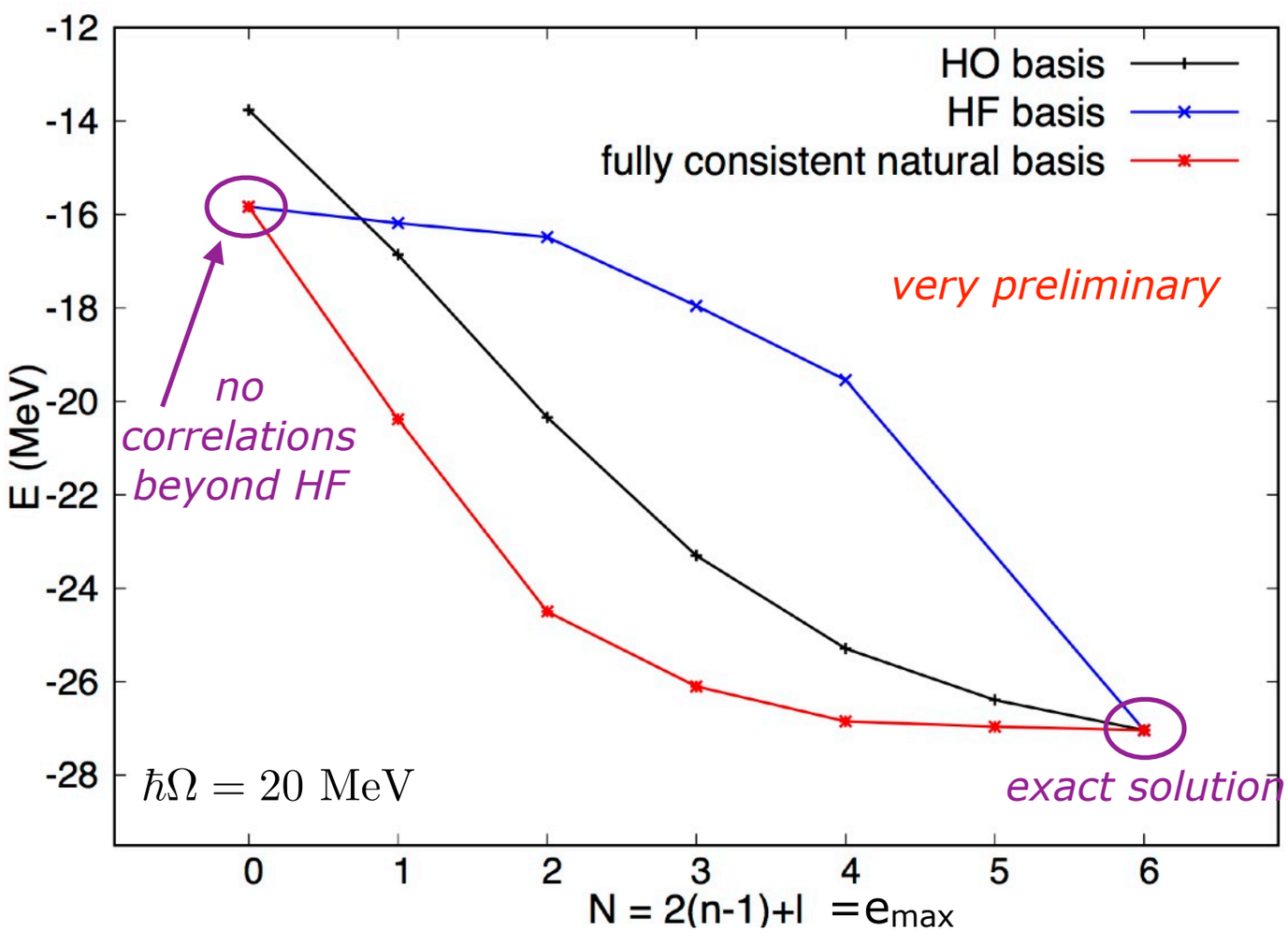
Interaction matrix elements and NCSM results : courtesy of Petr Navrátil

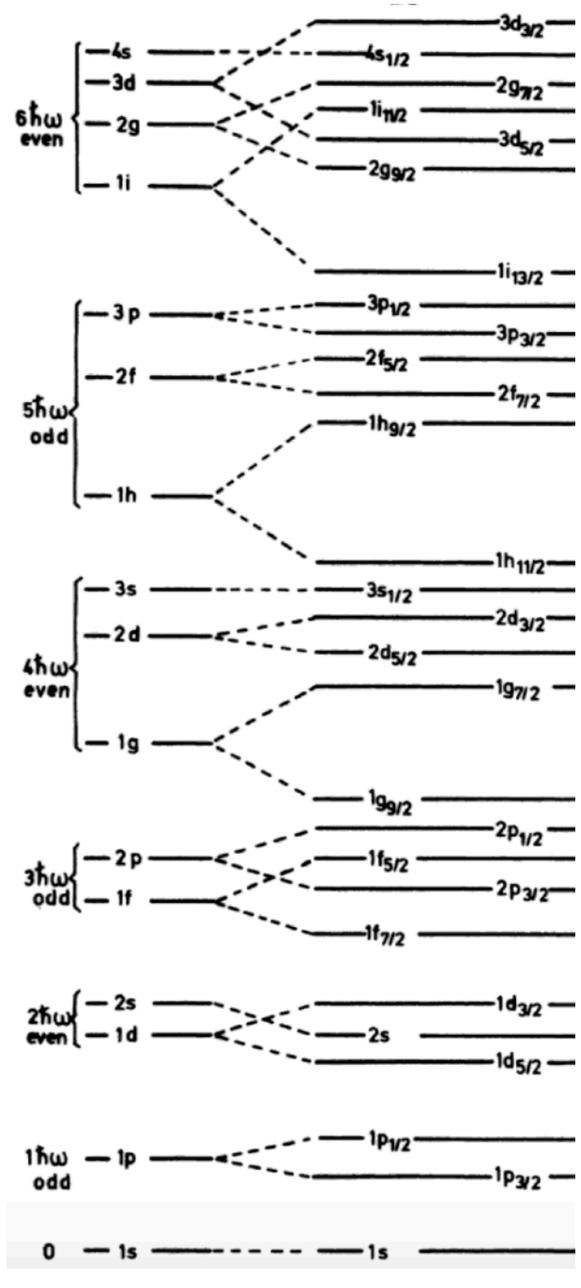
2-body Hamiltonian matrix dimensions (m-scheme)

0:	1
1:	75
2:	2 068
3:	25 257
4:	191 301
5:	1 026 664
6:	4 555 918

single-particle basis expanded on 7 HO shells [N_{tot} =6]

full diagonalization in active space with N ≤ N_{tot}





✳ *much faster convergence with variational natural orbitals (gain of ~ 2 shells compared to HO basis ➡ large gain in dimensionality)*

✳ *Hartree-Fock orbitals are not a good basis in this case (also seen in Tichai et al. PRC 99, 034021, (2019).)*

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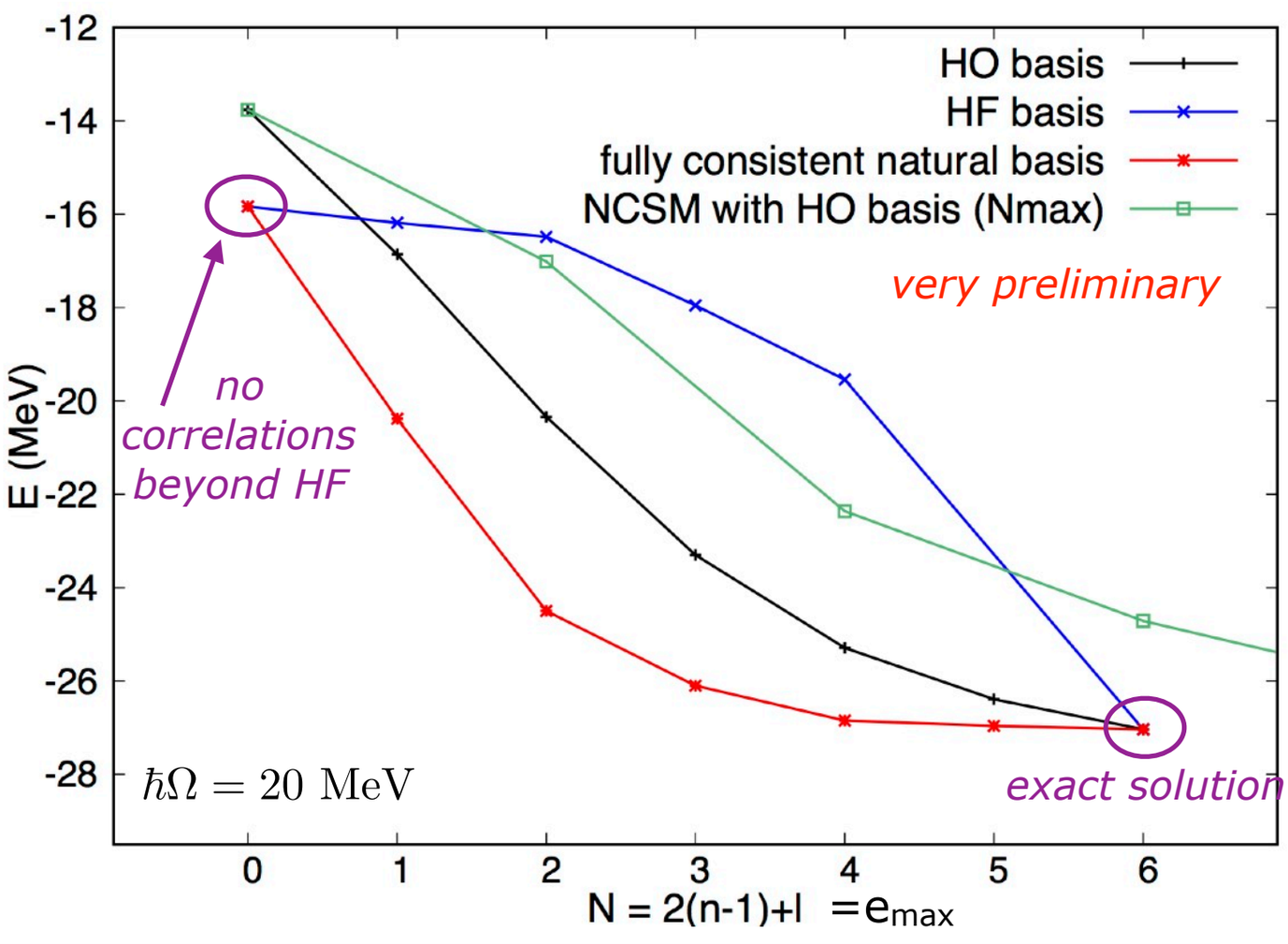

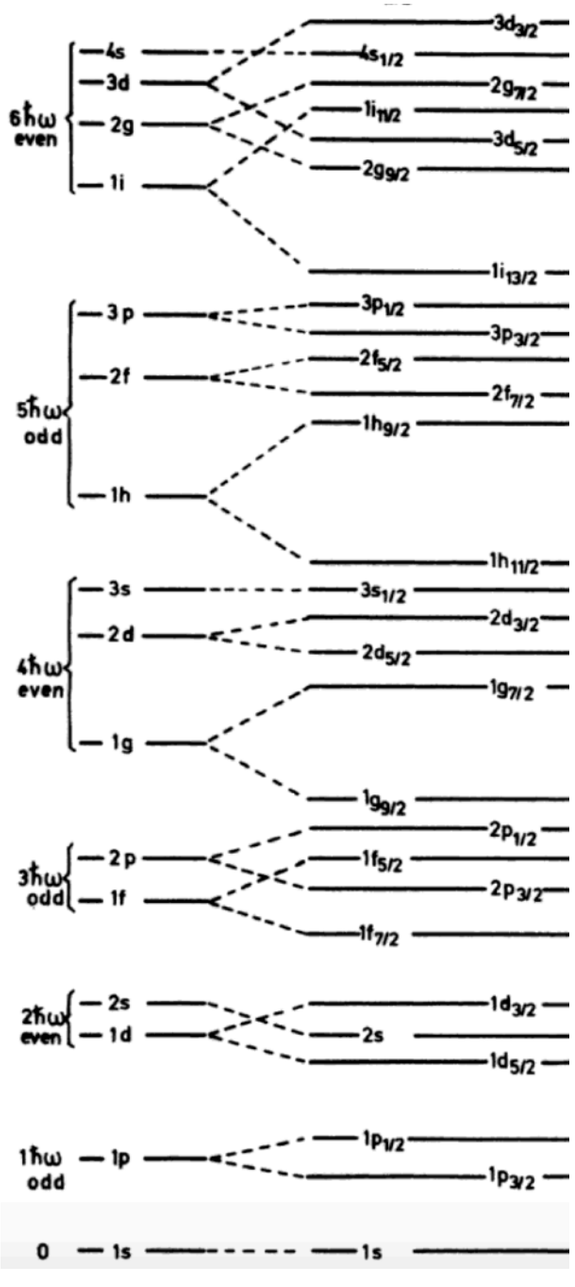

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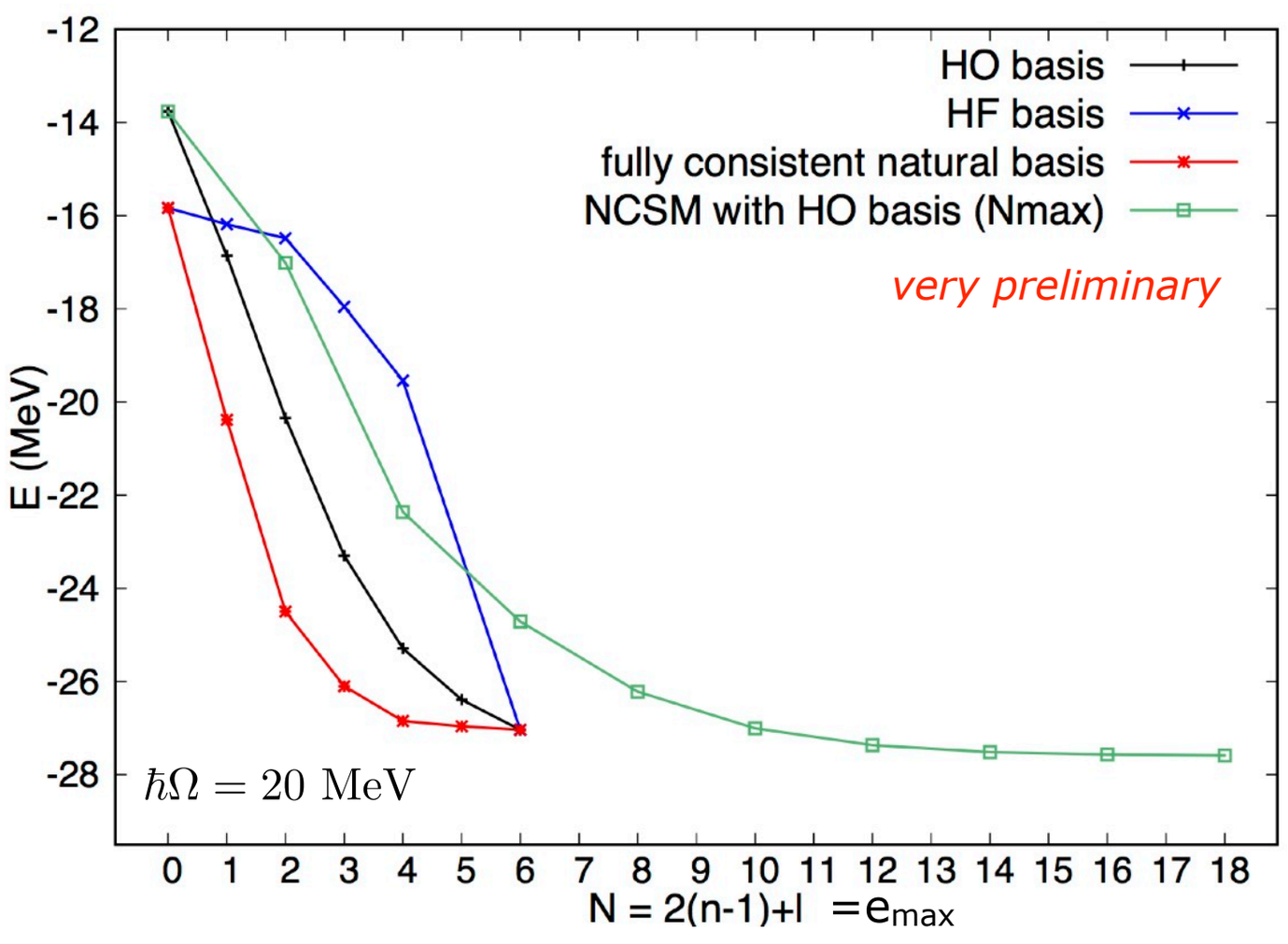

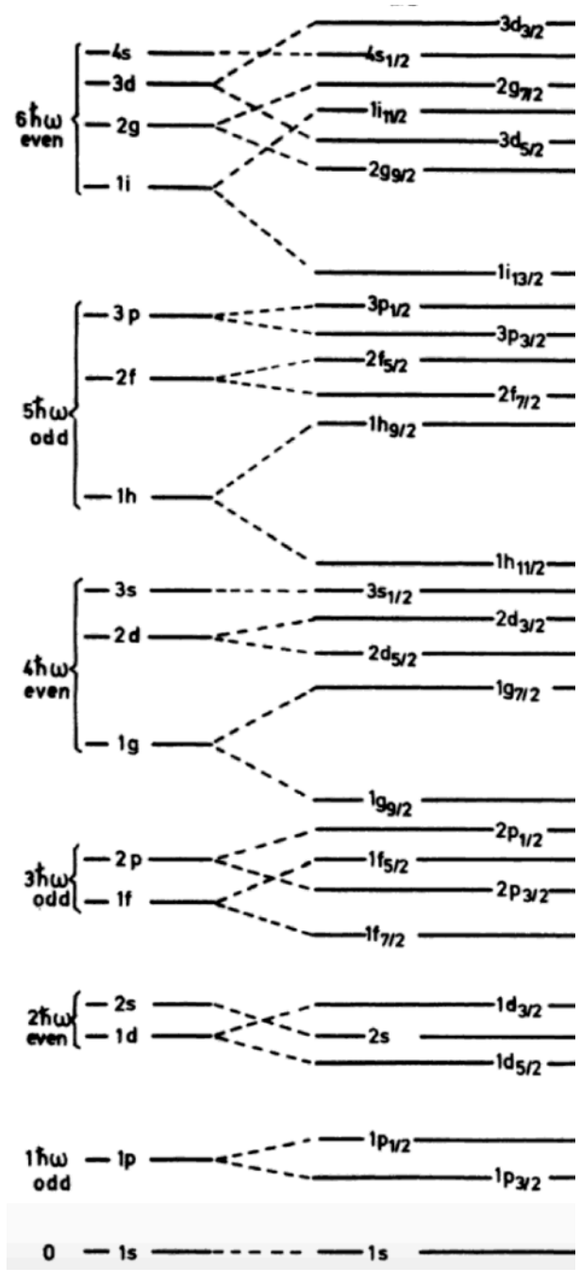

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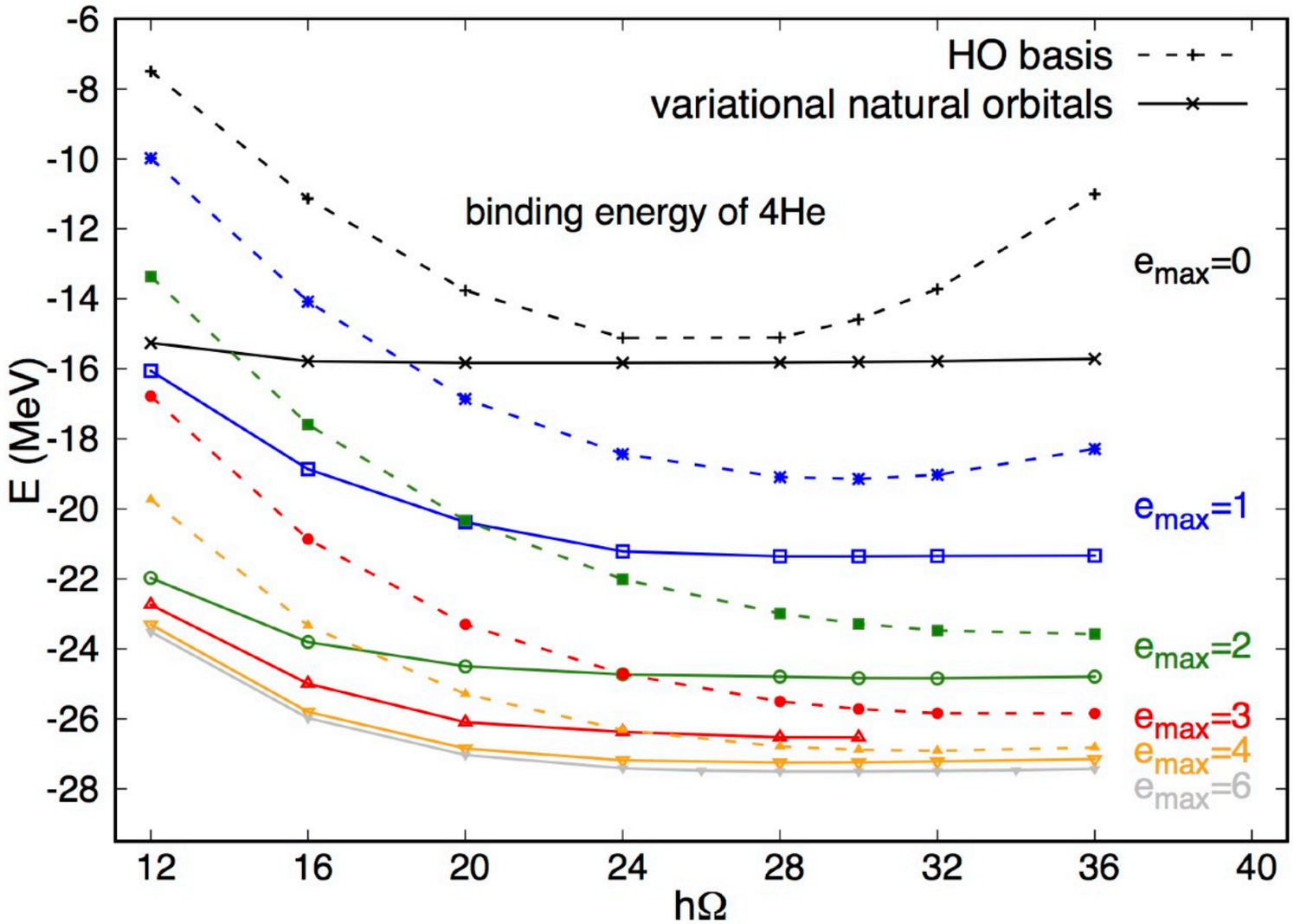
Test application to ^{4}He with a chiral interaction

✱ ***Binding energy: convergence with respect to the oscillator frequency***



✳ *The variational natural orbitals are less dependent on ħΩ*

Test application to ^{4}He with a chiral interaction

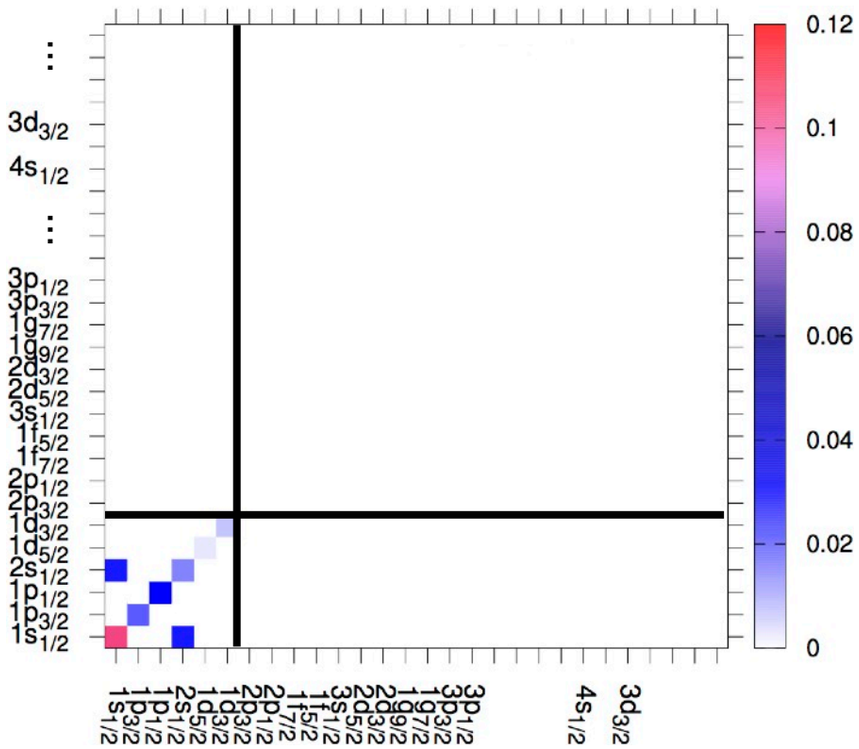
e_{max} =2

✱ One-body density matrix (neutrons):

Representation of $\Delta\rho_{ij} = |\rho_{ij} - \rho_{ij}^{0p0h}|$ in the HO basis:

Equation 1 - iteration 1

$$\rho_{ij} \begin{cases} \in [0,1] \text{ if } i,j \in \text{valence} \\ 0 \text{ otherwise} \end{cases}$$



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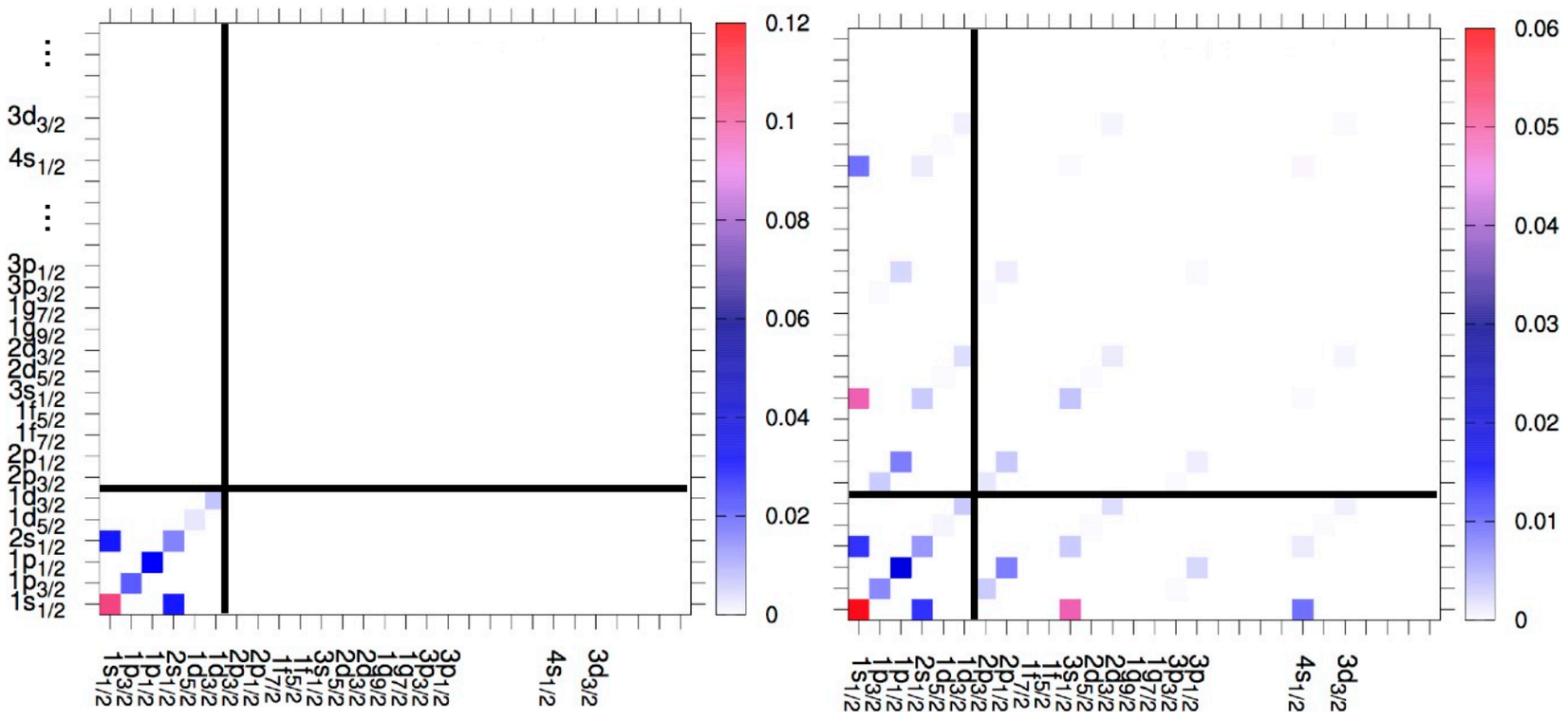
Eqs 1&2 - after convergence

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

single-particle energies



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Eqs 1&2 - after convergence

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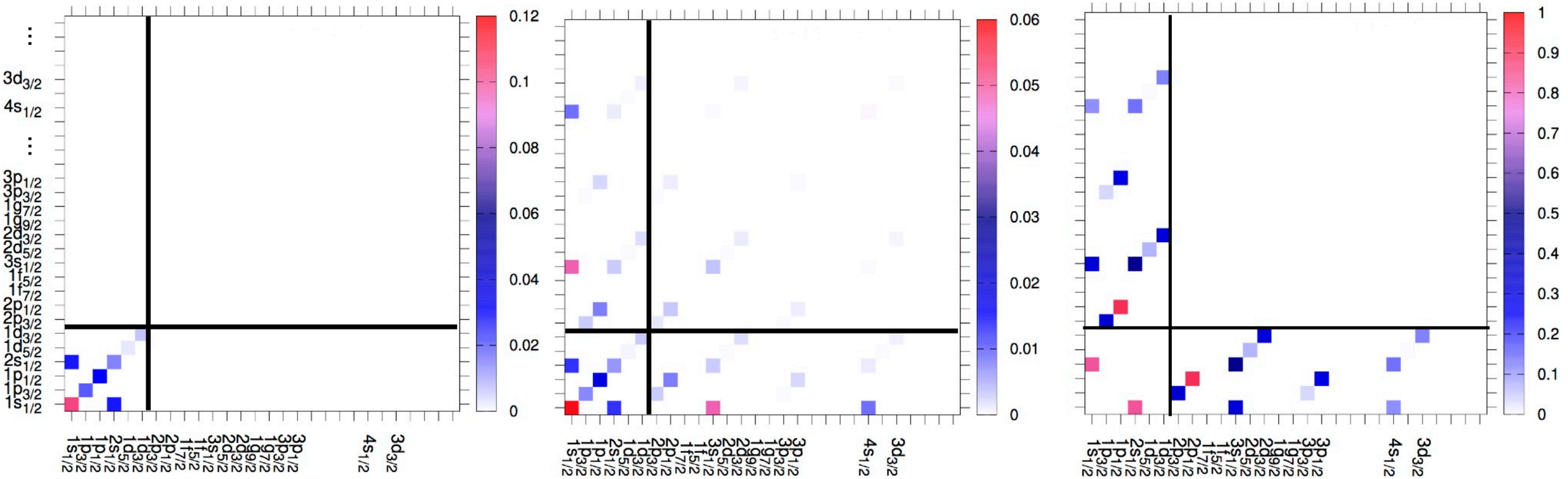
single-particle energies

✱ Source term of the orbital equation:

$$G_{ij}(\sigma) = \frac{1}{2}\sum_{klm} \widetilde{V}_{kmjl}\sigma_{kiml} - \frac{1}{2}\sum_{klm} \widetilde{V}_{kiml}\sigma_{jlkm}$$

$\in$ whole basis $\in$ valence space

➡ *Couples the active space to the rest of the single-particle basis.*



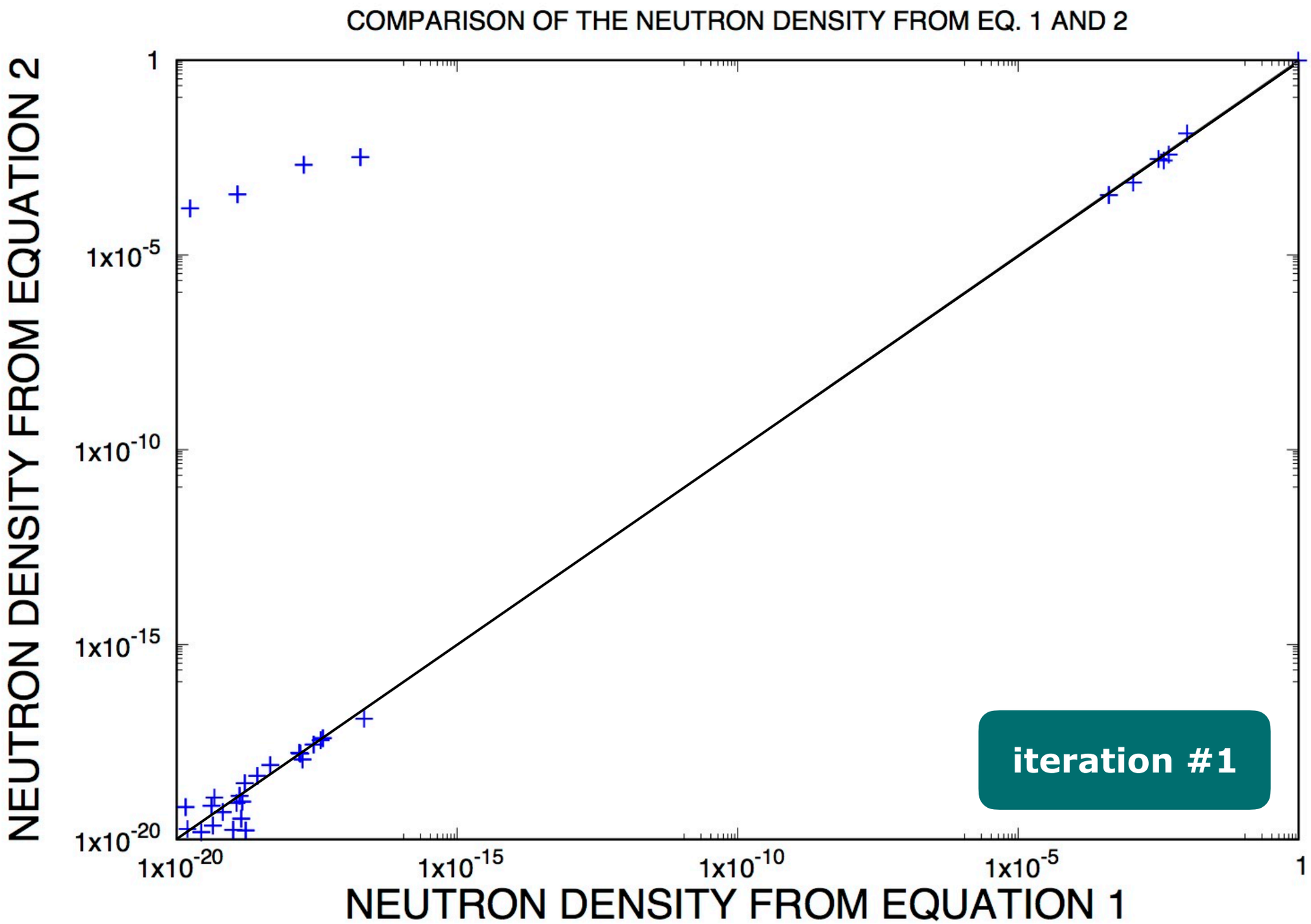
- *the source term introduces couplings outside of the active space*
- *states outside of the initial active become occupied*

} extra features compared to regular "natural orbitals"

Test application to ^{4}He with a chiral interaction

e_{max} =2

* ***Convergence of the one-body density matrix (neutrons):***



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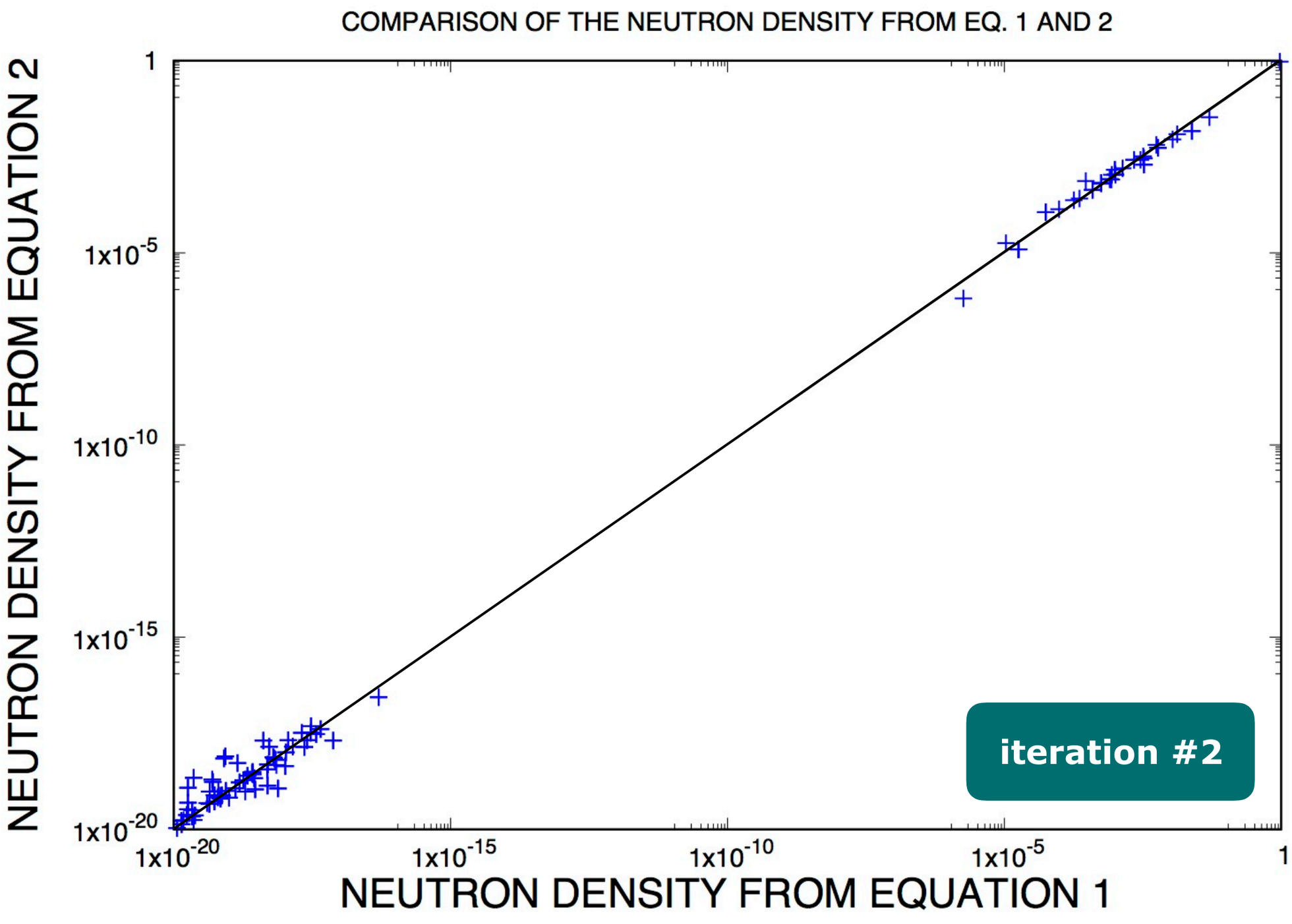

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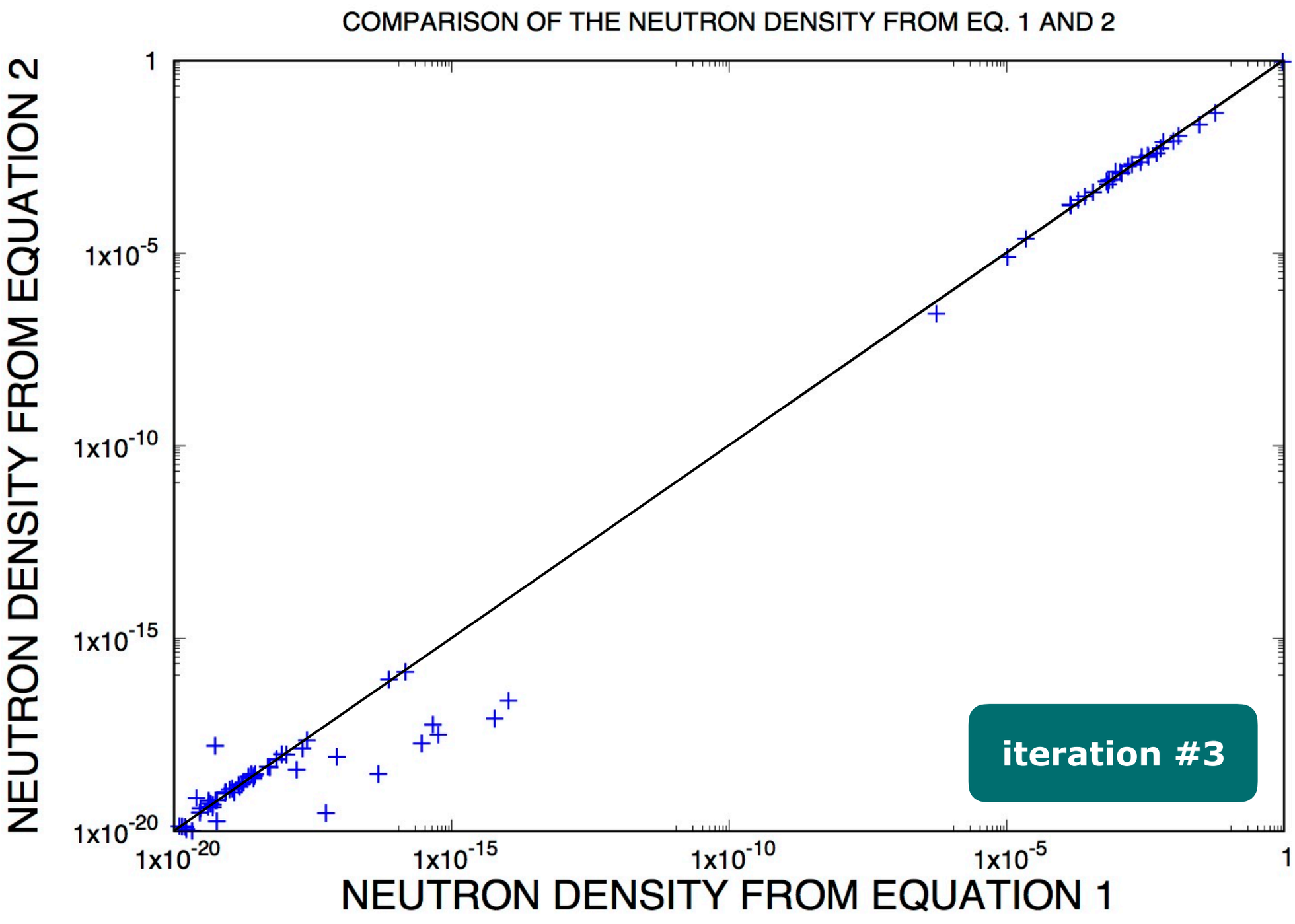
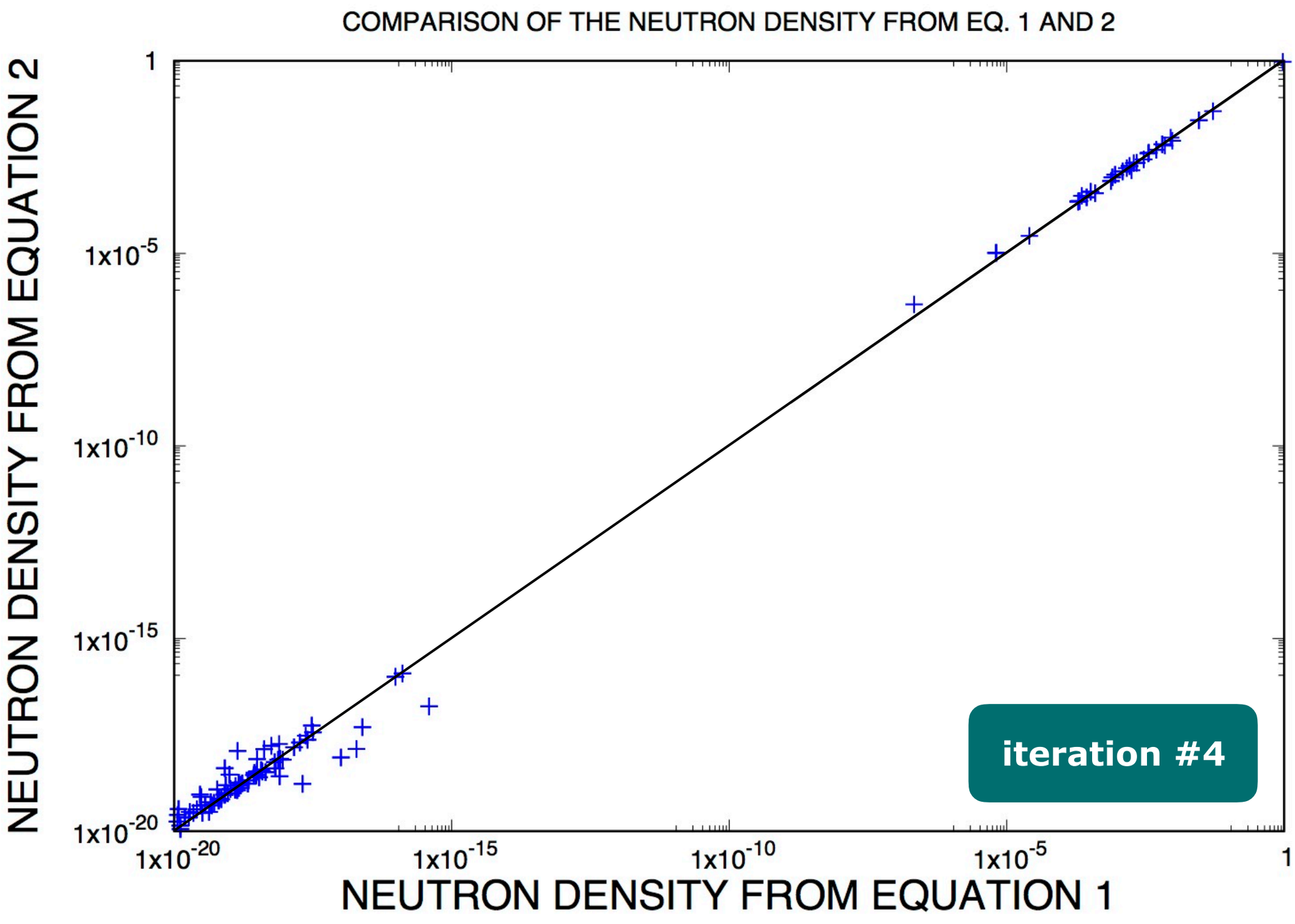


Test application to ^{4}He with a chiral interaction

e_{max} =2

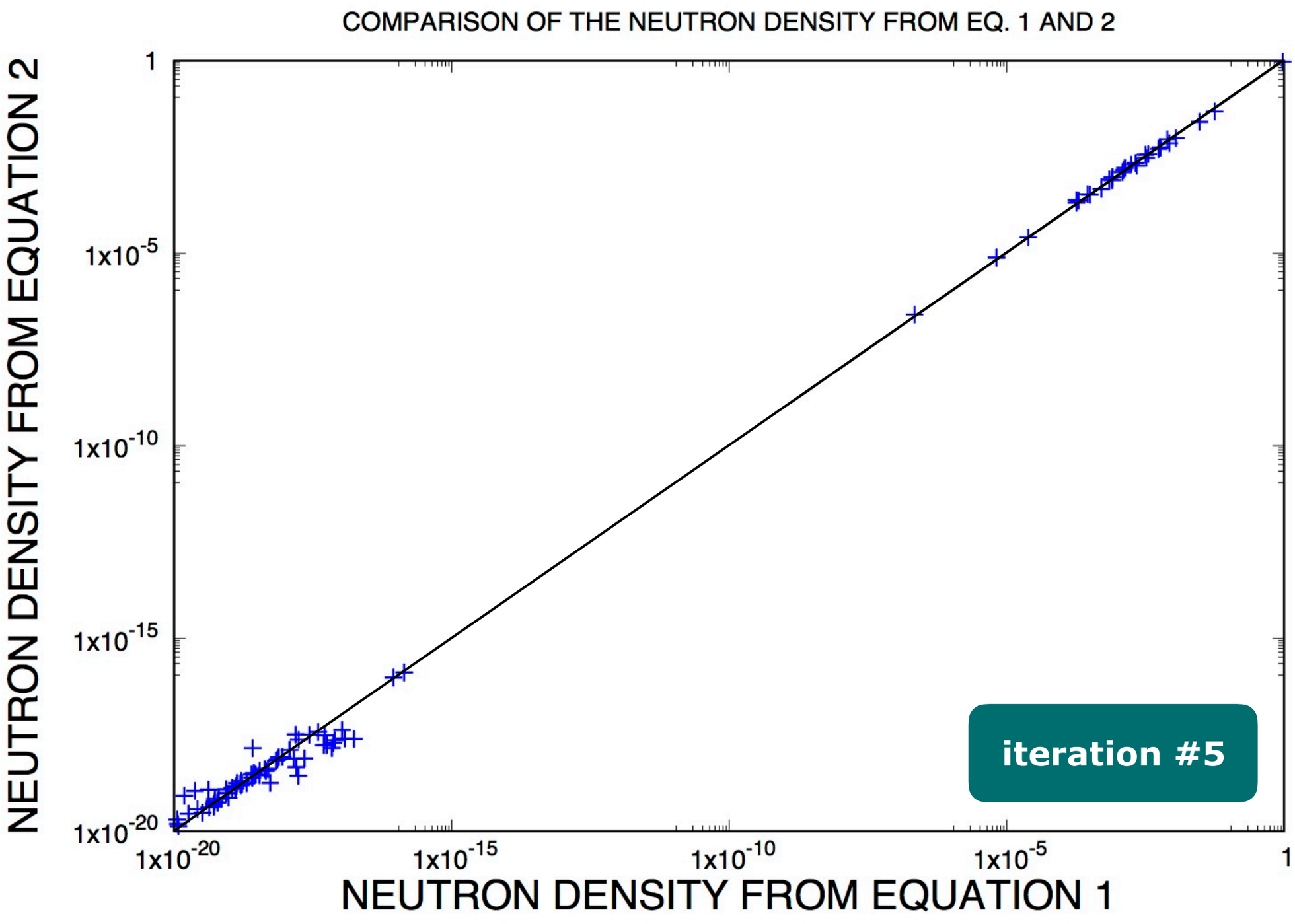
✱ ***Convergence of the one-body density matrix (neutrons):***



Test application to ^{4}He with a chiral interaction

e_{max} =2

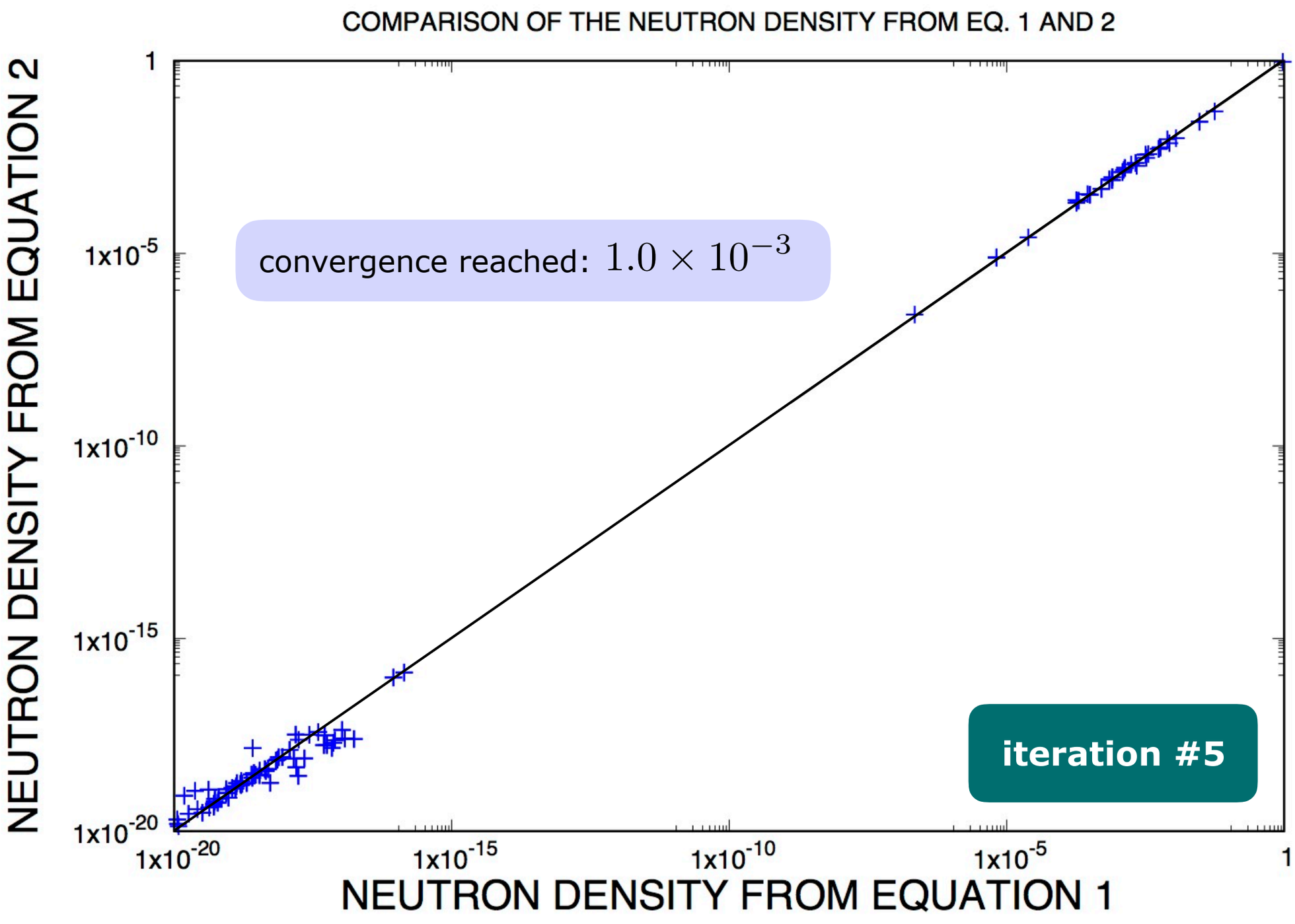
* ***Convergence of the one-body density matrix (neutrons):***



Test application to ^{4}He with a chiral interaction

e_{max} =2

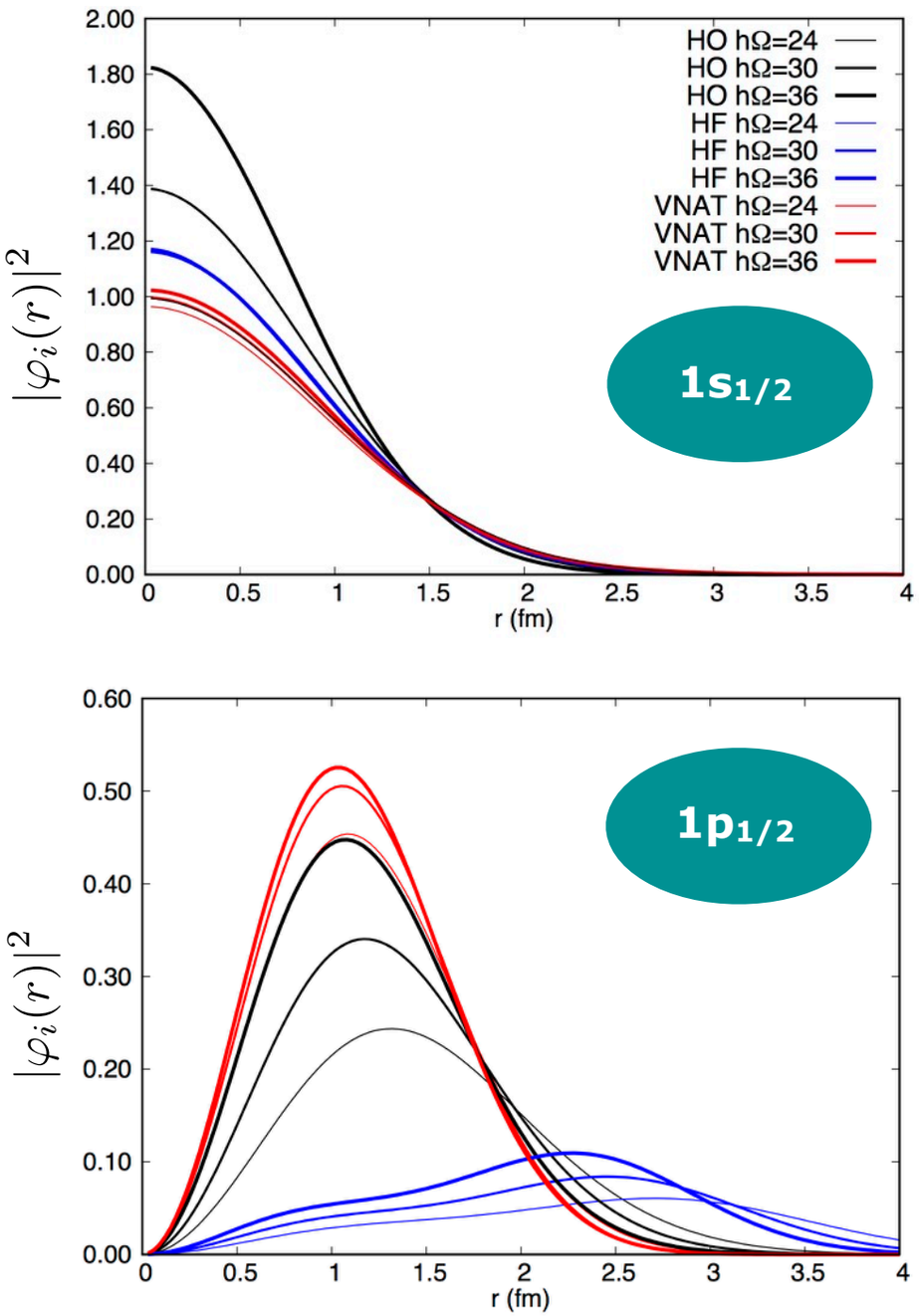
✱ ***Convergence of the one-body density matrix (neutrons):***

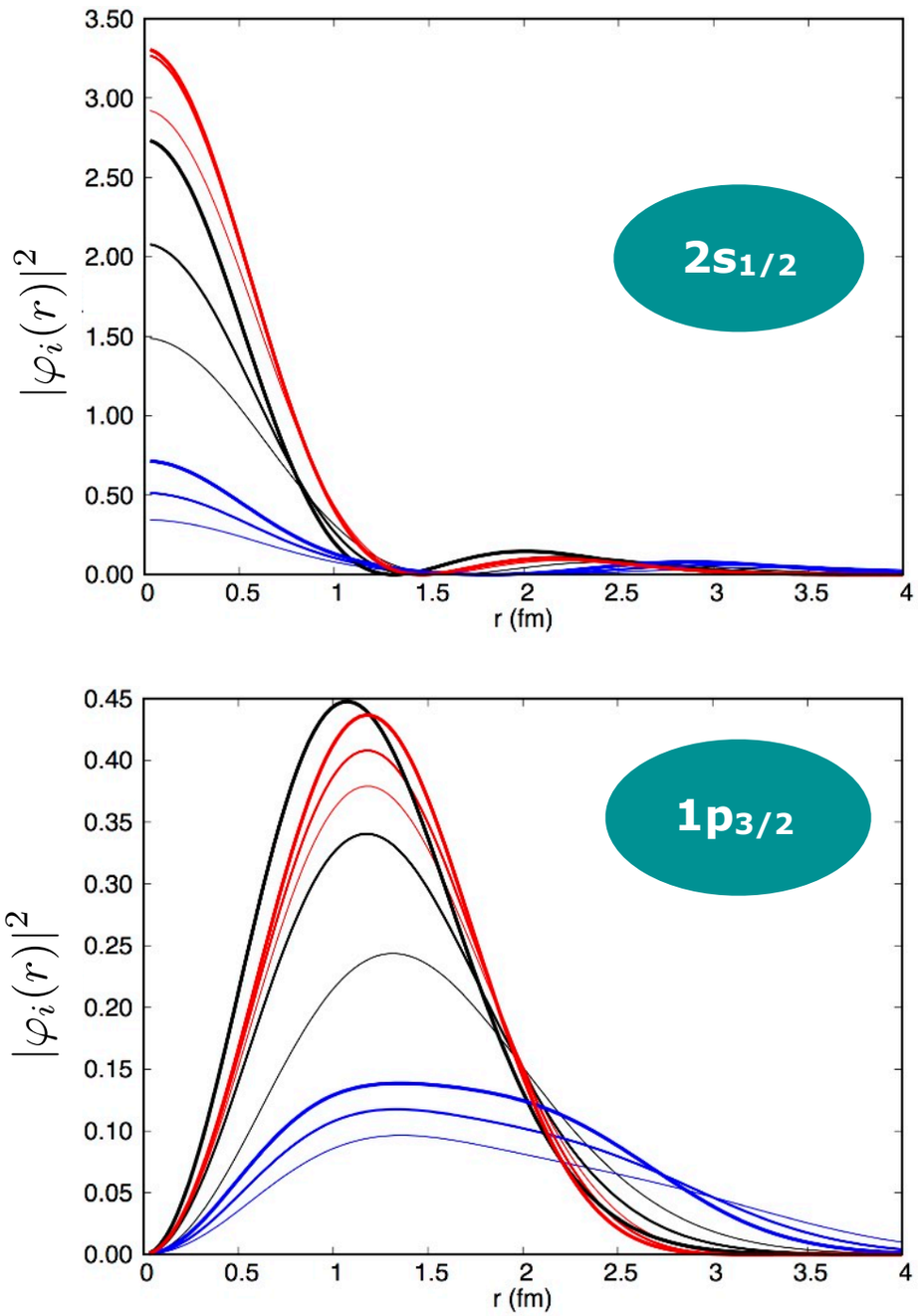


Test application to ^{4}He with a chiral interaction

e_{max} =2

✱ Single-particle orbitals (radial part):





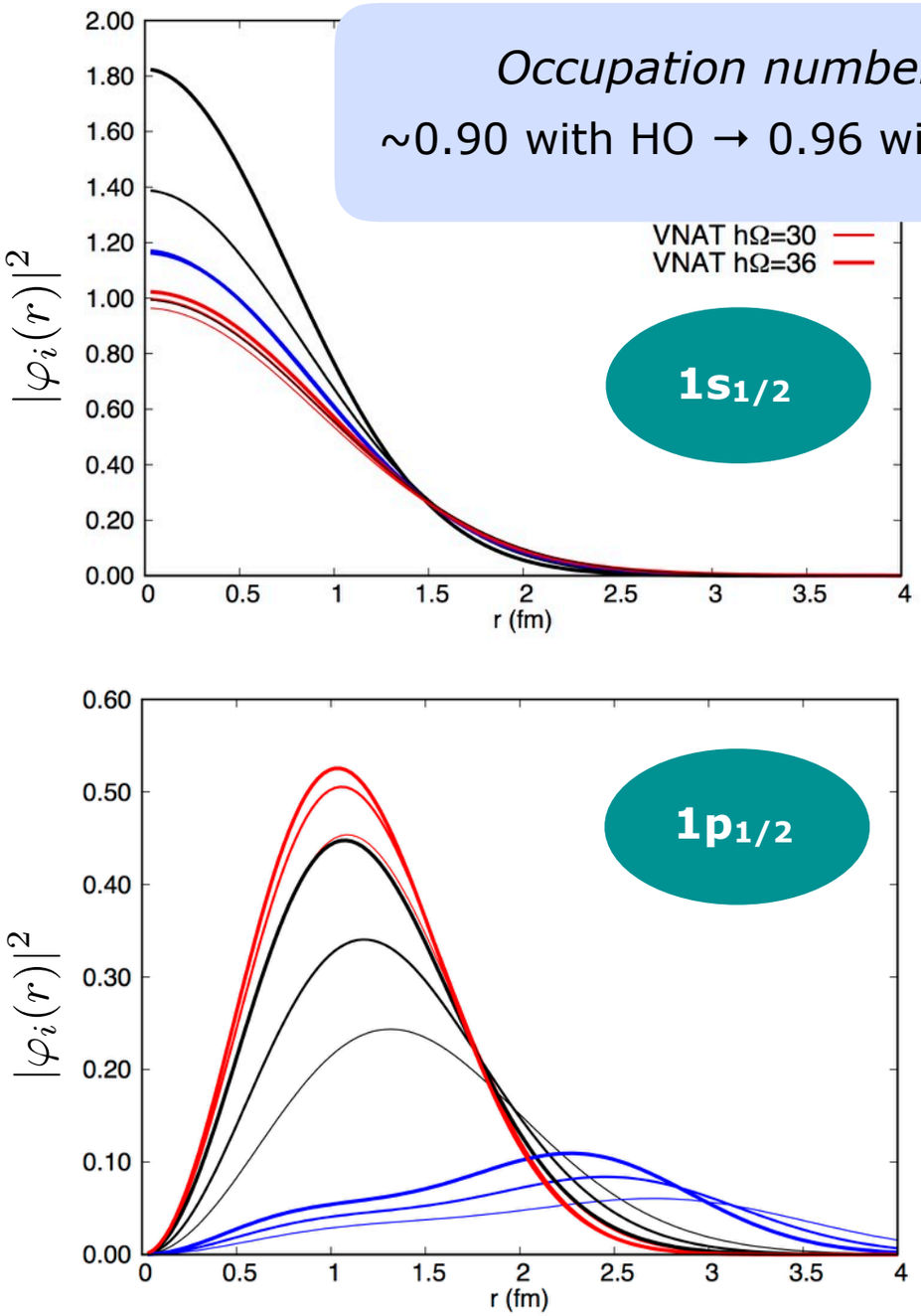
- *dependence on HO frequency reduced with VNAT orbitals*
- *weird behavior of the HF orbitals above the Fermi level, in accordance with Tichai et al. PRC 99, 034321 (2019)*

Test application to ^{4}He with a chiral interaction

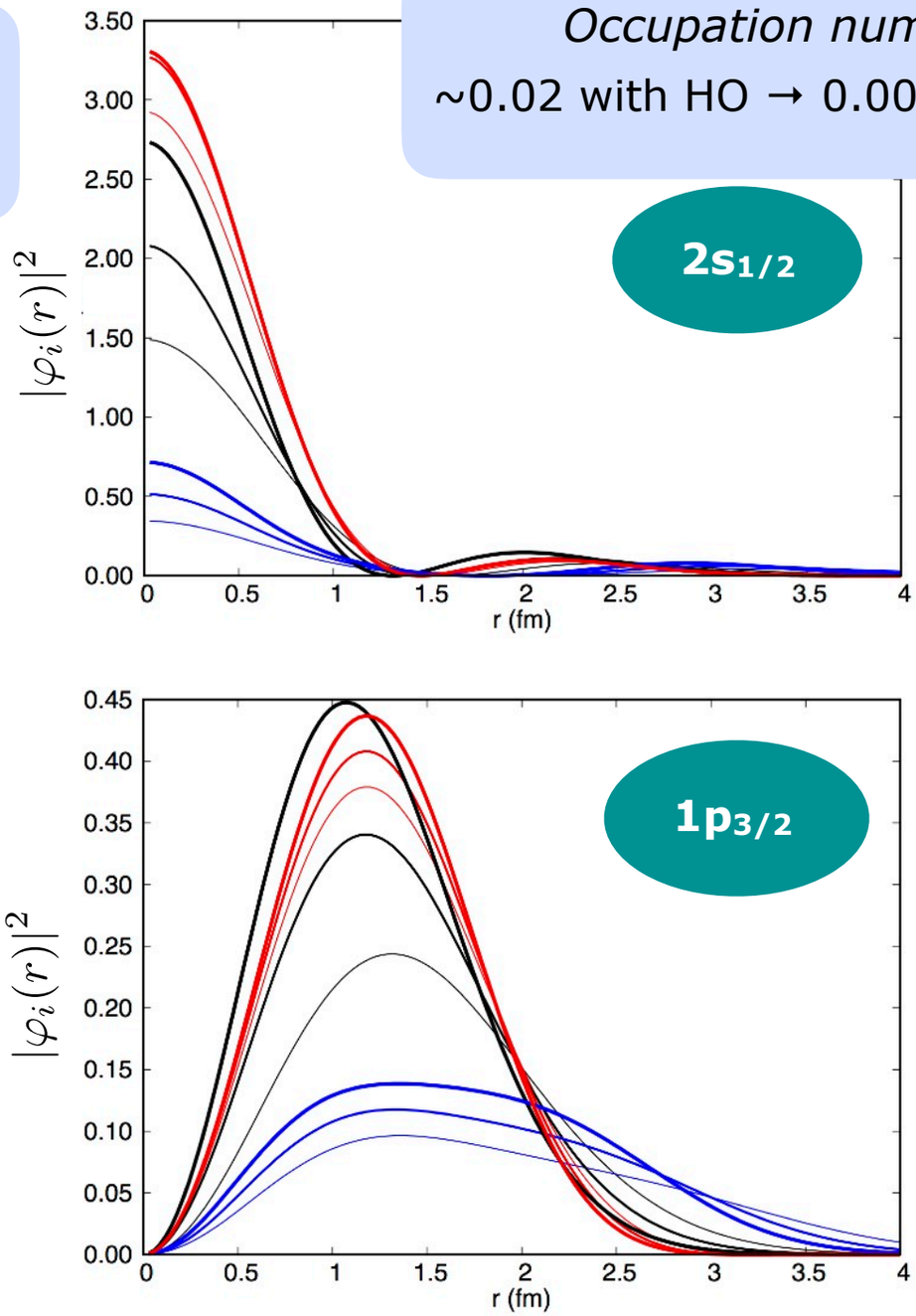
e_{max} =2

✱ *Single-particle orbitals (radial part):*

Occupation numbers:
~0.90 with HO → 0.96 with VNAT



Occupation numbers:
~0.02 with HO → 0.006 with VNAT

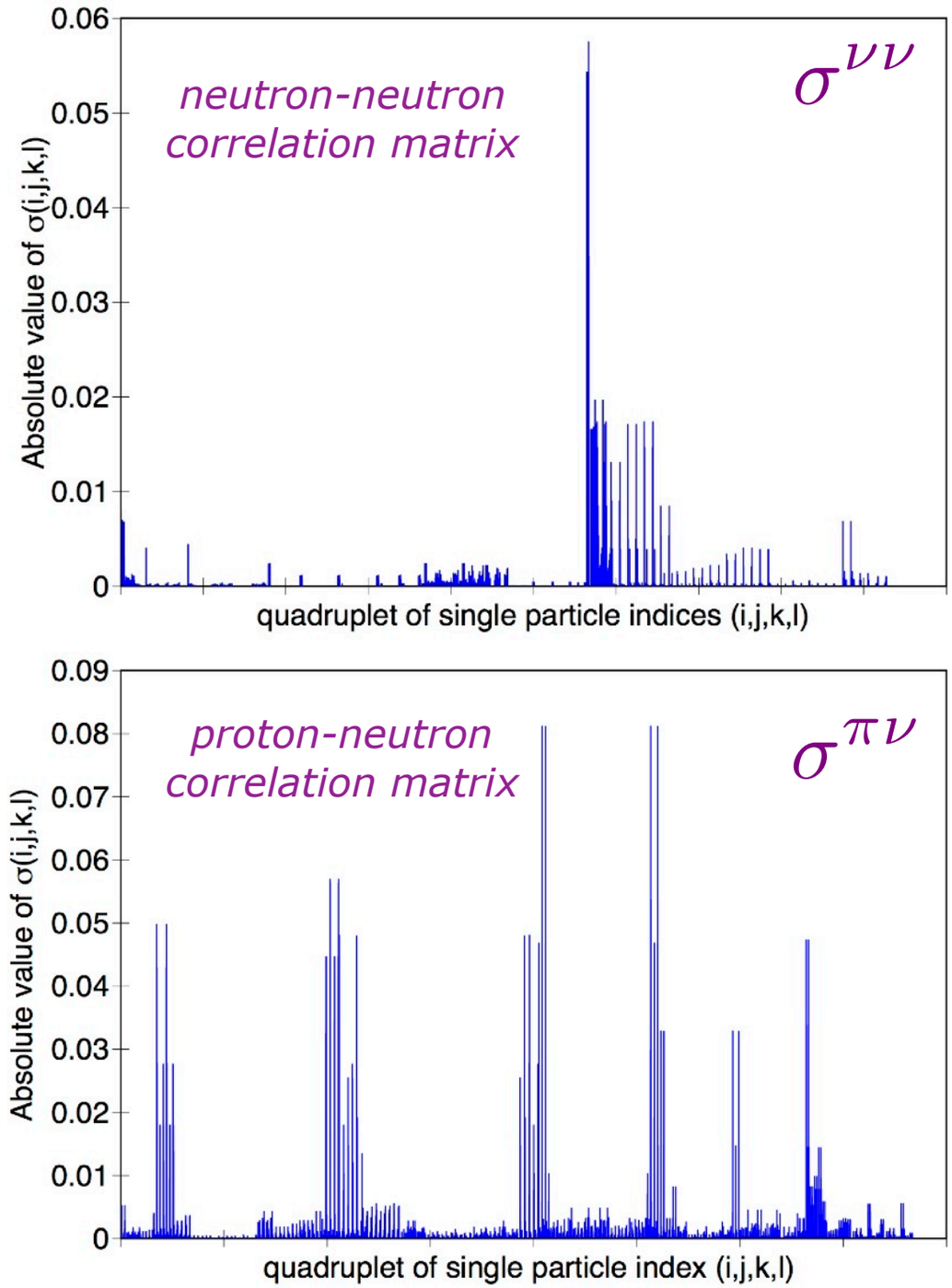


- *dependence on HO frequency reduced with VNAT orbitals*
- *weird behavior of the HF orbitals above the Fermi level, in accordance with Tichai et al. PRC 99, 034321 (2019)*
- *occupation of the $1s_{1/2}$ increases ↠ better 0p0h state*

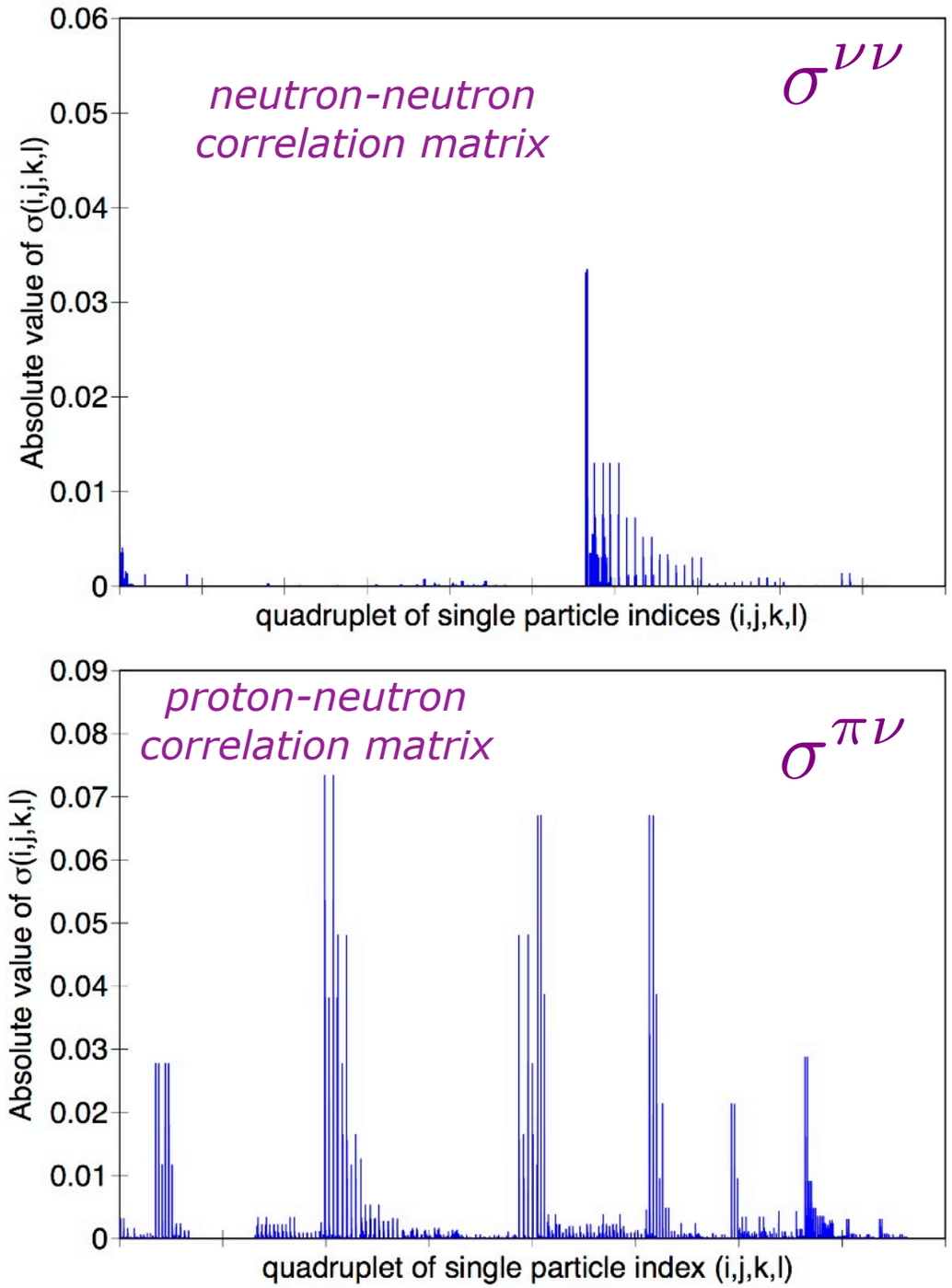
Test application to ^{4}He with a chiral interaction

e_{max} =2

with HO orbitals



with variational natural orbitals



- decrease by factor ~2 in the neutron-neutron sector
- pn correlations remain strong, only little change

Test application to ^{4}He with a chiral interaction

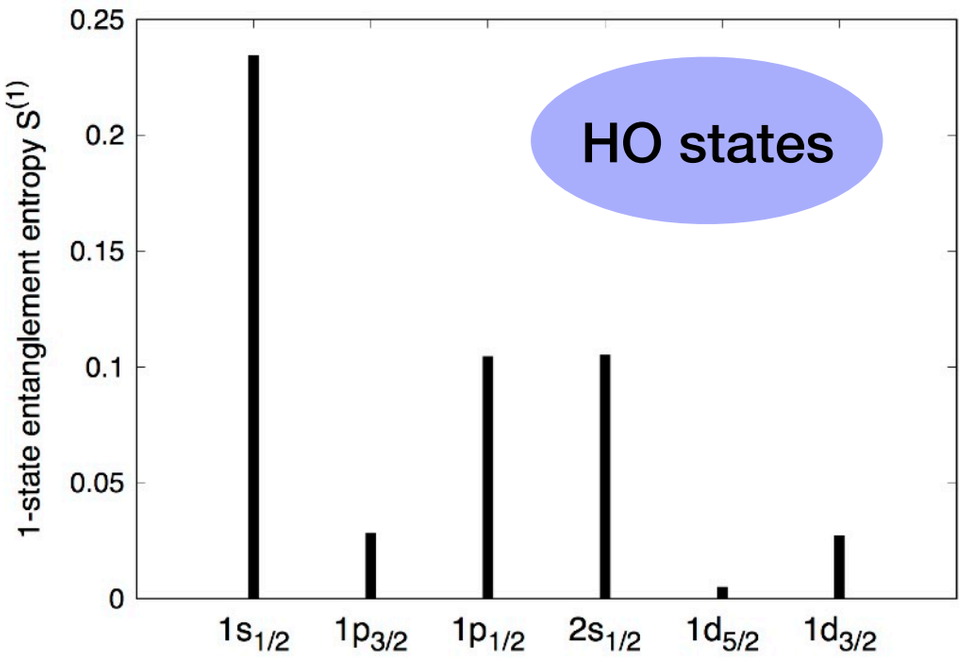
e_{max} =2

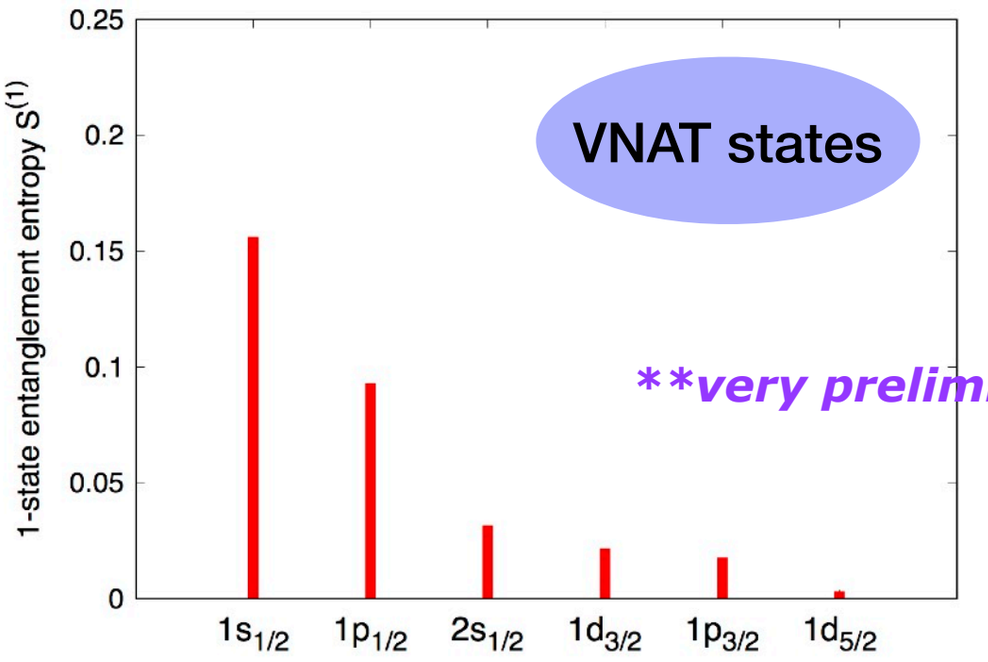
✱ ***Entanglement of single-particle states*** $(i) \equiv \{\alpha_i, l_i, j_i, m_i, \tau_i\}$ ***with M. Savage (INT)***

- write the wave function in terms of occupation numbers: $|\Psi\rangle = \sum_{n_1 \ldots n_i \ldots n_N} A_{n_1 \ldots n_i \ldots n_N} |n_1 n_2 \ldots n_i \ldots n_N\rangle$
- "one-state" reduced density matrix: $\widetilde{\rho}^{(i)} = \begin{pmatrix} 1-\rho_{ii} & 0 \\ 0 & \rho_{ii} \end{pmatrix}$

$\rho_{ii} = \langle \Psi | a_i^\dagger a_i | \Psi \rangle$
one-body density

- Entropy of entanglement of a single-particle state with the rest: $S^{(1)}_{(i)} = -\widetilde{\rho}^{(i)} \ln \widetilde{\rho}^{(i)}$





very preliminary*

✳ *The variational natural orbitals appear naturally organized by decreasing entanglement*

Test application to ^{4}He with a chiral interaction

e_{max} =2

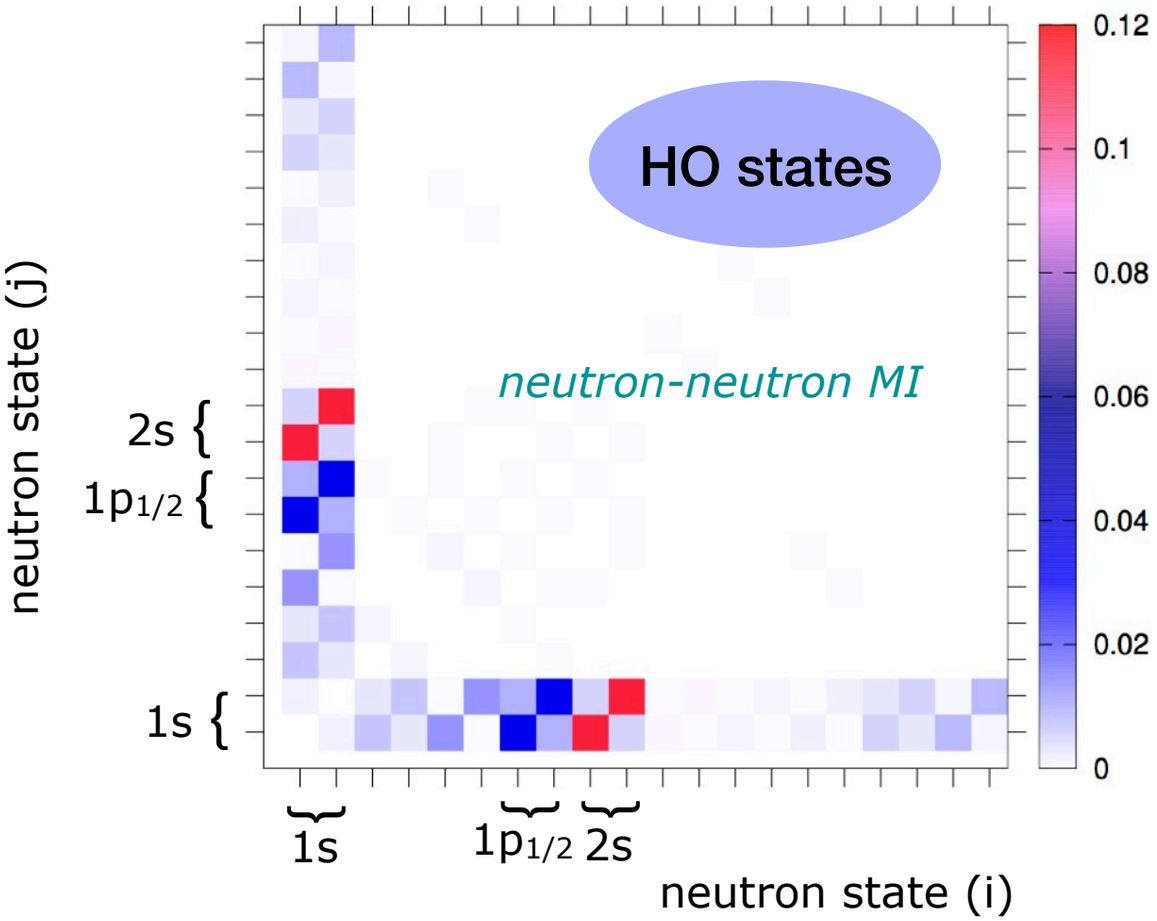
✱ ***Entanglement of single-particle states*** ***with M. Savage (INT)***

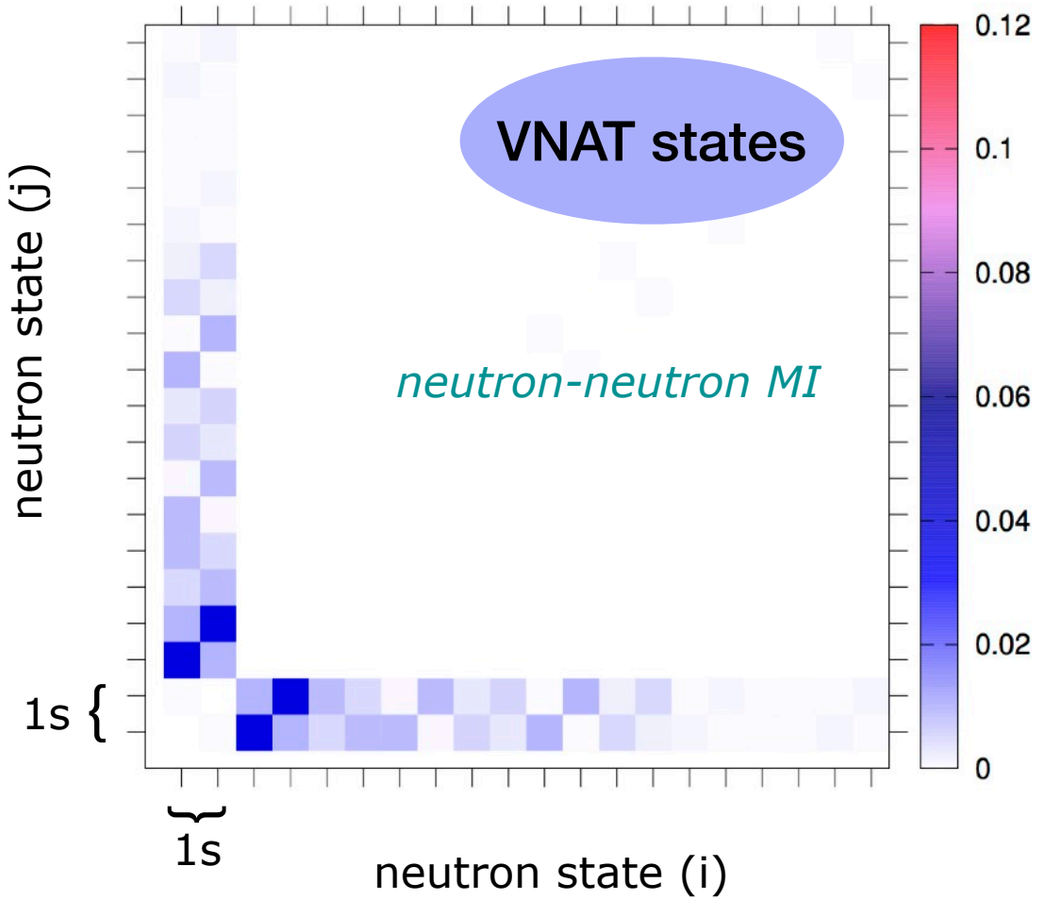
- "Two-state" reduced density matrix: $\widetilde{\rho}^{(ij)} = \begin{pmatrix} 1-\rho_{ii}-\rho_{jj}+\rho_{ijij} & 0 & 0 & 0 \\ 0 & \rho_{jj}-\rho_{ijij} & \rho_{ji} & 0 \\ 0 & \rho_{ij} & \rho_{ii}-\rho_{ijij} & 0 \\ 0 & 0 & 0 & \rho_{ijij} \end{pmatrix}$

- Entropy of entanglement of two single-particle states with the rest: $S^{(2)}_{(ij)} = -\widetilde{\rho}^{(ij)} \ln \widetilde{\rho}^{(ij)}$

- Mutual information between two states: $I_{ij} = -\left(S^{(2)}_{(ij)} - S^{(1)}_{(i)} - S^{(1)}_{(j)}\right)(1-\delta_{ij})$

*****very preliminary*****





Test application to ^{4}He with a chiral interaction

e_{max} =2

✱ *Entanglement of single-particle states*

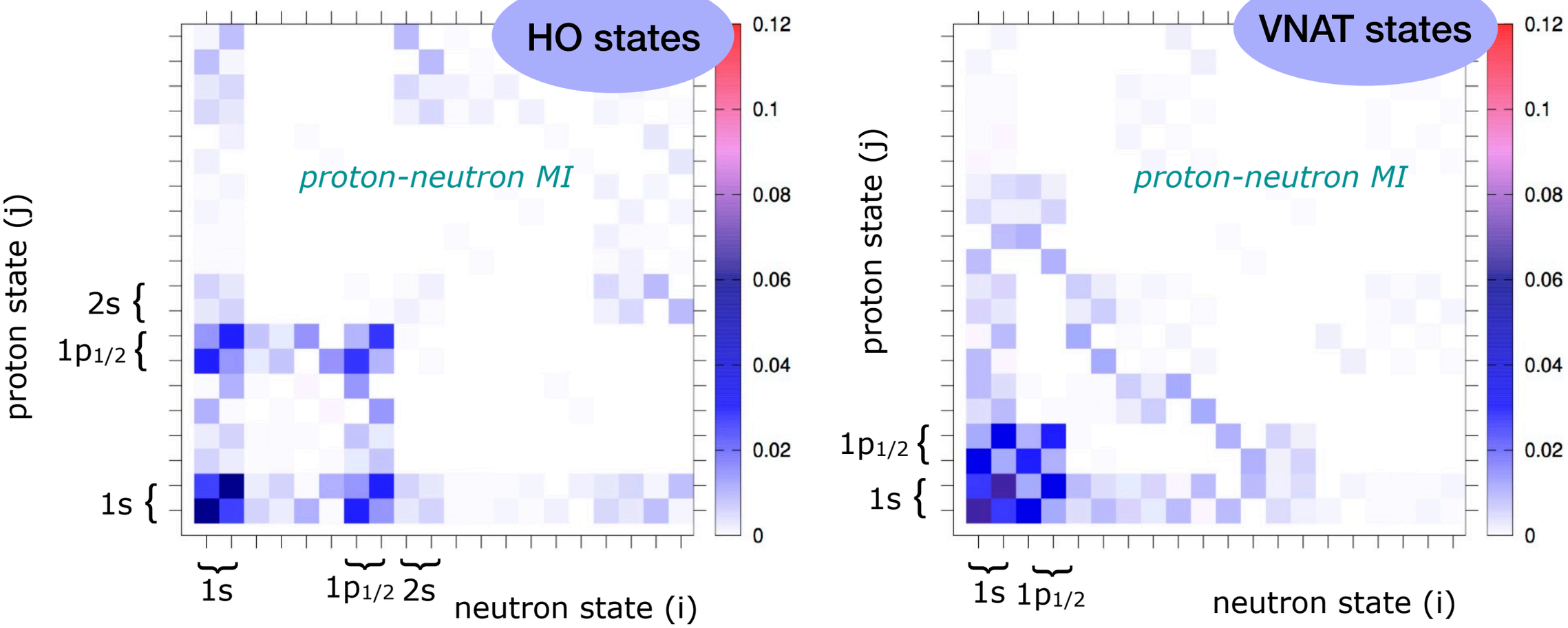
with M. Savage (INT)

- "Two-state" reduced density matrix: $\widetilde{\rho}^{(ij)} = \begin{pmatrix} 1-\rho_{ii}-\rho_{jj}+\rho_{ijij} & 0 & 0 & 0 \\ 0 & \rho_{jj}-\rho_{ijij} & \rho_{ji} & 0 \\ 0 & \rho_{ij} & \rho_{ii}-\rho_{ijij} & 0 \\ 0 & 0 & 0 & \rho_{ijij} \end{pmatrix}$

- Entropy of entanglement of two single-particle state with the rest: $S^{(2)}_{(ij)} = -\widetilde{\rho}^{(ij)} \ln \widetilde{\rho}^{(ij)}$

- Mutual information between two states: $I_{ij} = -\left(S^{(2)}_{(ij)} - S^{(1)}_{(i)} - S^{(1)}_{(j)}\right)(1-\delta_{ij})$

very preliminary



Conclusion, perspectives

Conclusion

✱ First application of the fully self-consistent multiparticle-multihole configuration mixing method with a chiral interaction ($N2LO_{opt}$)

- ✦ Construction of a general mean-field and variational natural orbitals consistent with the correlation of the system (convergence of the iterative procedure ~ 10^{-3} on the density matrices).
- ✦ Fast convergence of the binding energy in terms of the model space and less dependence on the oscillator frequency.

To do next:

★ calculations of radii and excited states

★Three-body forces and comparison with other ab-initio methods using the same interactions.

★ Gaussians expansions of local potentials (with Ingo Tews, LANL)
➡ comparison with quantum Monte Carlo calculations

★Implement smarter truncation schemes (excitation energies, weight of the configurations, entanglement-based?)

Conclusion, perspectives

Thanks to my collaborators:

- *Nathalie Pillet (CEA, DAM, DIF, France)*
- *Guillaume Hupin (IPN Orsay, France)*
- *M. Savage (INT, Seattle)*
- *P. Navrátil (TRIUMF, Canada)*
- *Ingo Tews (LANL, USA)*
- *Rémi Bernard (ANU, Australia)*

Thank you!

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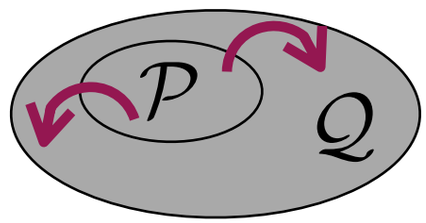
INT US-DOE Grant DE-FG02-00ER41132 and JINA-CEE US-NSF Grant PHY-1430152

SCMPMH method: Formalism

★ Role of the orbital equation:
II) Partial compensation of the truncation P/Q



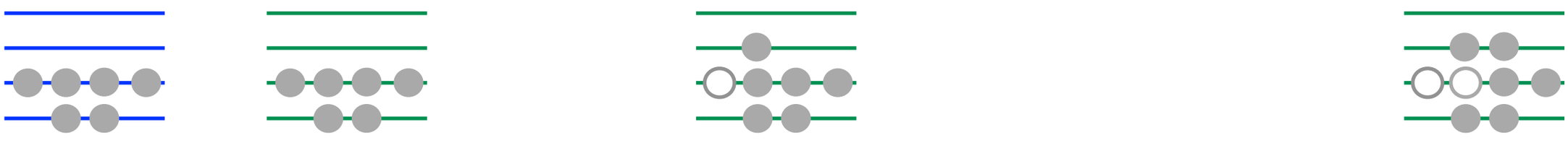
- Ex: truncation in term of the excitation order NpNh

orbital transformation: $b_i^\dagger = e^{i\hat{T}}\ a_i^\dagger\ e^{-i\hat{T}}$

$\Longrightarrow$ effect on the reference state:

$$|\phi^{(f)}\rangle = e^{i\hat{T}}\,|\phi^{(i)}\rangle$$

$$= |\phi^{(i)}\rangle + i\sum_{ph} T_{ph}\ a_p^\dagger a_h|\phi^{(i)}\rangle - \frac{1}{2}\sum_{php'h'} T_{ph}T_{p'h'}\ a_p^\dagger a_h a_{p'}^\dagger a_{h'}|\phi^{(i)}\rangle + \ldots$$

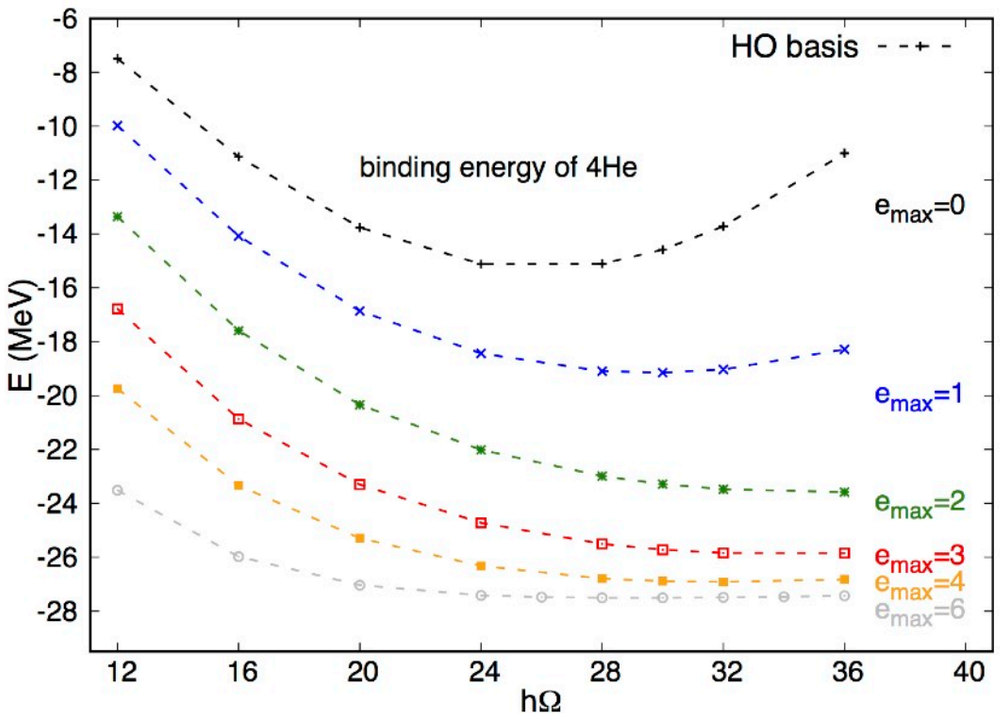


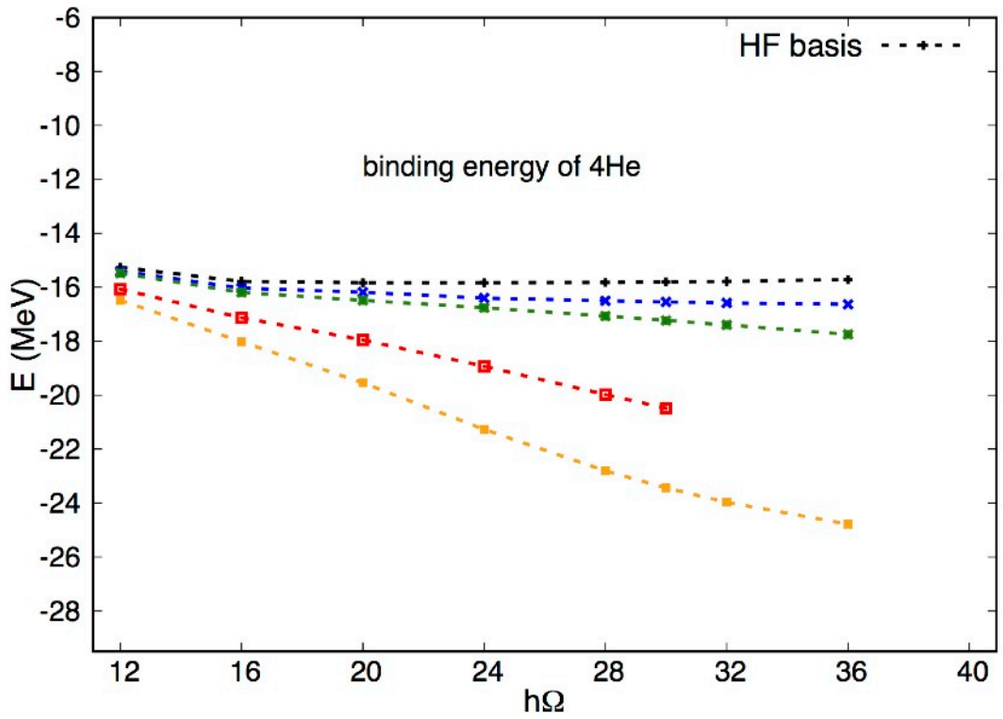
➡ final reference state = superposition of mpmh excitations on the initial reference state = richer

➡ should have a higher weight in the correlated wave function than the initial one

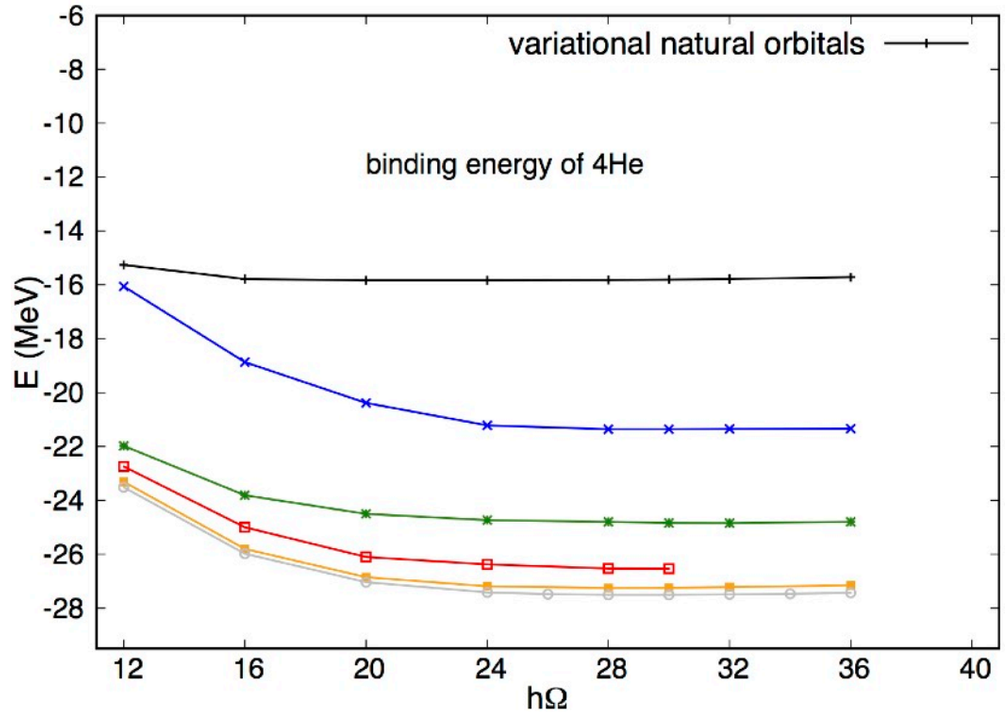
Test application to ^{4}He with a chiral interaction

✱ ***Binding energy: convergence with respect to the oscillator frequency***





✳ *The variational natural orbitals are less dependent on ħΩ*



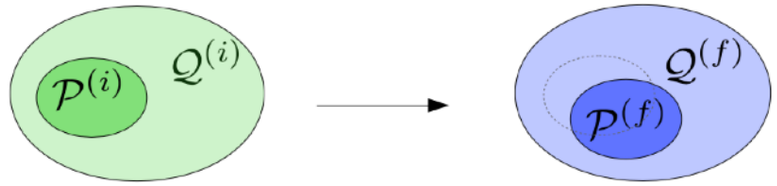
Application to sd-shell nuclei with the Gogny force

✱ ***Effect on the many-body wave function:*** Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$

➡ $|\Psi^{(f)}\rangle = \sum_{\alpha\in\mathcal{P}^{(f)}} A_\alpha^{(f)} |\phi_\alpha^{(f)}\rangle$

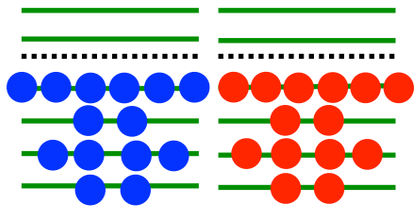
$= \sum_{\beta\in\mathcal{P}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle + \sum_{\beta\in\mathcal{Q}^{(i)}} A_\beta^{(i)} |\phi_\beta^{(i)}\rangle$

How big?



	1st equation only		1st+2nd equations Starting from HF orbitals		1st+2nd equations Starting from HO orbitals	
nucleus	Weight of $P^{(i)}$	Weight of $Q^{(i)}$	Weight of $P^{(i)}$	Weight of $Q^{(i)}$	Weight of $P^{(i)}$	Weight of $Q^{(i)}$
^{20}Ne	100%	0%	98%	2%	66%	34%
^{24}Mg	100%	0%	97%	3%	61%	39%
^{28}Si	100%	0%	95%	4%	55%	45%
^{32}S	100%	0%	93%	7%	61%	39%
^{28}Ne	100%	0%	85%	15%	78%	22%

- ***Main component:***

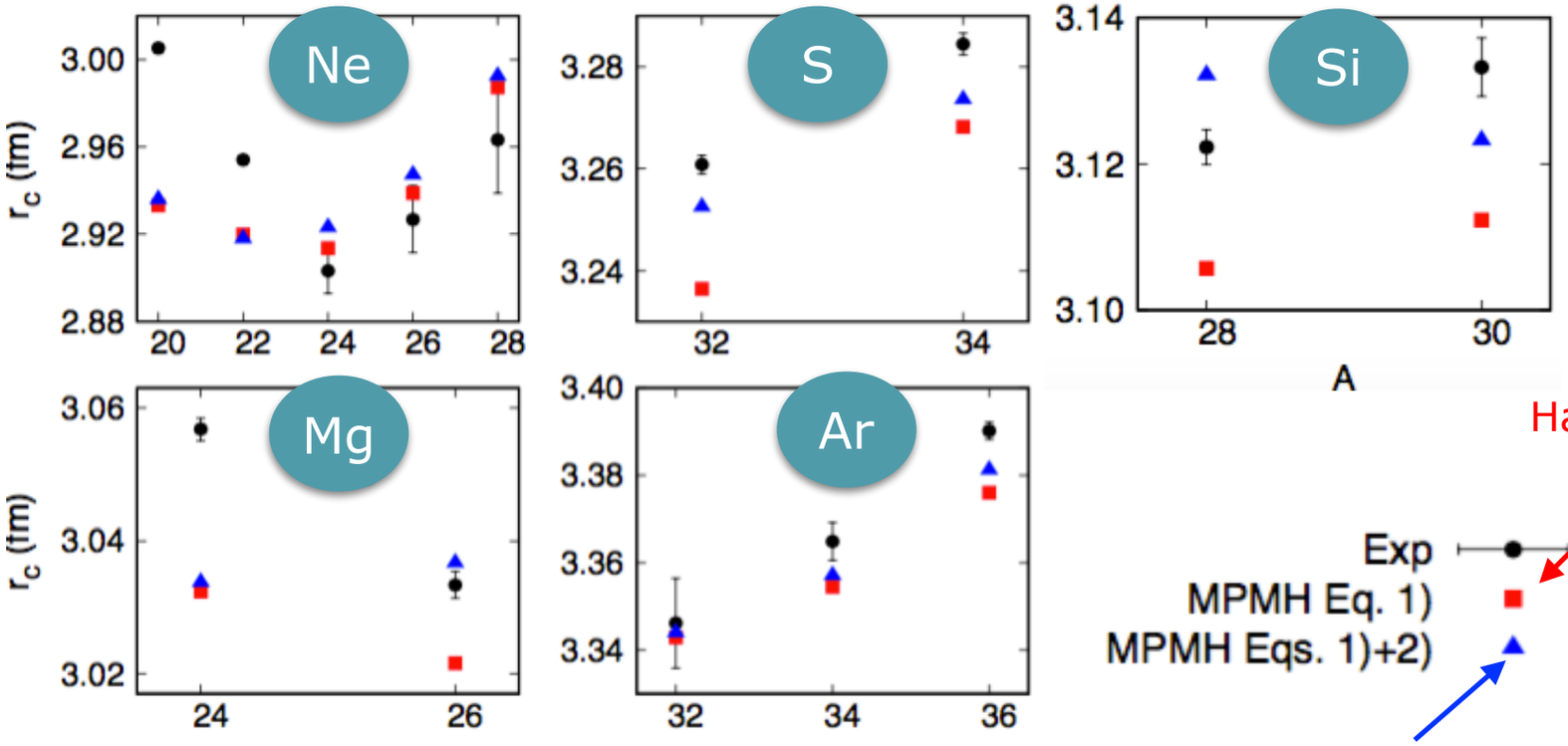


Pure Hartree-Fock component in correlated ground state		
nucleus	1st equation only	1st + 2nd equations
^{20}Ne	71%	62%
^{28}Si	60%	24%
^{32}S	58%	39%
^{34}S	39%	17%

➡ Pure HF component decreases: self-consistent procedure appears to fragment the wave function

Application to sd-shell nuclei with the Gogny force

✦ Charge radii:



- *Average difference:*

$$\langle \Delta r_c \rangle = 0.021 \text{ fm} \rightarrow 0.018 \text{ fm}$$

- *Standard deviation*:

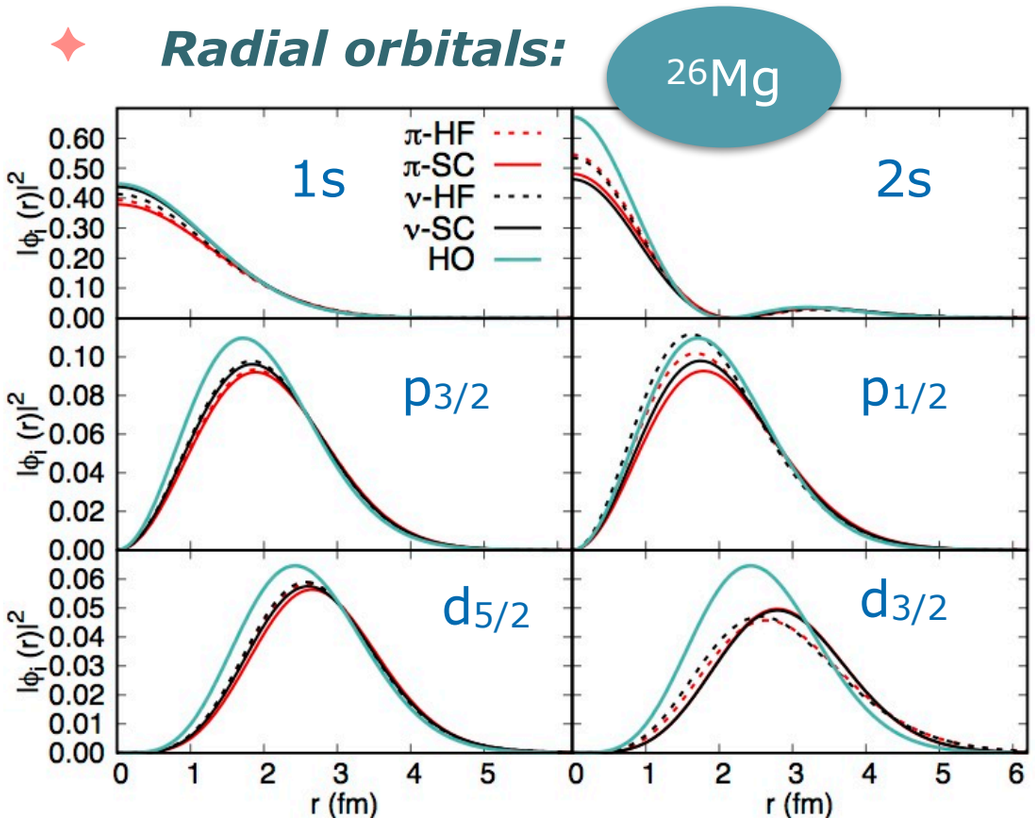
$$\sigma(\Delta r_c) = 0.017 \text{ fm} \rightarrow 0.018 \text{ fm}$$

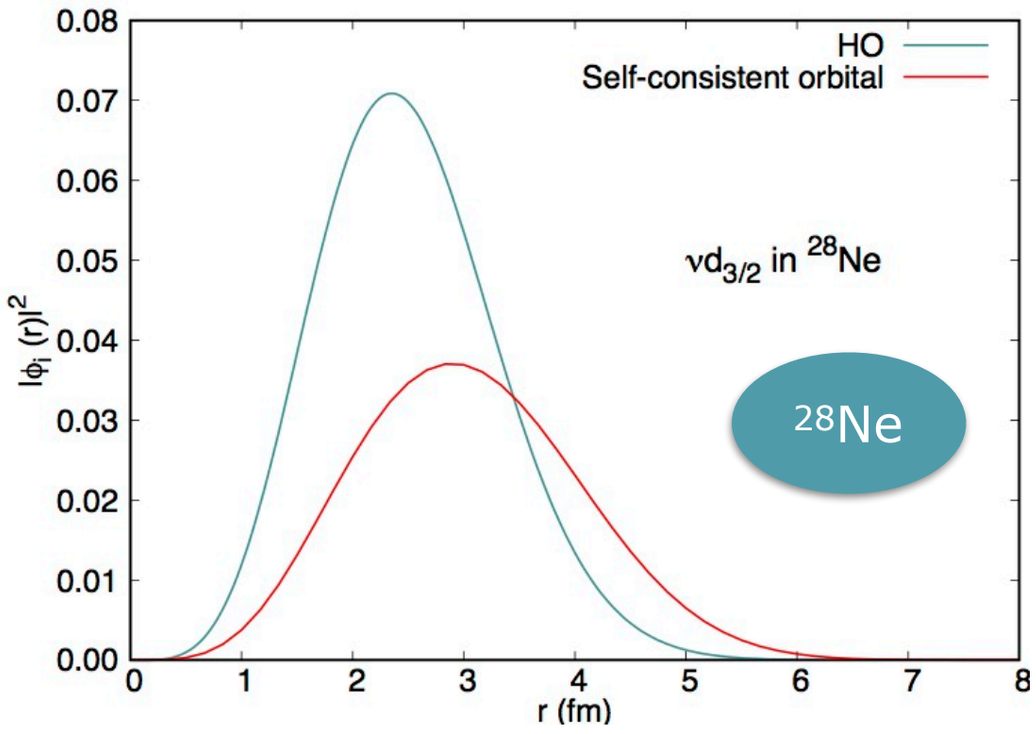
Hartree-Fock orbitals

Exp
MPMH Eq. 1)
MPMH Eqs. 1)+2)

self-consistent natural orbitals

✦ Radial orbitals:

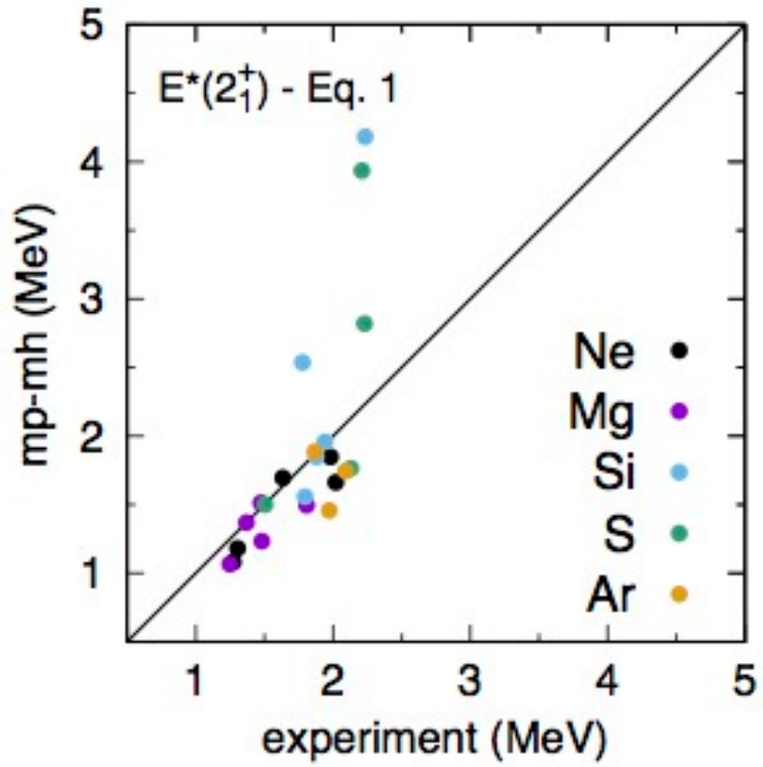




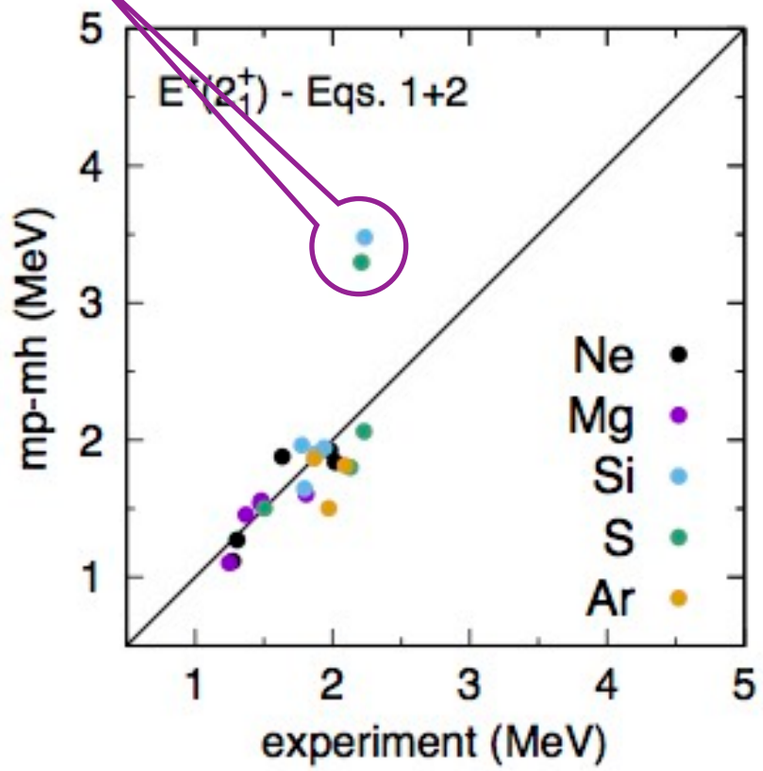
Application to sd-shell nuclei with the Gogny force

✦ ***Excitation energies:***

T=0 component of the Gogny force
(lack of tensor term, *Pillet et al. PRC 85, 044315 (2012)*)



Orbital optimization



All $\begin{cases} \langle \Delta E^* \rangle = 373 \text{ keV} \\ \sigma(\Delta E^*) = 517 \text{ keV} \end{cases}$

^{30}S & ^{30}Si excluded $\begin{cases} \langle \Delta E^* \rangle = 226 \text{keV} \\ \sigma(\Delta E^*) = 214 \text{ keV} \end{cases}$

All $\begin{cases} \langle \Delta E^* \rangle = 235 \text{ keV} \\ \sigma(\Delta E^*) = 323 \text{ keV} \end{cases}$

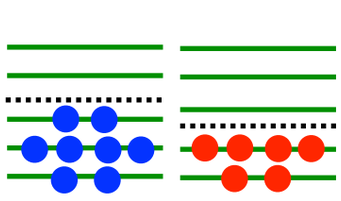
^{30}S & ^{30}Si excluded $\begin{cases} \langle \Delta E^* \rangle = 142 \text{ keV} \\ \sigma(\Delta E^*) = 122 \text{ keV} \end{cases}$

Application to sd-shell nuclei with the Gogny force

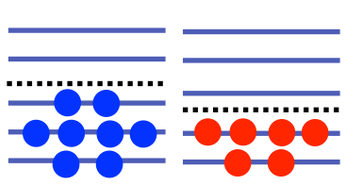
✱ ***Effect on the many-body wave function:*** Orbital transformation: $b_i^\dagger = e^{i\hat{T}} a_i^\dagger e^{-i\hat{T}}$

Pure Hartree-Fock component in correlated ground state		
nucleus	1st equation only	1st + 2nd equations
^{26}Ne	71%	62%
^{28}Si	60%	24%
^{32}S	58%	39%
^{34}S	39%	17%

New reference-state componentd state
1st + 2nd equations
69%
26%
47%
18%



➡ Pure HF component decreases: self-consistent procedure appears to fragment the wave function



Reference state built on optimized orbitals

➡ "better" than HF state

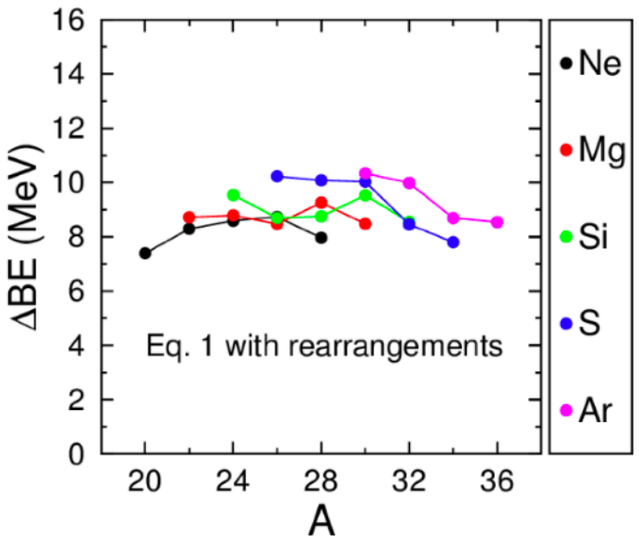
✱ ***Correlation energies:*** $E_{corr} = E(\Psi) - E(\Phi_{HF}^{(0)})$

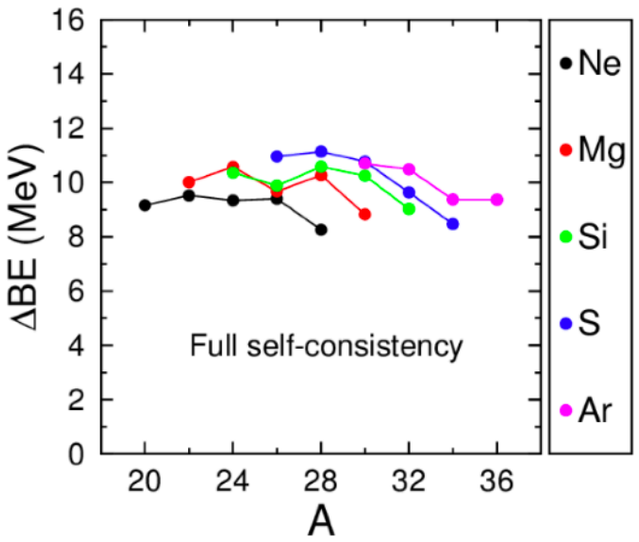
Correlation energy E_{corr} (MeV)			
nucleus	1st equation only	1st + 2nd equations	ΔE_{corr}
^{28}Ne	1.17	1.59	**0.42**
^{26}Ne	7.32	8.46	**1.14**
^{24}Ne	5.75	6.98	**1.23**
^{22}Ne	10.48	12.12	**1.64**
^{20}Ne	10.93	13.30	**2.37**

Correlation energy E_{corr} (MeV)			
nucleus	1st equation only	1st + 2nd equations	ΔE_{corr}
^{28}S	8.05	10.05	**2.00**
^{30}S	0.59	2.06	**1.47**
^{32}S	2.82	5.22	**2.40**
^{34}S	4.27	5.62	**1.35**

Systematic study of sd-shell nuclei

- Ground state properties:
  - ⋆ Binding & separation energies (difference to experiment)





- *Average difference:*

$$\langle \Delta BE \rangle = 8.91 \text{ MeV} \rightarrow 9.84 \text{ MeV}$$

→ Expected over-binding due to fitting of the D1S Gogny force.

- *Standard deviation*:

$$\sigma(\Delta BE) = 0.793 \text{ MeV} \rightarrow 0.789 \text{ MeV}$$

- *Average difference:*

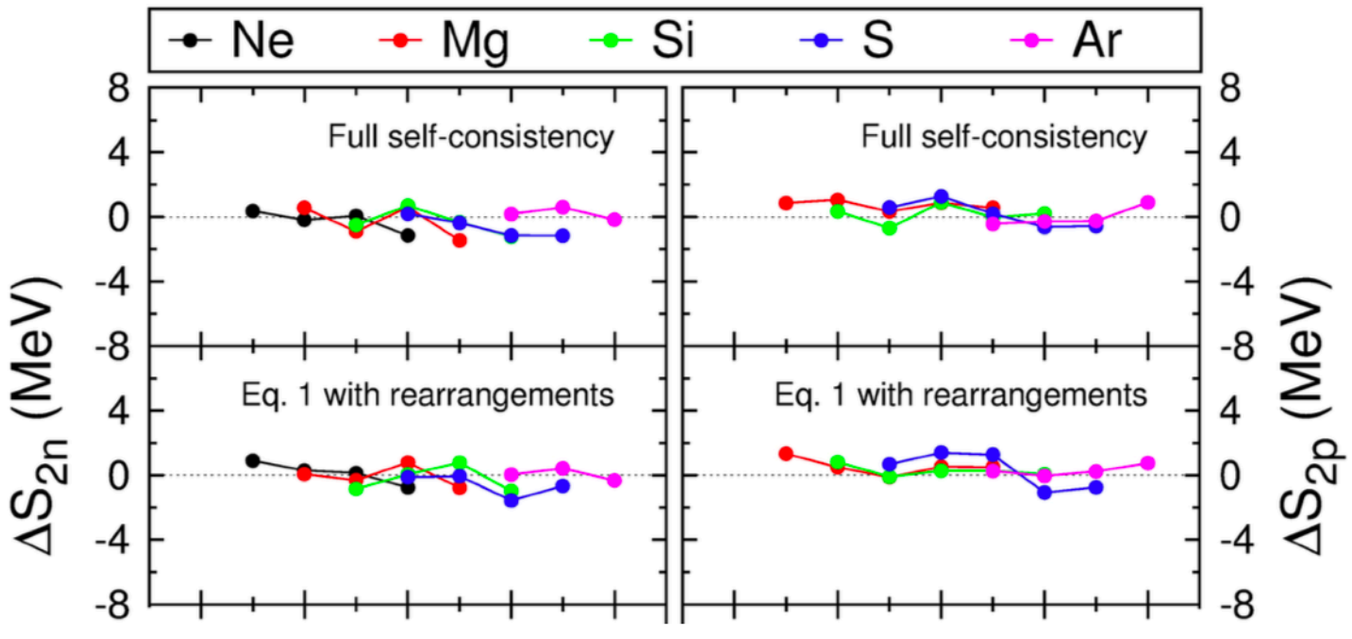
$$\langle \Delta S_{2n} \rangle = 577 \text{ keV} \rightarrow 641 \text{ keV}$$

$$\langle \Delta S_{2p} \rangle = 578 \text{ keV} \rightarrow 577 \text{ keV}$$

- *Standard deviation*:

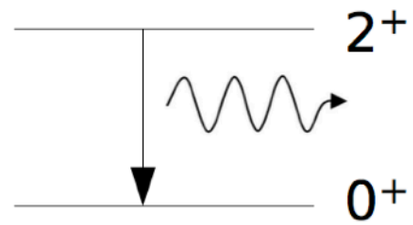
$$\sigma(\Delta S_{2n}) = 446 \text{ keV} \rightarrow 453 \text{ keV}$$

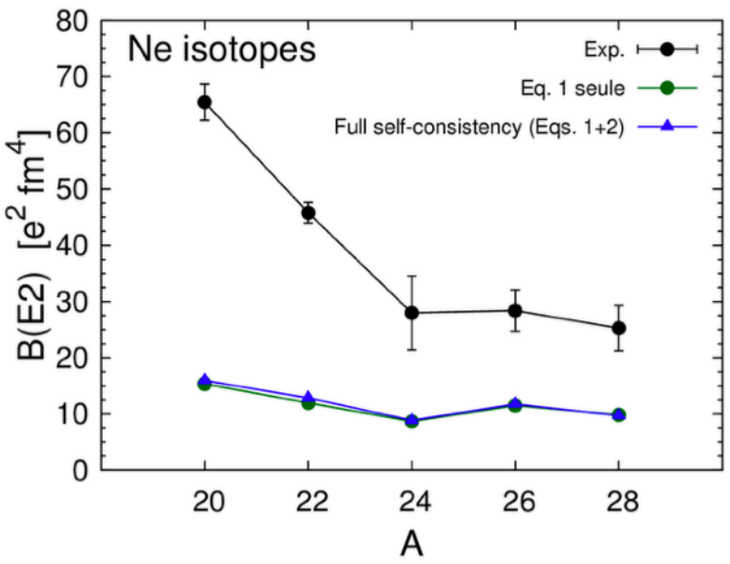
$$\sigma(\Delta S_{2p}) = 440 \text{ keV} \rightarrow 332 \text{ keV}$$

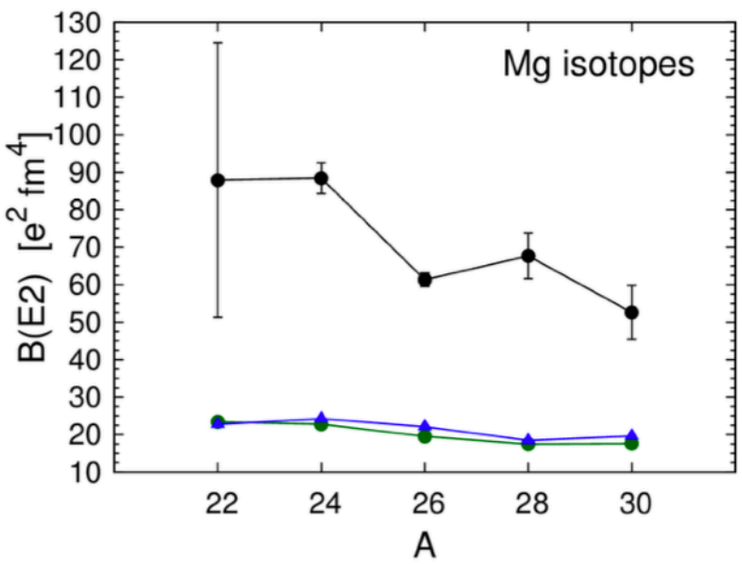


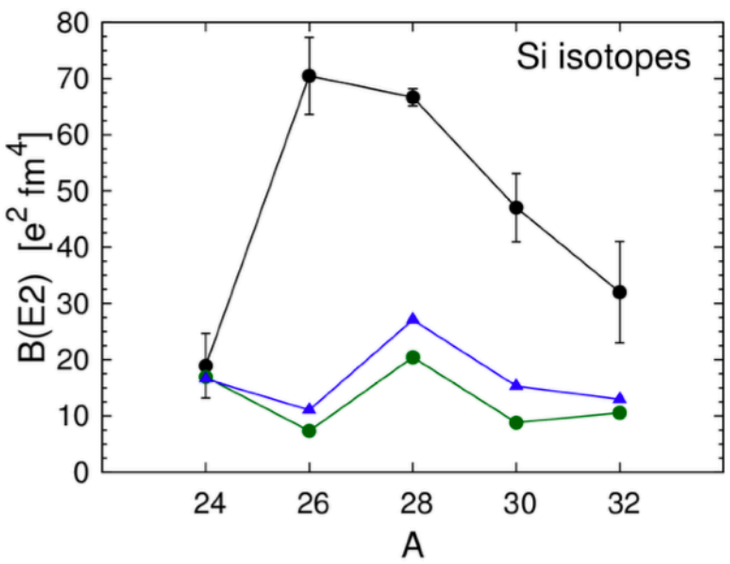
Systematic study of sd-shell nuclei

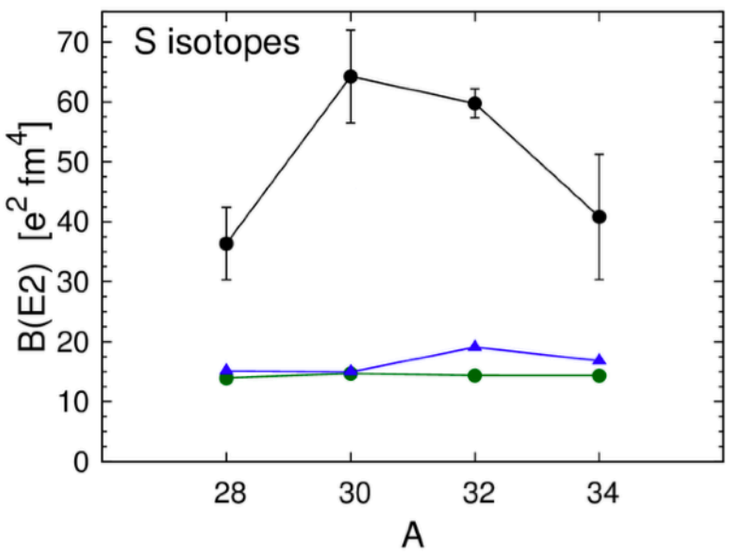
- Spectroscopic properties:
  - Transition probabilities B(E2):

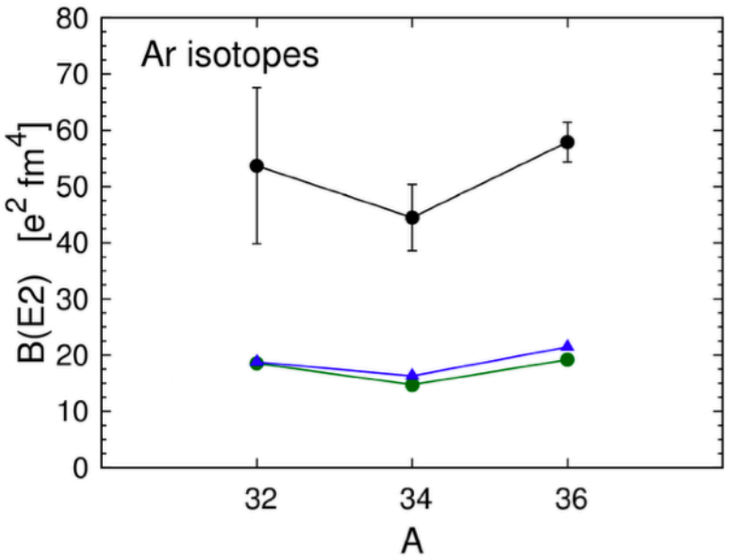












- Experimental trends globally well reproduced but...
- Clear lack of collectivity du the restricted valence space
- Positive but little effect from optimization of orbitals

→ Gain factor ~1.7 in ^{30}Si, ~1.3 in ^{28}Si and ^{32}S

Systematic study of sd-shell nuclei

★ **Excitation energies:**

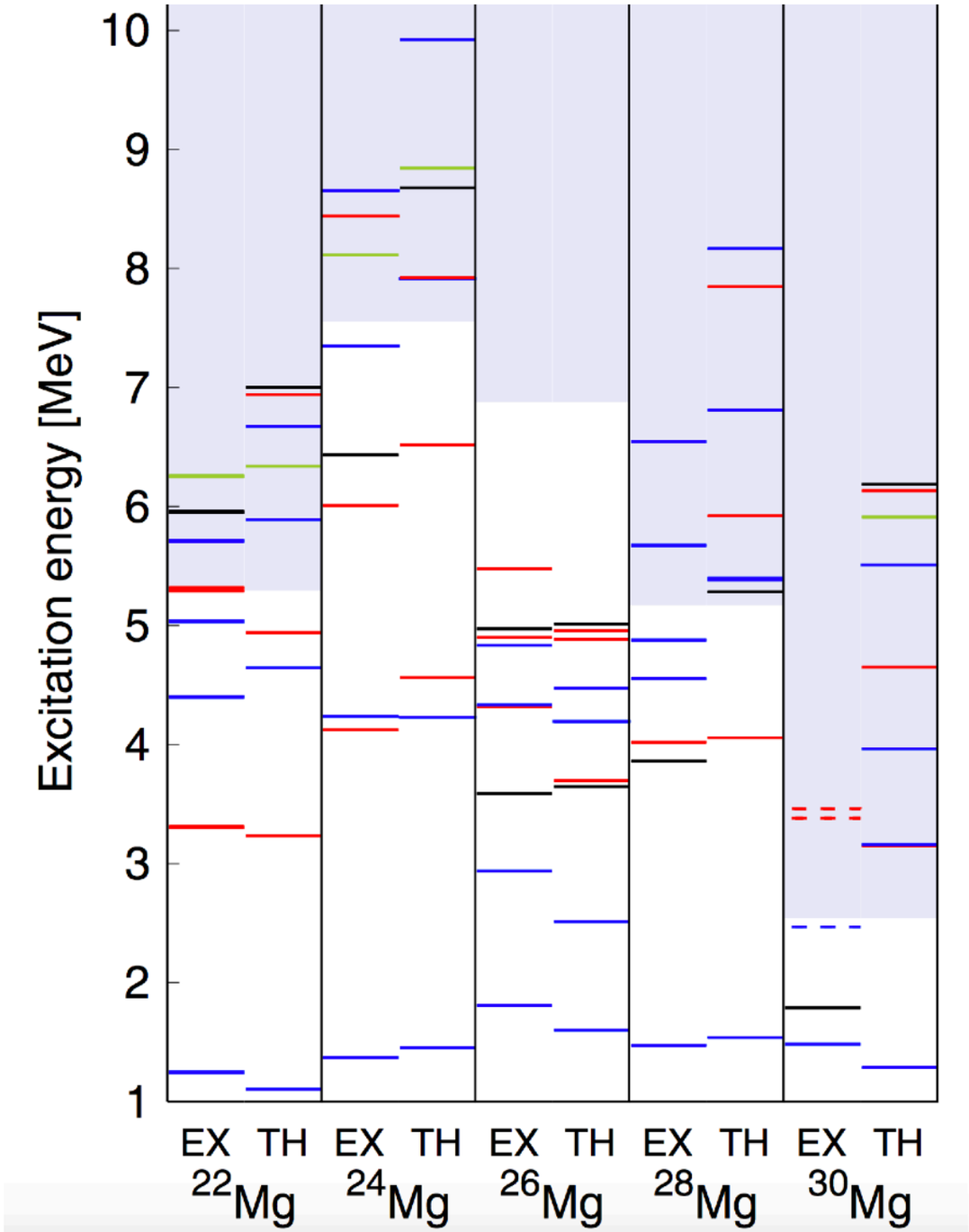


TABLE IV. Comparison between the low-energy states of ^{24}Mg calculated by the MPMH method, the GCM method of Ref. [44], and the experimental data [42]. The energies are in MeV.

State	EXP	MPMH	Ref. [44]
2_1^+	1.369	1.453	1.202
2_2^+	4.238	4.230	5.616
2_3^+	7.349	7.914	12.686
4_1^+	4.123	4.564	3.875
4_2^+	6.011	6.518	7.990
4_3^+	8.439	7.923	14.363
6_1^+	8.114	8.843	8.256
0_2^+	6.432	8.676	11.265

[44] T. R. Rodríguez and J. L. Egido, Phys. Rev. C **81**, 064323 (2010).

[42] National Nuclear Data Center (NNDC) database, www.nndc.bnl.gov.

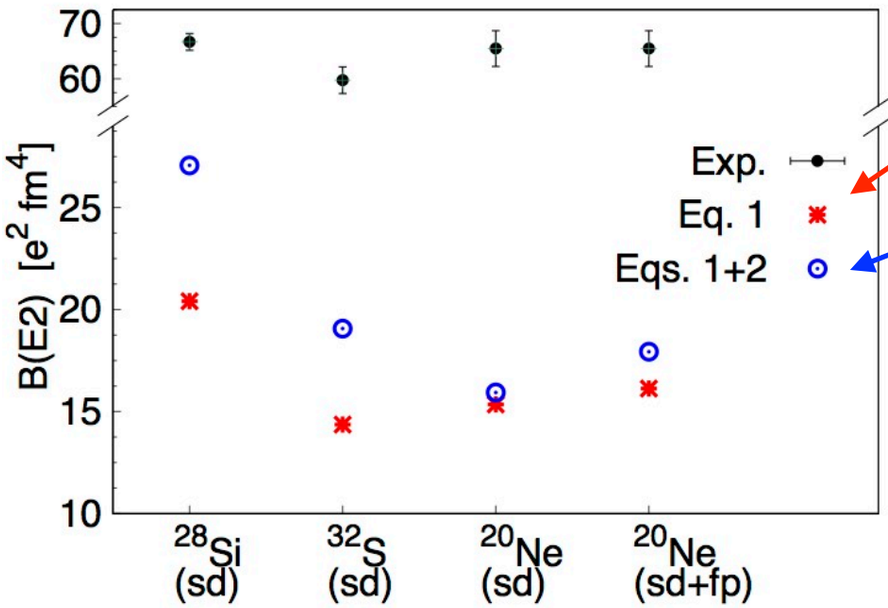
C.R. et al. PRC 95 044315 (2017).

Application to sd-shell nuclei with the Gogny force

✦ Transition probabilities B(E2)

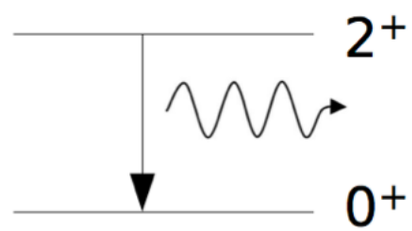
Improvement
by a factor up to ~1.7
but still clear lack of
collectivity

No effective charges



Hartree-Fock orbitals

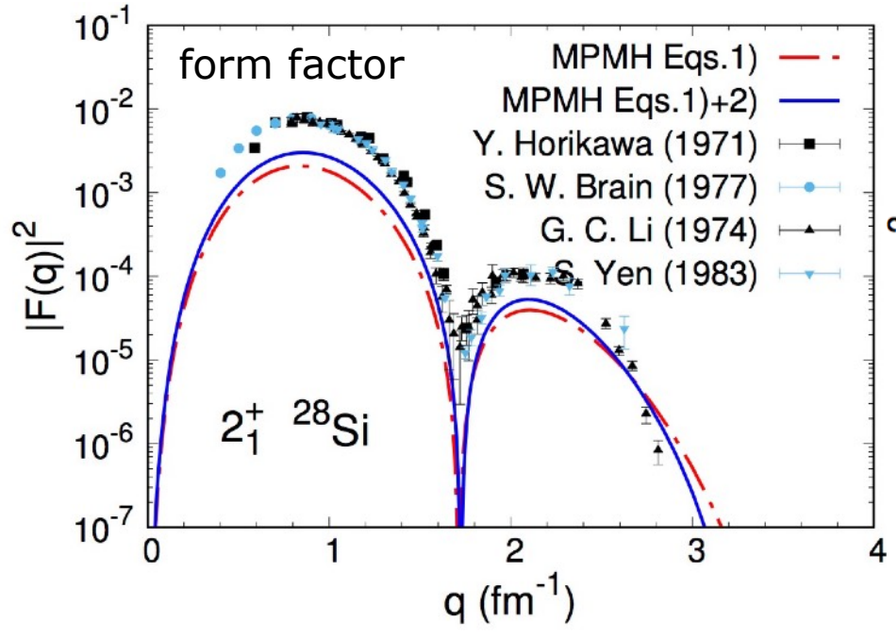
self-consistent
natural orbitals

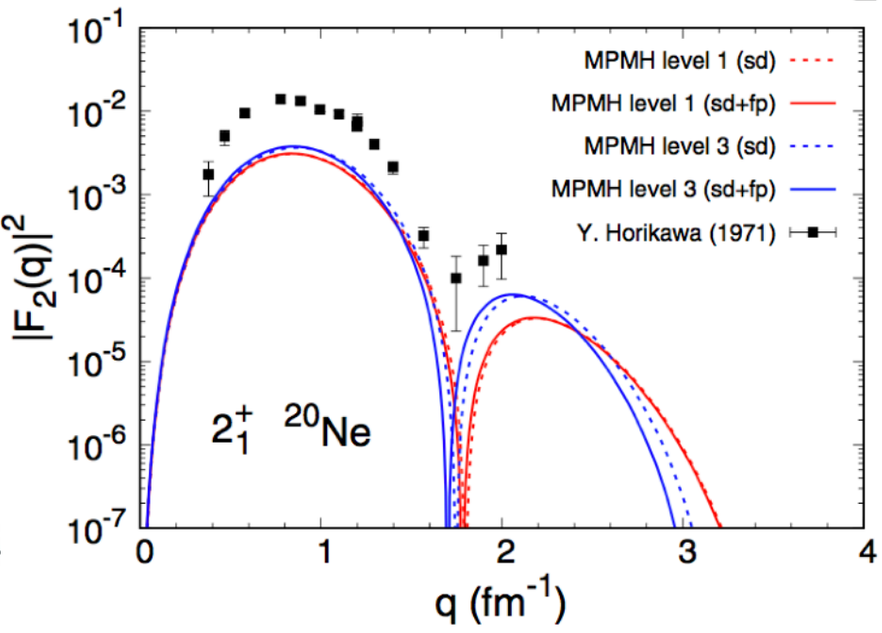


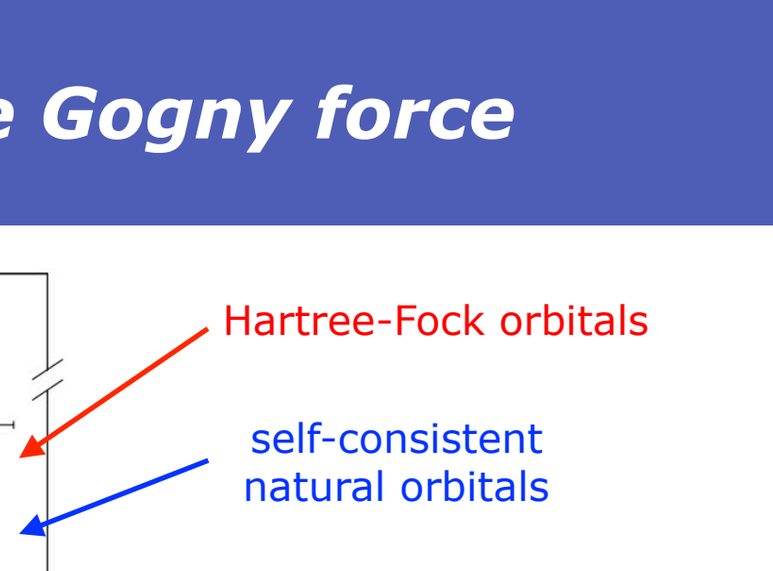
✦ Electron inelastic scattering on discrete states

Form factor: $F_\lambda(q) = \frac{\sqrt{4\pi}}{Z}\sqrt{\frac{2J_f+1}{2J_i+1}}\int_0^\infty r^2\, dr\; j_\lambda(qr)\,\rho_{tr}(r)$

From MPMH:







With optimized states:

- Small increase of the magnitude
- Improvement of the trend at high q

with M. Dupuis, CEA,DAM,DIF

Application of the MPMH method with a chiral interaction

(II) Chiral interaction with local analytical form

- In MPMH, we have to do the calculation of the mean field/source term at each iteration

  ↠ use matrix elements as only input will become inefficient for mid-mass nuclei

  ↠ need potential in coordinate space and ideally Gaussians

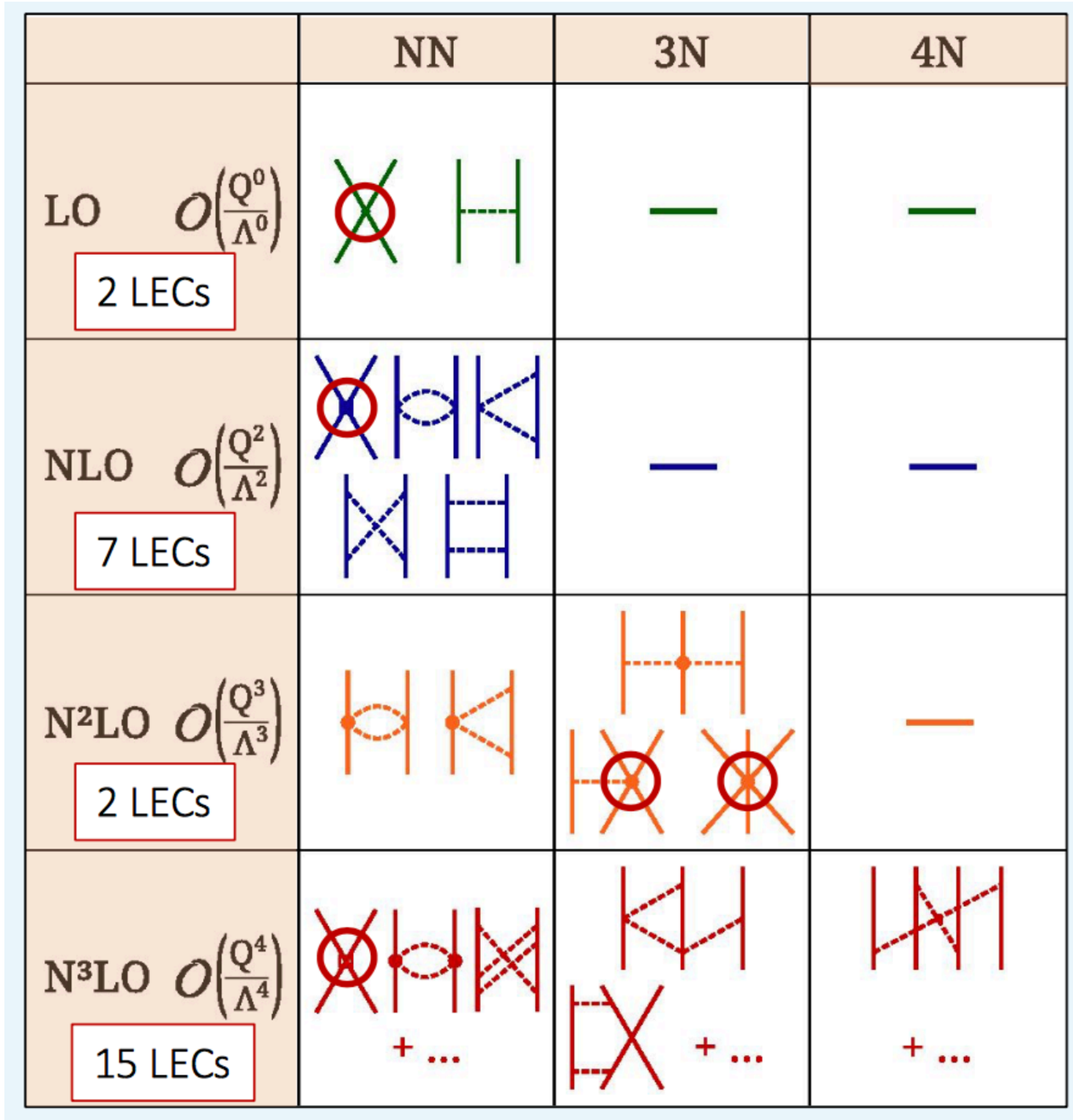
- Ingo Tews and collaborators have developed **local** chiral interactions with **Gaussian regulators** that can be written in coordinate space

See e.g. A. Gezerlis, I. Tews, E. Epelbaum et al., Phys. Rev. C 90, 054323 (2014)

At each order:

contact terms
+
long-range pion-exchange terms

Chiral expansion:



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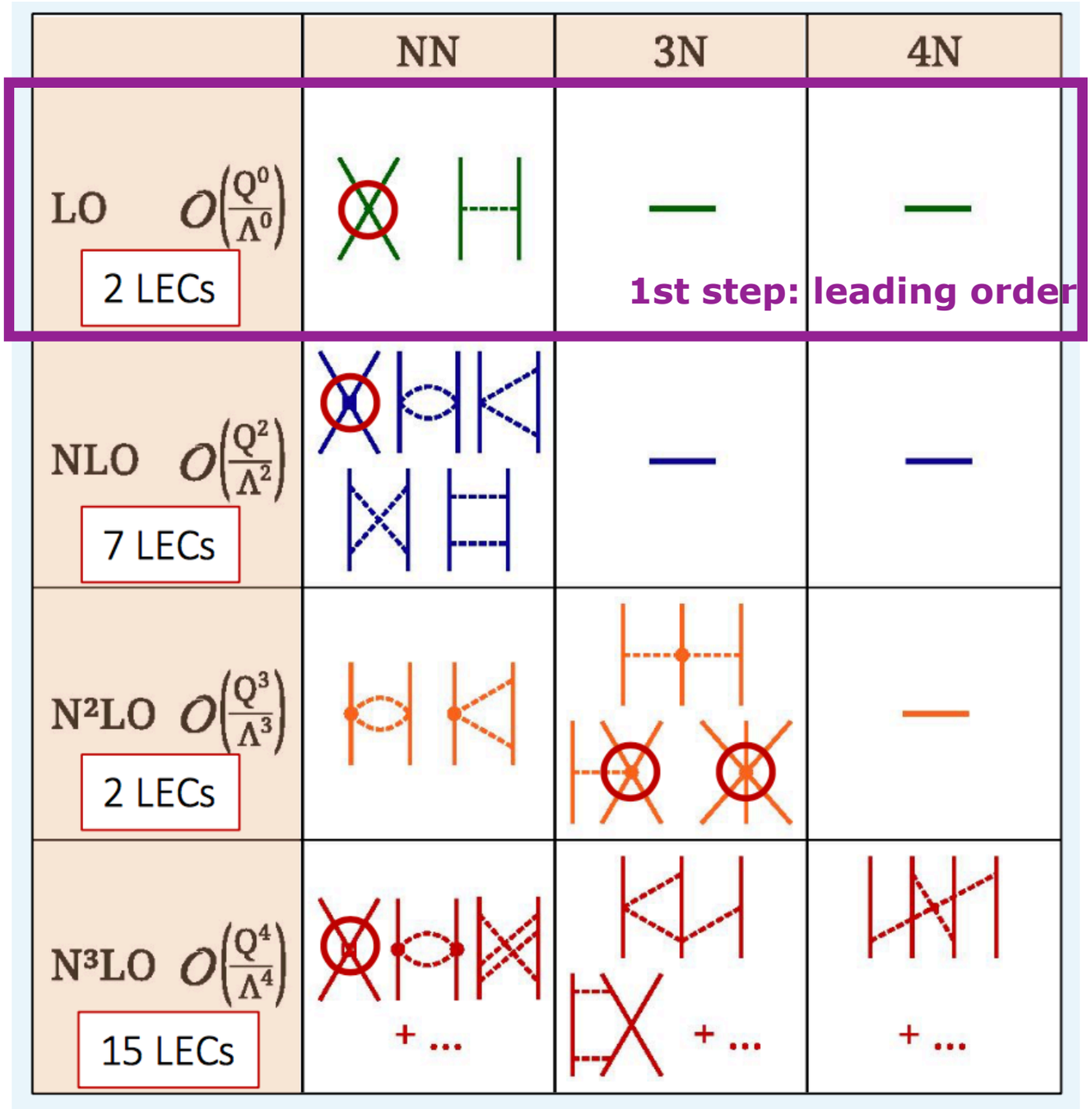
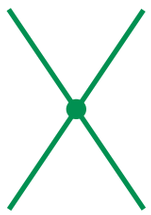


Application of the MPMH method with a chiral interaction

★ Chiral interaction at leading order with Gaussian regulators:

cut-off R_0= 1 fm

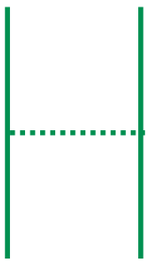
✦ contact term:



$$V_{contact}^{LO}(r) = (C_S + C_T \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \times \underbrace{\left(\alpha\, e^{-(r/R_0)^2}\right)}_{\text{regulator}}$$

↠ purely gaussian

✦ long-range one-pion exchange:



$$V_{OPE}^{LO}(r) = \left(W_S^{(0)}(r)\, \vec{\tau}_1 \cdot \vec{\tau}_2\, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + W_T^{(0)}(r)\, \vec{\tau}_1 \cdot \vec{\tau}_2\, S_{12}\right) \times \underbrace{\left(1 - e^{-(r/R_0)^2}\right)^2}_{\text{regulator}}$$

central spin-isospin term:

$$W_S^{(0)}(r) = \frac{M_\pi^3}{12\pi} \left(\frac{g_A}{2F_\pi}\right)^2 \frac{e^{-M_\pi r}}{M_\pi r}$$

tensor isospin term:

$$W_T^{(0)}(r) = \frac{M_\pi^3}{12\pi} \left(\frac{g_A}{2F_\pi}\right)^2 \frac{e^{-M_\pi r}}{M_\pi r} \left(1 + \frac{3}{M_\pi r} + \frac{3}{(M_\pi r)^2}\right)$$

↠ Yukawa or Yukawa-like x Gaussians

Application of the MPMH method with a chiral interaction

★ Strategy: fit the regularized Yukawa or Yukawa-like functions to a sum of Gaussians

$$W^{(0)}_{S,reg}(r) \propto \frac{e^{-M_\pi r}}{r} \times (1 - e^{-(r/R_0)^2})^2 \simeq \sum_i a_i^S e^{-(r/b_i^S)^2}$$

$$W^{(0)}_{T,reg}(r) \propto \frac{e^{-M_\pi r}}{r} \left(1 + \frac{3}{M_\pi r} + \frac{3}{(M_\pi r)^2}\right) \times (1 - e^{-(r/R_0)^2})^2 \simeq \sum_i a_i^T e^{-(r/b_i^T)^2}$$

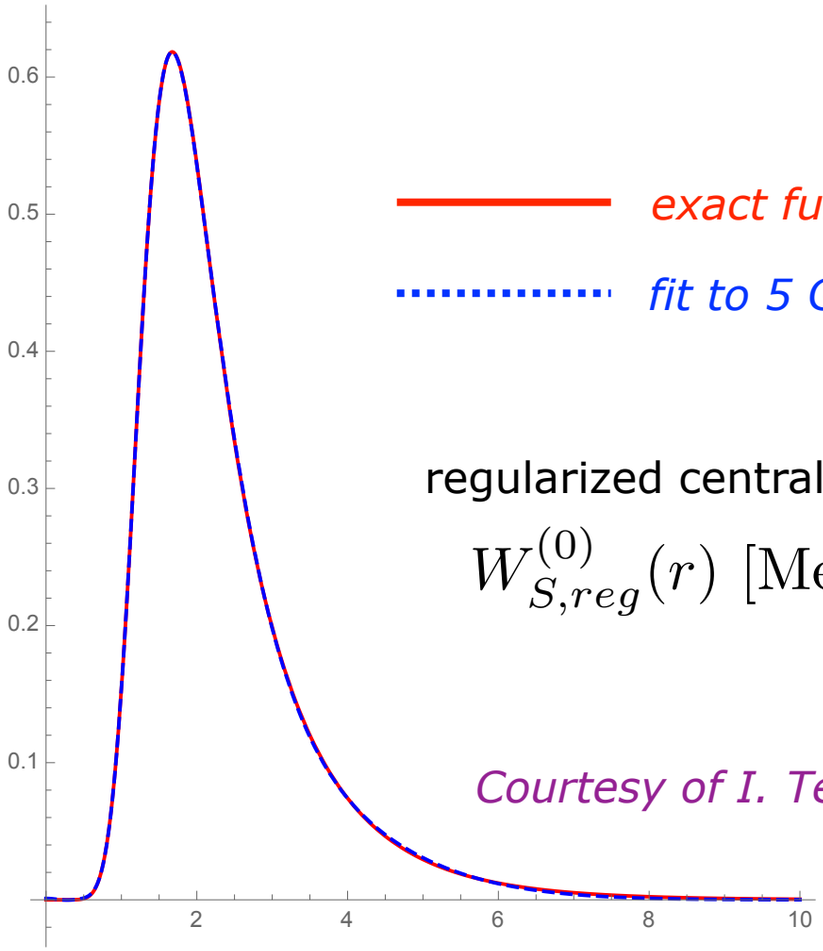
to use the machinery already developed in the original code for the Gogny interaction

Note:
such fits of Yukawa to Gaussians already applied in *J. Dobaczewski & J. Engel, Phys. Rev. Lett. 94, 232502 (2005), or more recently in e.g. R. Navarro Pérez et al. PRC 97, 054304 (2018).*

Application of the MPMH method with a chiral interaction

➛ **Ex: Central term**

Very preliminary!



exact function

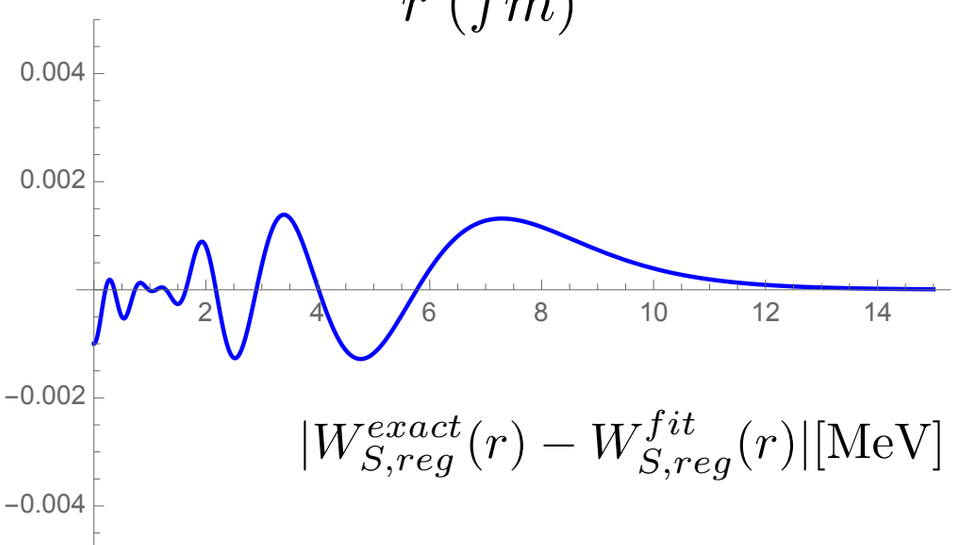
fit to 5 Gaussians

regularized central term

$$W^{(0)}_{S,reg}(r)\ [\mathrm{MeV}]$$

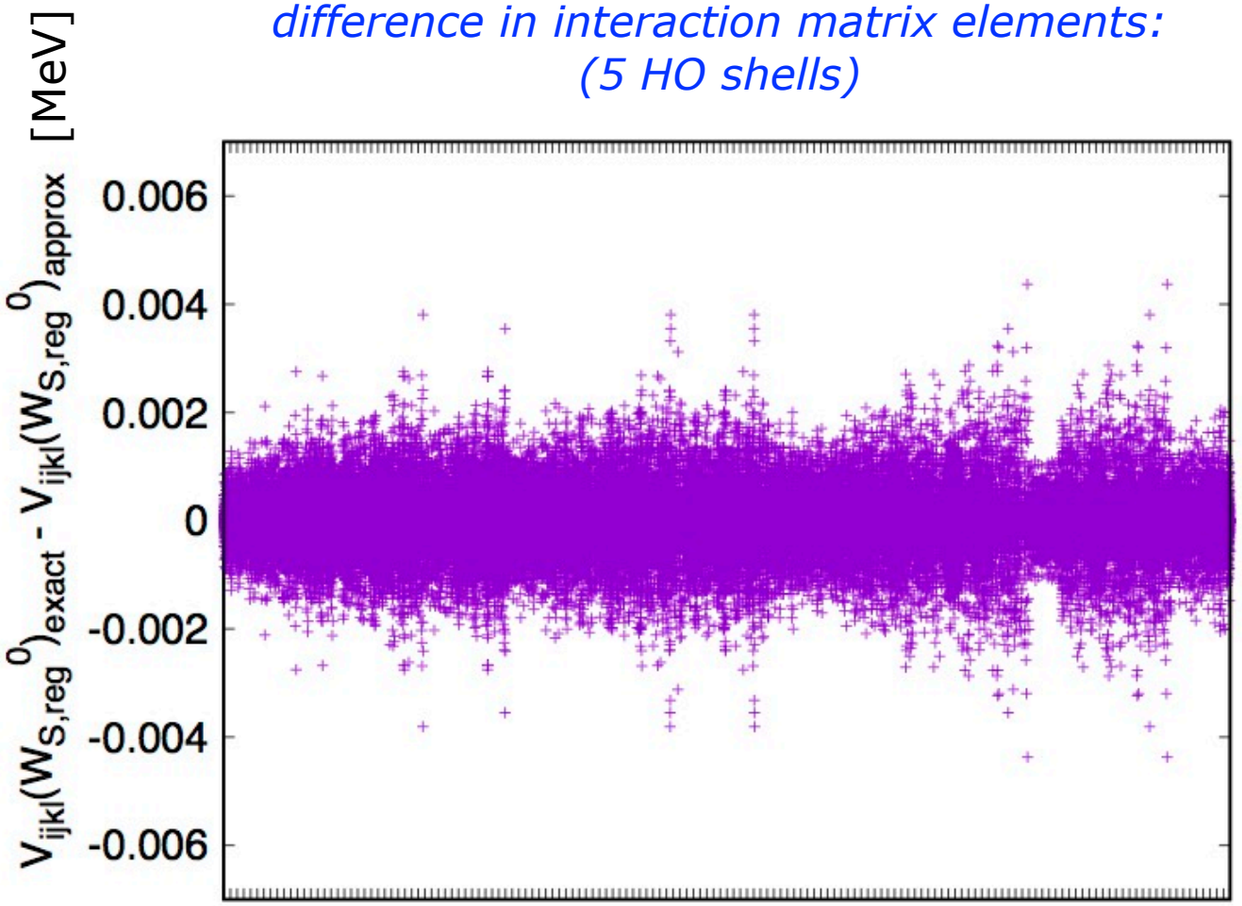
Courtesy of I. Tews

$r\ (fm)$



$$|W^{exact}_{S,reg}(r) - W^{fit}_{S,reg}(r)|[\mathrm{MeV}]$$

difference in interaction matrix elements: (5 HO shells)



✳ Average difference:

$$\langle \Delta\widetilde{V} \rangle = \frac{1}{N} \sum_{\{ijkl\}=1}^{N} |\widetilde{V}^{exact}_{ijkl} - \widetilde{V}^{fit}_{ijkl}|$$

$$= 2.10 \times 10^{-5}\ \mathrm{MeV}$$

✳ standard deviation:

$$s = \sqrt{\langle \Delta\widetilde{V}^2 \rangle - \langle \Delta\widetilde{V} \rangle^2} \quad = 1.20 \times 10^{-4}\ \mathrm{MeV}$$

➡ *<4 keV difference on the binding energy of ^{4}He (no self-consistency)*