Natural orbital methods for *ab initio* nuclear structure

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Natural orbitals for Nuclear Structure – Outline

1. No-Core Configuration Interaction (NCCI) Overview
2. Natural Orbital Definition
3. Description of He Nuclei with Natural Orbitals

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Basics of NCCI

Begin with single-particle Hilbert space spanned by orthonormal single-particle basis $\{|\alpha\rangle\}$:

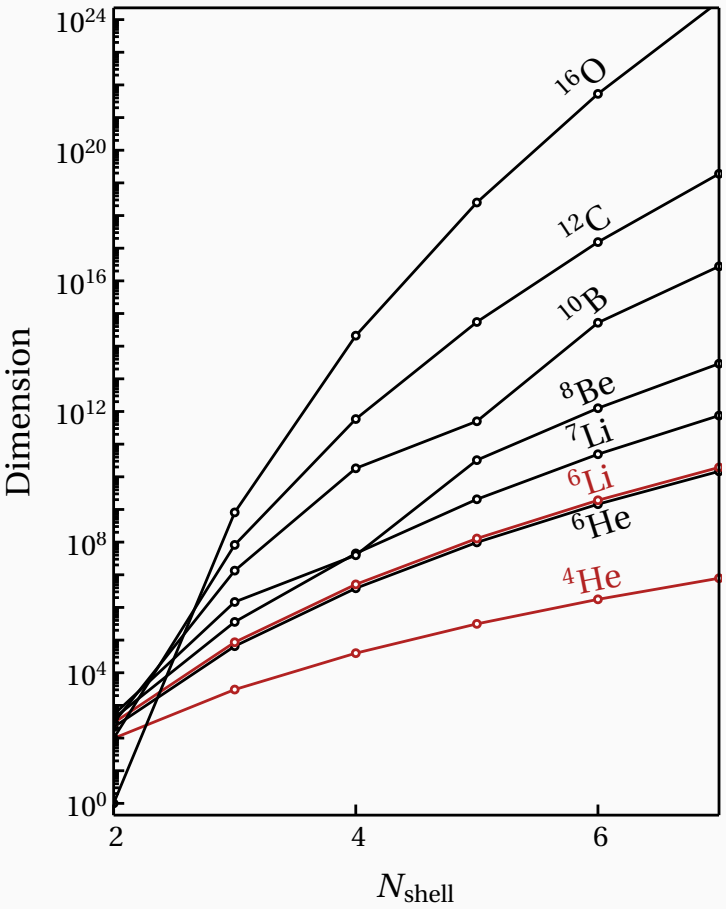
$$\hat{h}\,|nljm\rangle = \epsilon_{nljm}\,|nljm\rangle$$

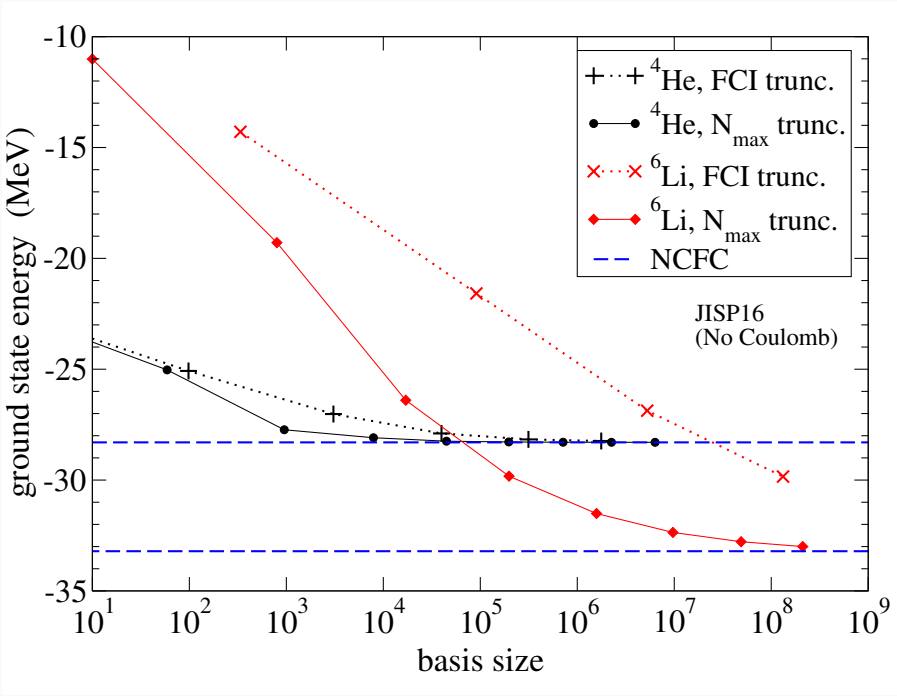
This space has an (countably) infinite dimension; computationally, we must truncate to a finite number of single-particle states.

Construct a many-body basis of Slater determinants with good M:

$$\{|\Psi_\alpha\rangle\} = \left\{ |\pi_{\alpha_1}\pi_{\alpha_2}\cdots\pi_{\alpha_Z}\nu_{\alpha_1}\nu_{\alpha_2}\cdots\nu_{\alpha_N}\rangle \middle| \sum_i m_i = M \right\}$$

Basics of NCCI – The Curse of Dimensionality





Basis grows too fast keeping all possible Slater determinants, i.e. Full Configuration Interaction (FCI).

→Can we eliminate some Slater determinants we don't need?

N_{max} Truncation

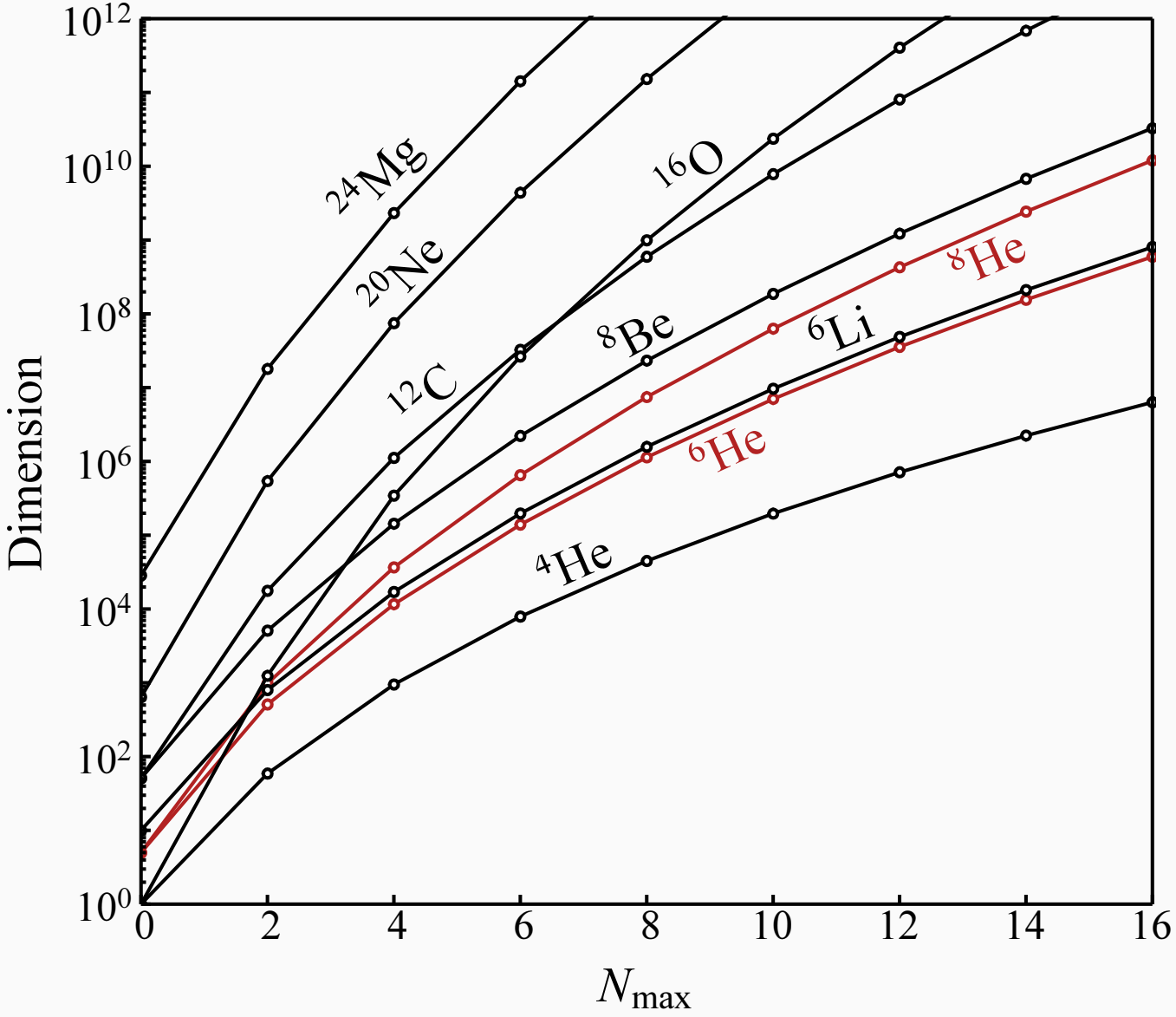
All Slaters with a total number of oscillator quanta

$$N = \sum_{\alpha=1}^{A} N_\alpha \leq N_0 + N_{max}$$

are included in the basis, where N_α is the oscillator quantum number of the $\alpha - th$ particle, and N_0 is the number of oscillator quanta in the lowest configuration.

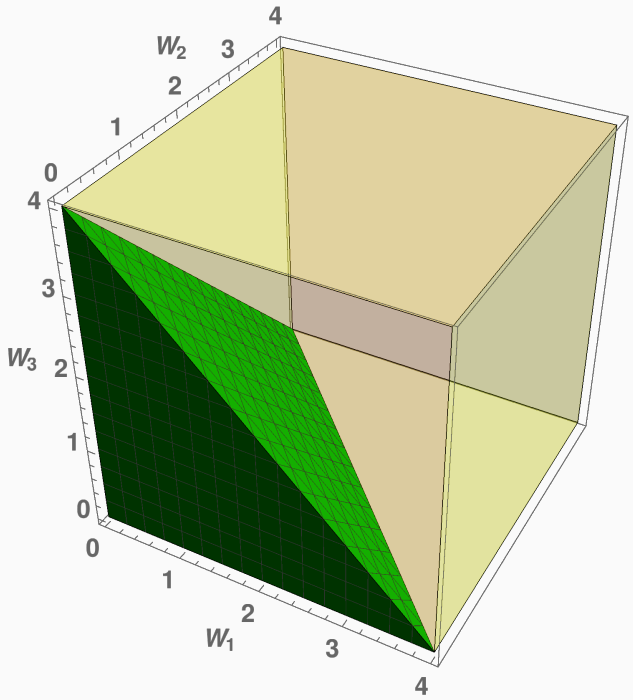
N_{max}-truncation has been preferred traditionally because it allows exact center-of-mass factorization, and can lead to faster convergence with respect to basis size than FCI-truncation.

NCCI Basis Size



Many-body truncation

1. Assign each single-particle state a weight w_α (e.g. harmonic oscillator quanta $N = 2n + \ell$) and sort orbitals by that weight.
2. Assign a weight to the Slater determinants by $W_\alpha = \sum w_{\alpha_i}$.
3. Truncate based on weight of Slater determinant $W_\alpha \leq W_{max}$.



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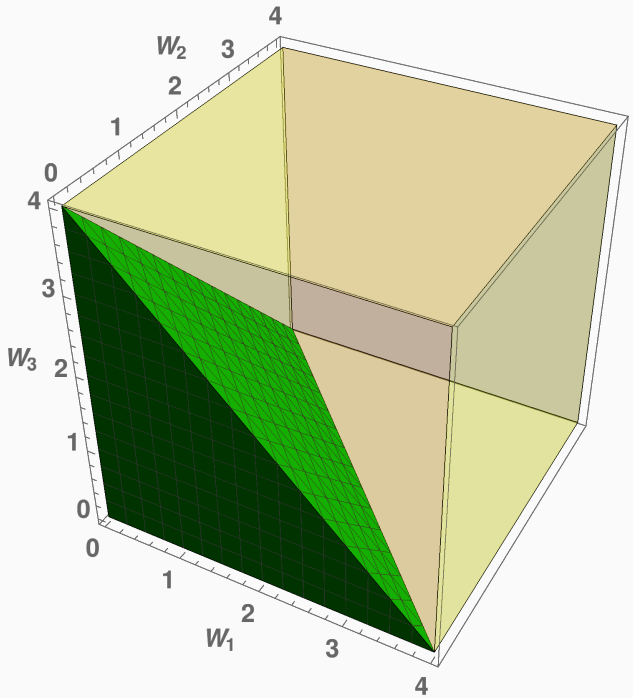

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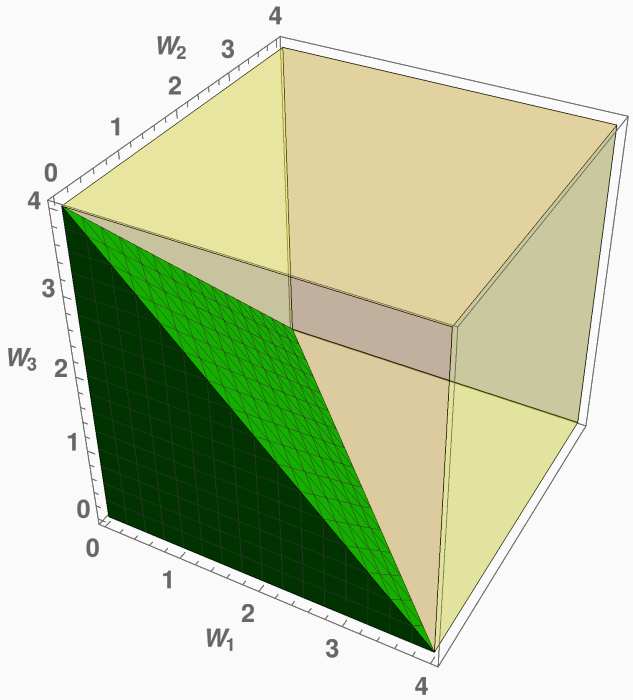
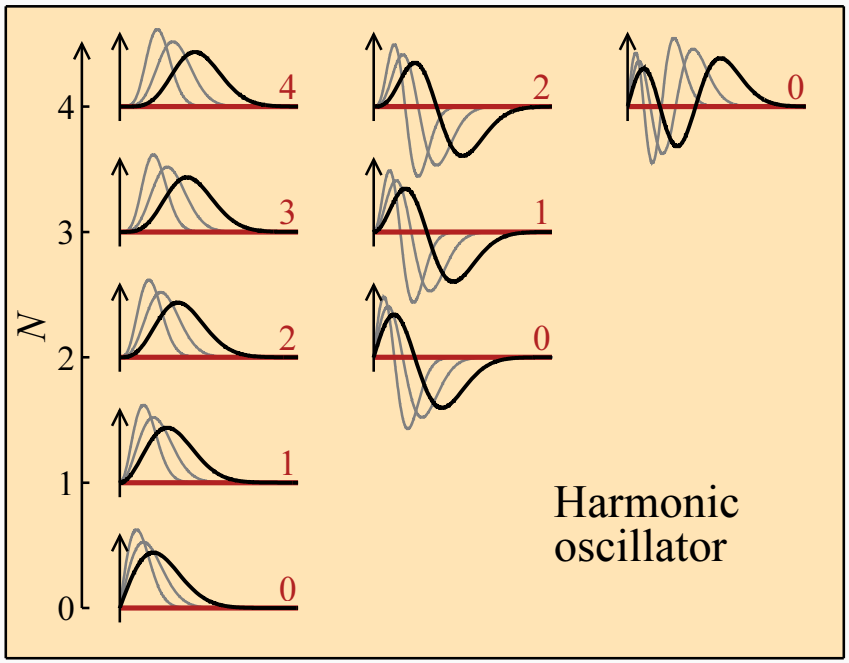


Convergence of NCCI Calculations

By completeness, a calculation in the infinite space $\rightarrow$ independence from parameters in the single-particle basis (i.e. $\hbar\omega$).

Convergence is signalled by independence of the calculated value from N_{max} and $b = (\hbar c)/\sqrt{(m_N c^2)(\hbar\omega)}$.



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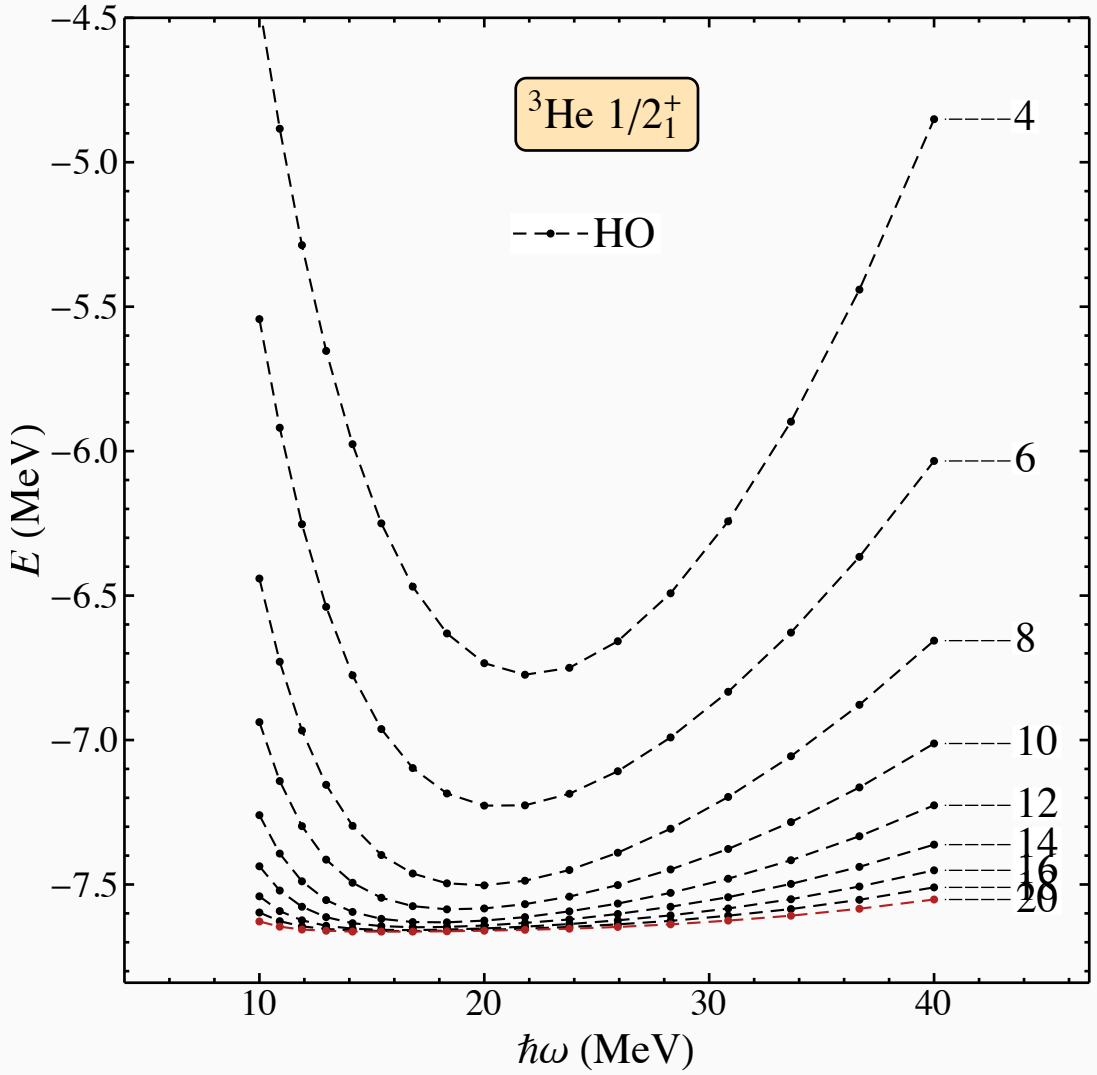

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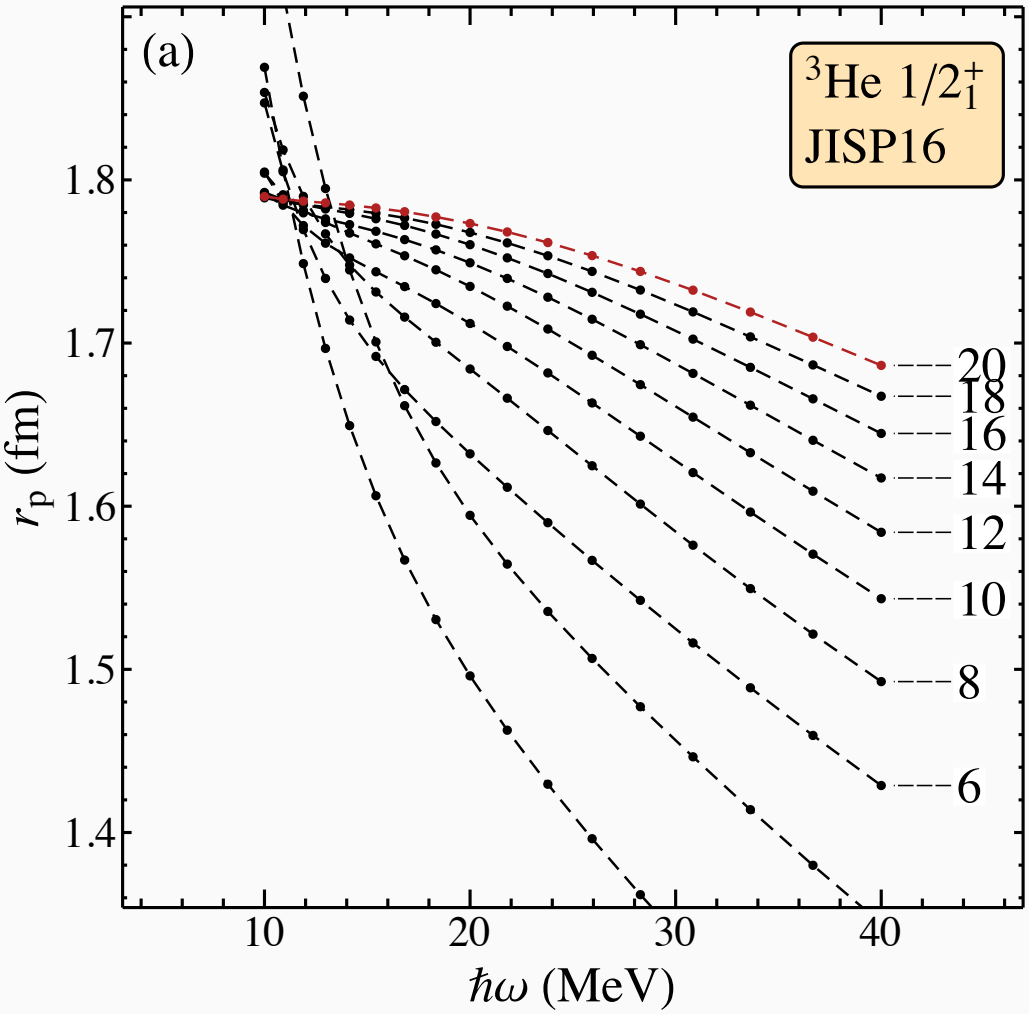

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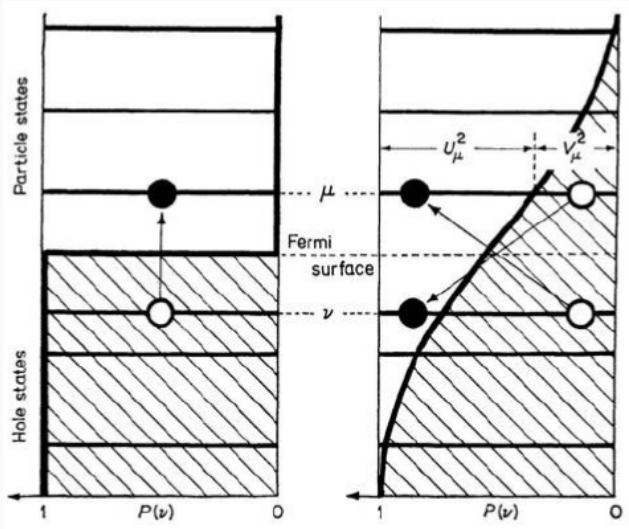
Natural Orbitals for Nuclear Physics

- Attempt to formulate a “natural” basis for performing NCCI calculations.
- Observables should converge faster in “natural” basis.
- Define “natural” $\rightarrow$ maximize occupation of lowest orbitals
- Minimizing depletion of Fermi sea, not minimizing energy!
- Built from many-body calculation, so maybe “aware” of correlations.



rowe2010:collective-motion

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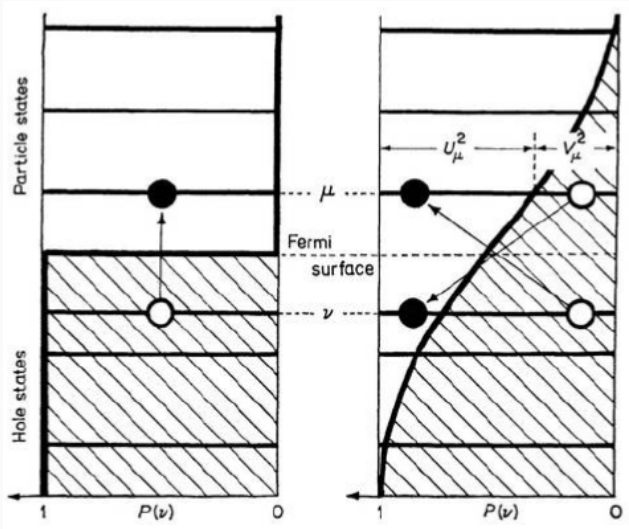

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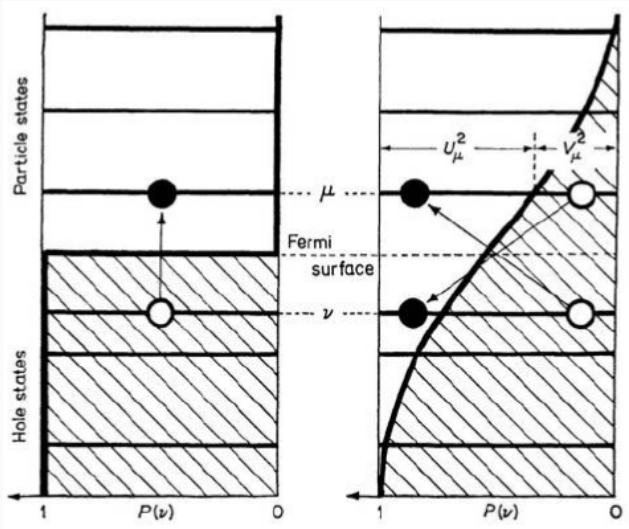

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Natural Orbitals for Nuclear Physics

Natural orbitals are the eigenvectors of the one-body RDM

$\rho_{\alpha\beta} = \langle\alpha|\,\hat{\rho}\,|\beta\rangle$

One-Body Reduced Density Matrix (RDM)

$$\hat{\rho} = \sum_{\alpha\beta} |\alpha\rangle \langle\Psi|\, a_\alpha^\dagger a_\beta \,|\Psi\rangle \langle\beta|$$

$$\rho(\mathbf{x}, \mathbf{x}') = A \int \Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_A)\Psi^*(\mathbf{x}', \mathbf{x}_2, \ldots, \mathbf{x}_A)\mathrm{d}\mathbf{x}_2 \cdots \mathrm{d}\mathbf{x}_A$$

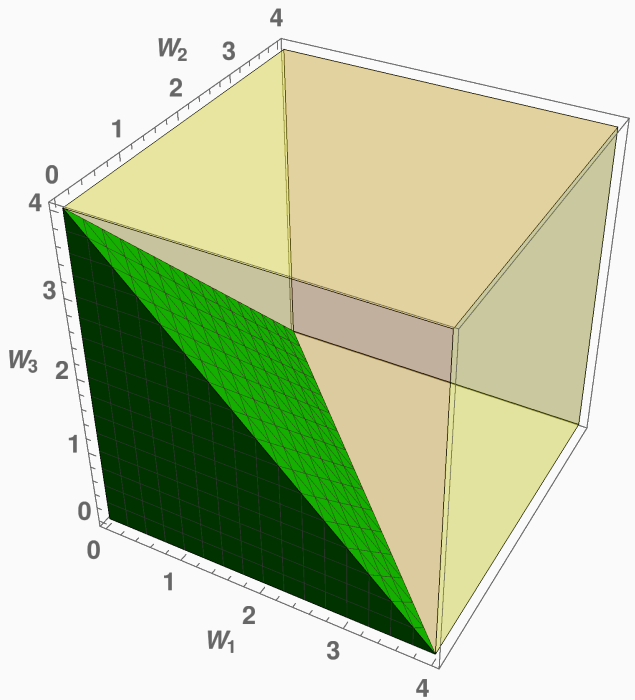
- Hermitian operator on the single-particle space;
- Depends on some reference many-body state $|\Psi\rangle$;
- Contains all single-particle behavior in $|\Psi\rangle$;
- Number operator expectation values on diagonal
  $\rho_{\alpha\alpha} = \langle\alpha|\Psi|\alpha\rangle = \langle\Psi|N_\alpha|\Psi\rangle$

Natural Orbitals for Nuclear Physics

A change of basis on the single-particle space:

- does not change the single-particle space;
- does not change the FCI many-body space;
- does change a truncated many-body space.

We must sort our new natural orbitals by occupation.



Natural Orbitals – Two examples

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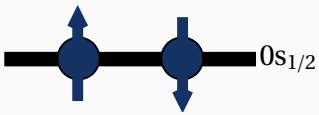
Eigenvector in initial basis:

$$|\Psi\rangle = \frac{1}{2}\Big(\underbrace{\big|(0s_\uparrow)(0s_\downarrow)\big\rangle}_{N=0} + \underbrace{\big|(0s_\uparrow)(1s_\downarrow)\big\rangle - \big|(0s_\downarrow)(1s_\uparrow)\big\rangle}_{N=2} + \underbrace{\big|(1s_\uparrow)(1s_\downarrow)\big\rangle}_{N=4}\Big)$$



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Density matrix:

$$\rho = \begin{pmatrix} 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \end{pmatrix}$$

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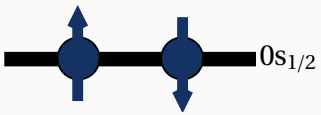

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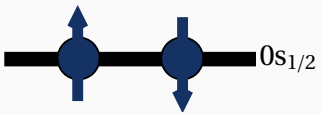

Eigenvector in natural orbital basis:

$$|\Psi\rangle = \left|(0s'_\uparrow)(0s'_\downarrow)\right\rangle$$

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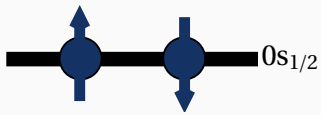

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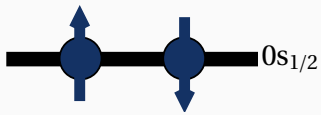

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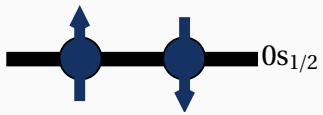

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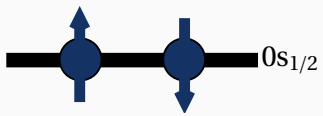

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Natural Orbitals for NCCI

How we use natural orbitals to accelerate convergence:

1. Perform an initial many-body NCCI calculation in an oscillator basis.
2. Compute an *approximate* one-body reduced density matrix from one of the many-body states.
3. Diagonalize the one-body reduced density matrix to obtain a new basis.
4. Transform all input Hamiltonian matrix elements.
5. Diagonalize many-body Hamiltonian in new many-body basis.

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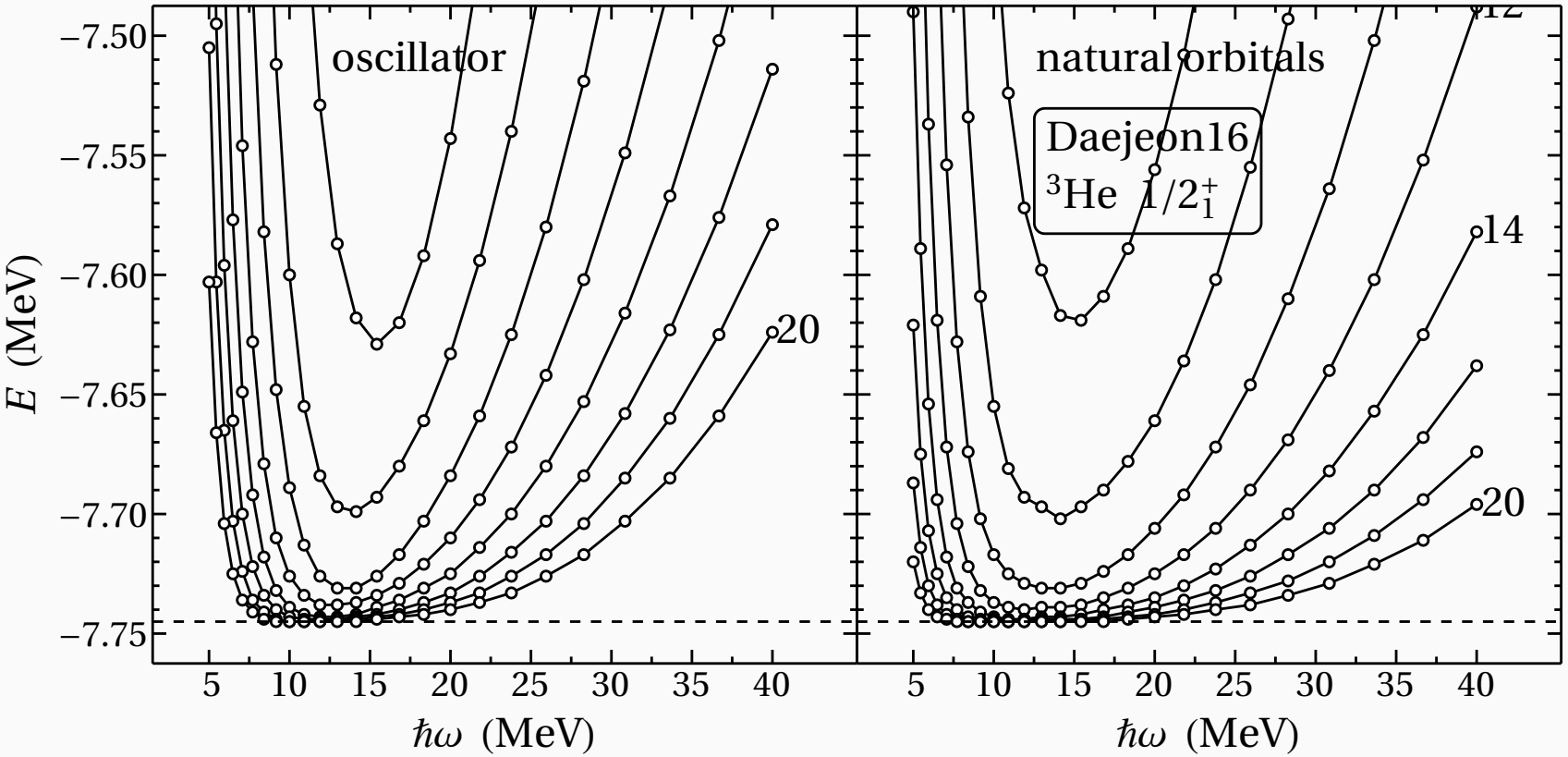

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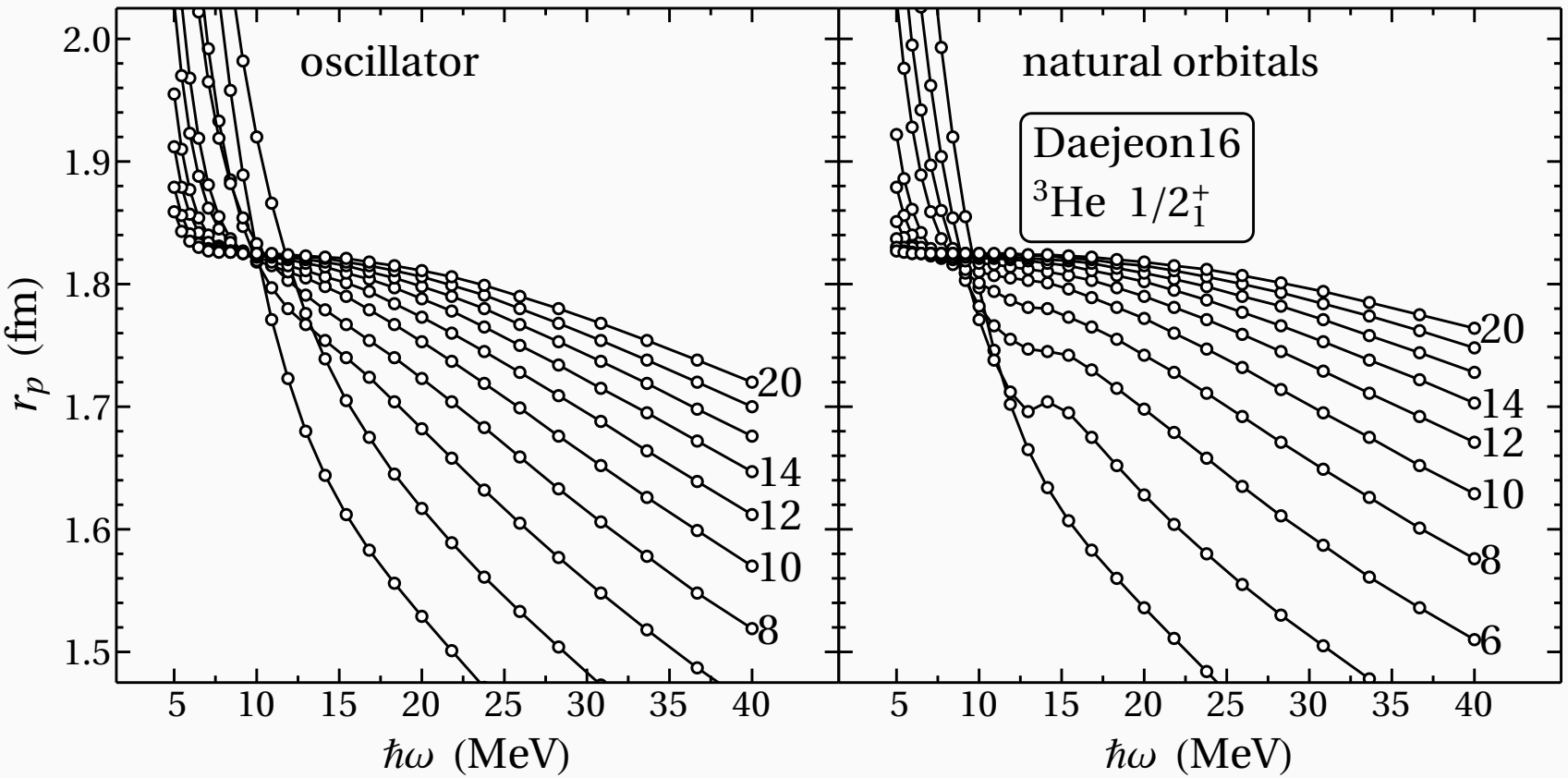

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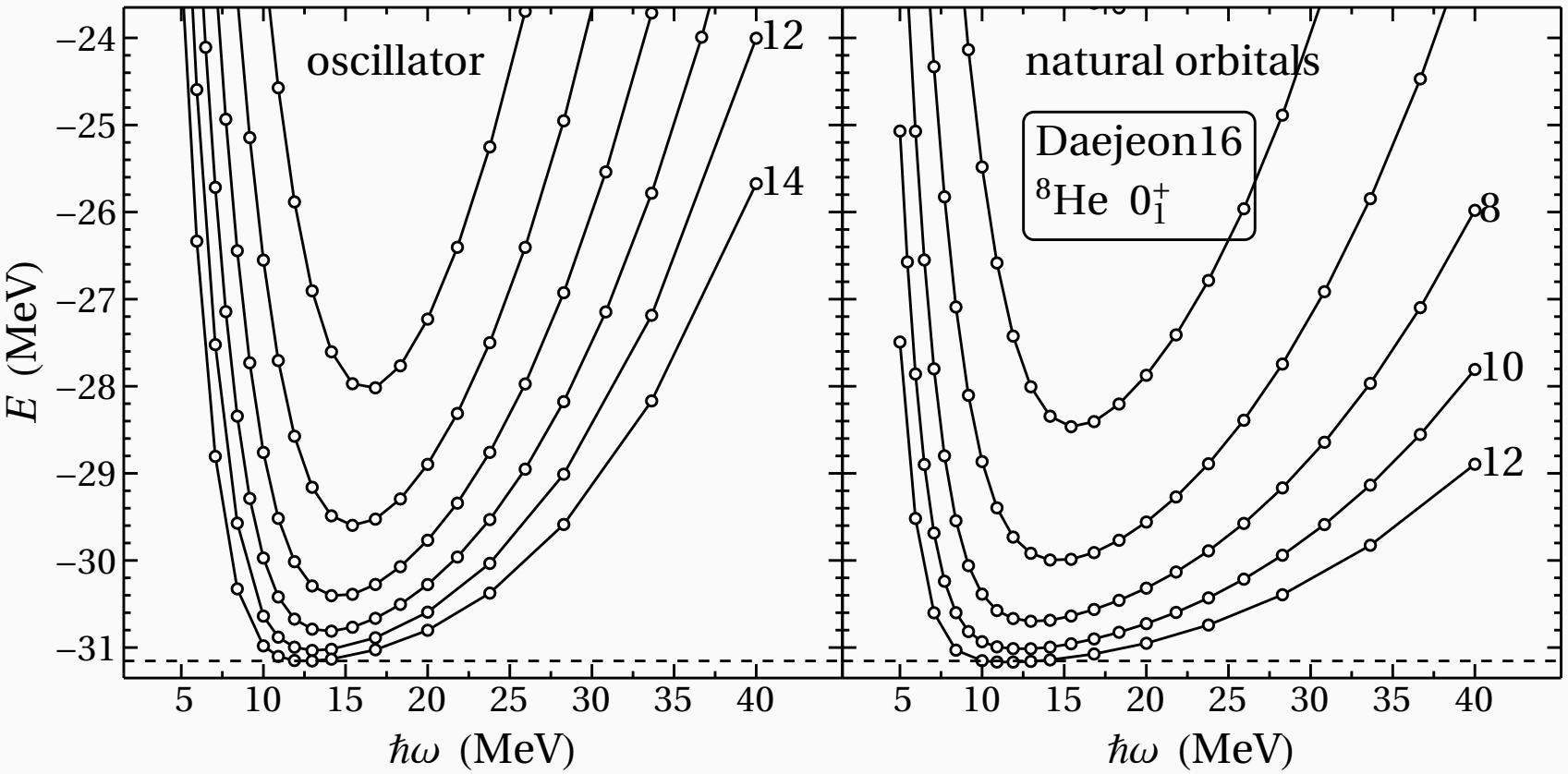

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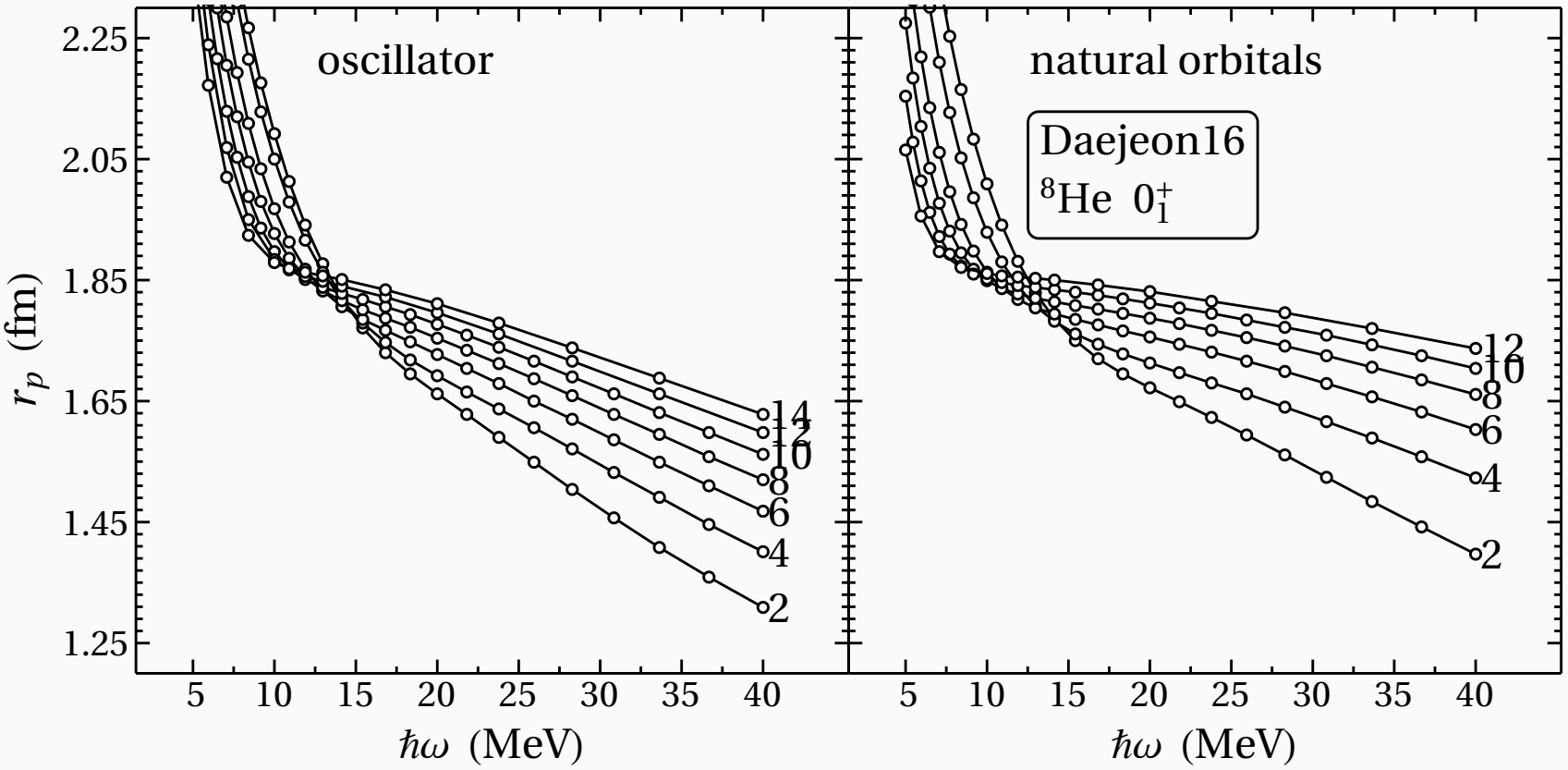

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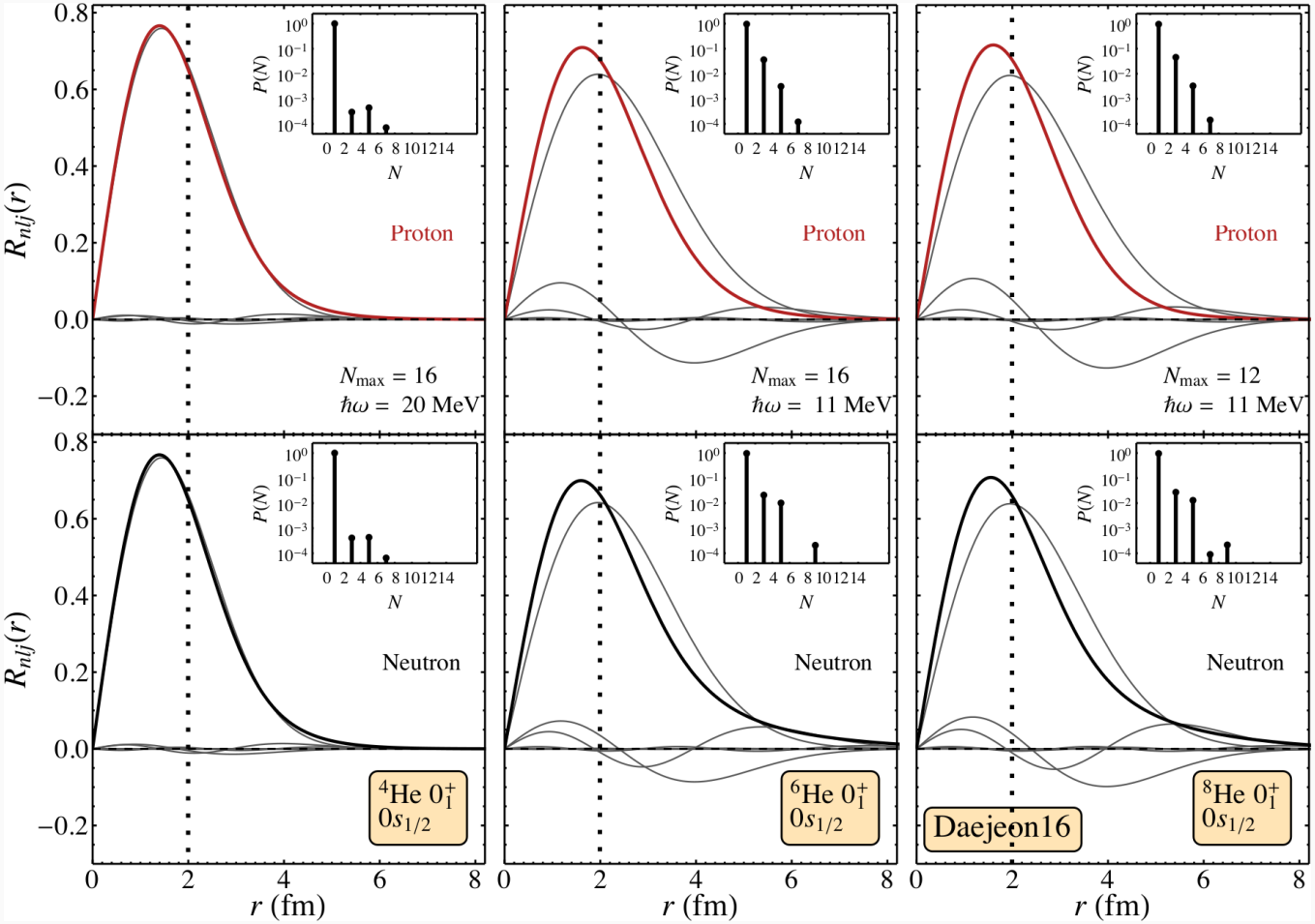
Natural Orbitals – Decompositions

Natural orbitals decomposed into harmonic oscillator functions:



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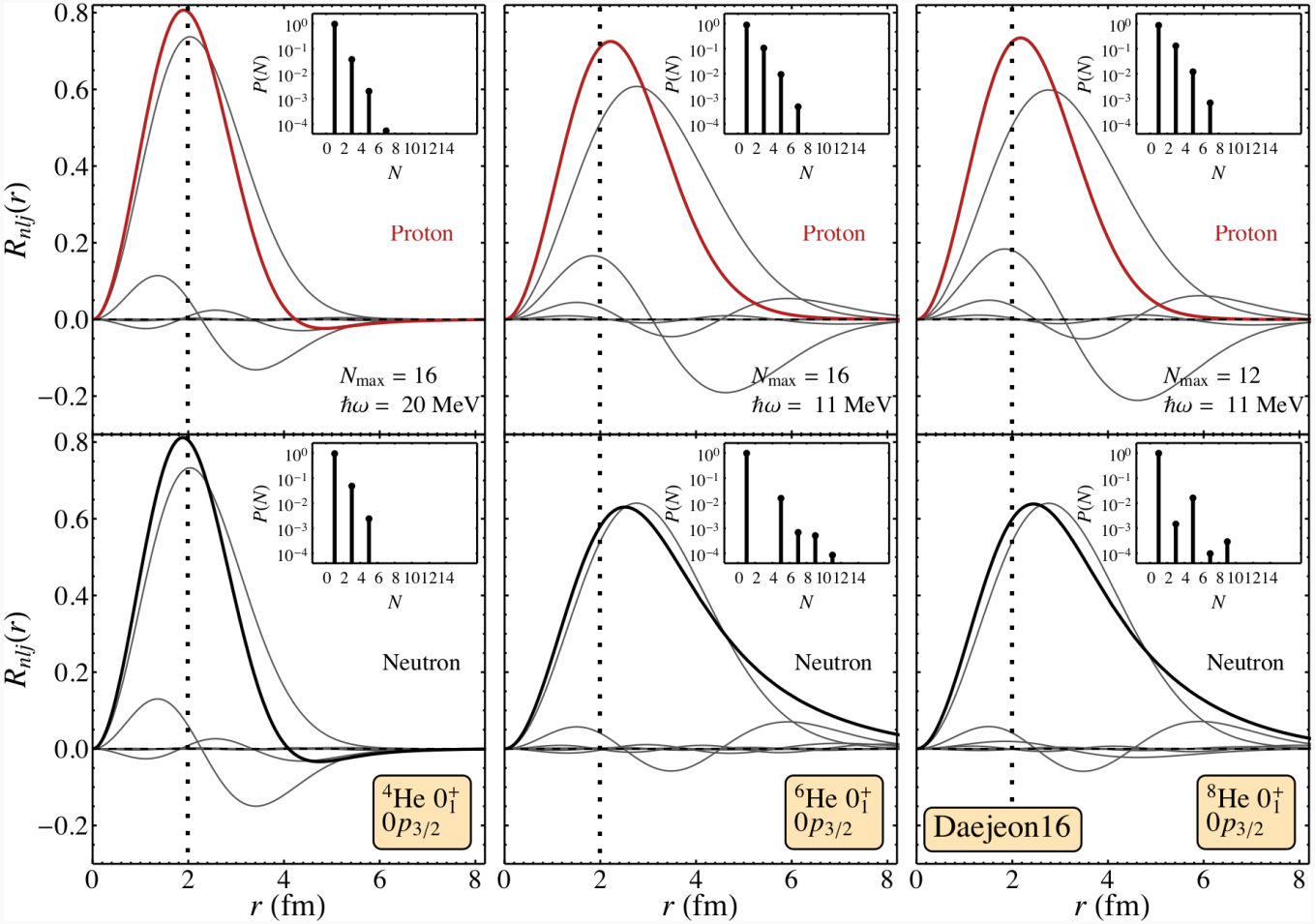

Ch. Constantinou *et al.*, in preparation

Collaborators

- Valentino Constantinou (U. Notre Dame, Monmouth College)
- Mark Caprio (U. Notre Dame)
- Pieter Maris (Iowa State U.)
- James Vary (Iowa State U.)

Summary

- Goal: Try to solve the many-body problem starting with a realistic NN (and 3N) interaction.
- Convergence assessed based on independence from single-particle basis and many-body truncation.
- Picking better basis functions leads to better convergence!