No-core configuration interaction methods for ab initio nuclear theory

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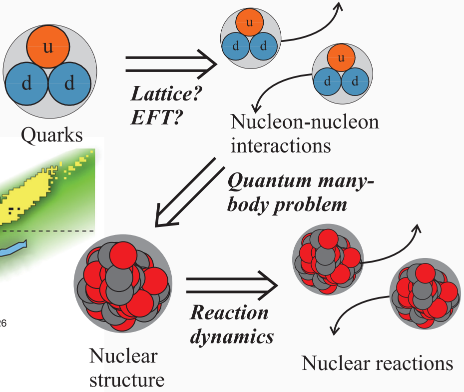
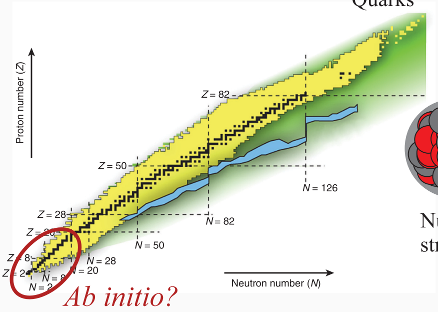
Goals of *ab initio* nuclear structure

First-principles understanding of nature *Nuclei from QCD*

What is the origin of simple patterns in complex nuclei?





B. Schwarzschild, Physics Today 63(8), 16 (2010).

Ab Initio Nuclear Theory

- *Ab initio* theory – start with a realistic NN (and maybe $3N$) interaction and solve the quantum many-body problem
- We want not only ground-state energies but many other low-energy observables:
  - energy spectra
  - spatial distributions
  - momentum distributions
  - inputs for reaction theory (spectroscopic overlaps, spectroscopic factors, asymptotic normalization factors)
  - electromagnetic observables (transition probabilities, magnetic moments, form factors)
  - weak observables (Fermi and Gamow-Teller probabilities)
  - nuclear equation of state parameters

Many techniques for solving nuclear Hamiltonians have been devised[1]:

- Few-body:
  - Fadeev-Yakubowski Equation
  - Hyperspherical Harmonics
- Many-body:
  - Coupled-cluster
  - Quantum Monte Carlo
  - No-Core Configuration Interaction (NCCI) model

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Basics of NCCI

Basic idea: configuration-interaction (CI) without a core!
All types of excitations are allowed.

Begin with an orthonormal single-particle basis:

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

Of course, we must truncate to a finite number of single-particle states.

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

$$|\Psi_\alpha\rangle = |\pi_{\alpha_1}\pi_{\alpha_2}\cdots\pi_{\alpha_Z}\nu_{\alpha_1}\nu_{\alpha_2}\cdots\nu_{\alpha_N}\rangle$$

Basics of NCCI

Full Configuration Interaction: include all possible Slaters. Dimension blows up:

N_{shell}	2	3	4	5	6	7
			M scheme			
^{4}He	98	3.06×10^3	3.98×10^4	3.14×10^5	1.77×10^6	7.84×10^6
^{6}He	216	6.51×10^4	3.86×10^6	9.80×10^7	1.45×10^9	1.47×10^{10}
^{6}Li	293	8.59×10^4	5.08×10^6	1.29×10^8	1.91×10^9	1.94×10^{10}
^{7}Li	400	3.60×10^5	4.51×10^7	2.05×10^9	4.91×10^{10}	7.50×10^{11}
^{8}Be	518	1.47×10^6	3.96×10^7	3.24×10^{10}	1.26×10^{12}	2.91×10^{13}
^{10}B	293	1.34×10^7	1.82×10^{10}	5.02×10^{11}	5.22×10^{14}	2.78×10^{16}
^{12}C	98	8.22×10^7	5.87×10^{11}	5.50×10^{14}	1.54×10^{17}	1.90×10^{19}
^{16}O	1	8.12×10^8	2.10×10^{14}	2.51×10^{18}	5.32×10^{21}	3.59×10^{24}

T. Abe et al., "Benchmarks of the full configuration interaction, monte carlo shell model, and no-core full configuration methods", Phys. Rev. C **86**, 054301 (2012)

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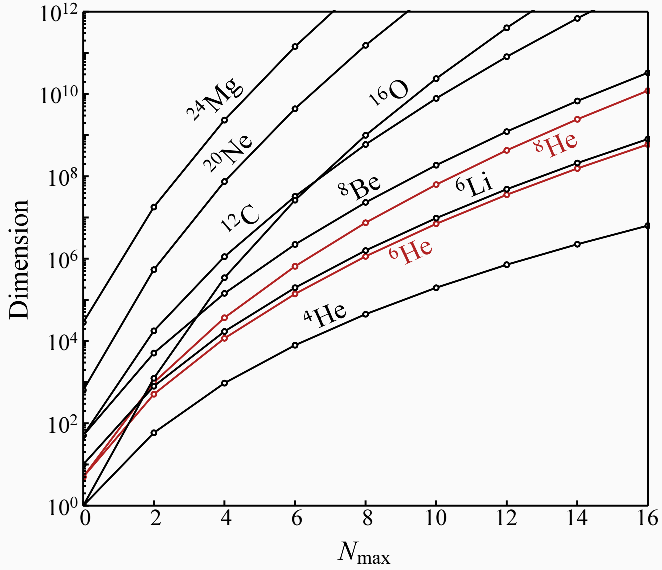
Truncate based on weight of Slater determinant.

NCCI Basis Size



N_{max} Truncation

For the case where $w = N = 2n + \ell$, we define the 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 Hamiltonian

No-Core Configuration Interaction Hamiltonian

$$H = T_{intr} + V + aN_{c.m.}$$

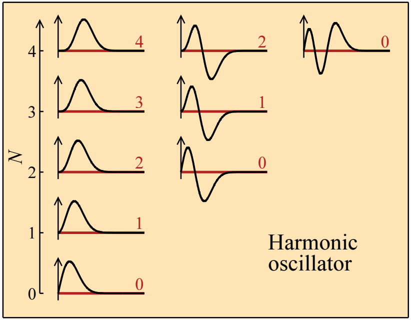
- T_{intr} – intrinsic kinetic energy ("upgraded" to a two-body operator)
- V – realistic nucleon-nucleon (NN) interaction
- $N_{c.m.}$ – center-of-mass number operator (Lawson term)

Take matrix elements of H from relative coordinates, Moshinksy transform into lab coordinates, and feed in as two-body matrix elements.

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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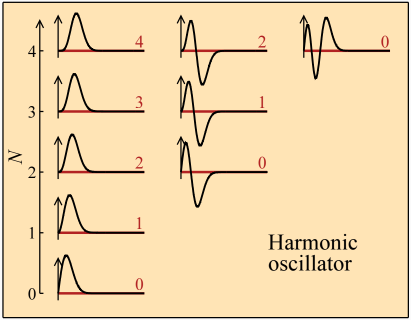

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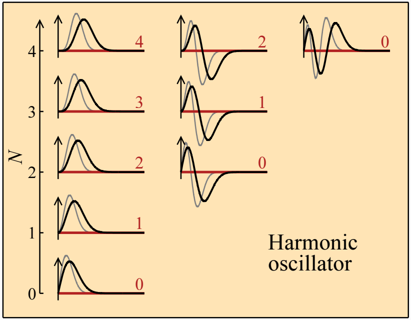

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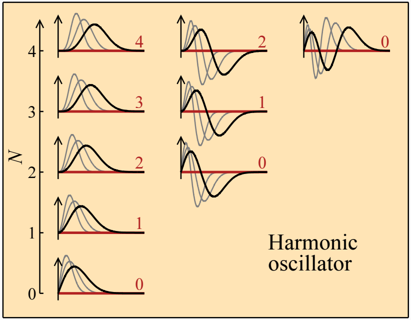

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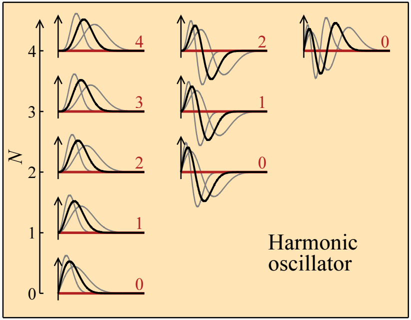

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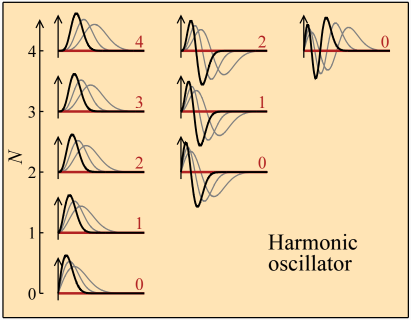

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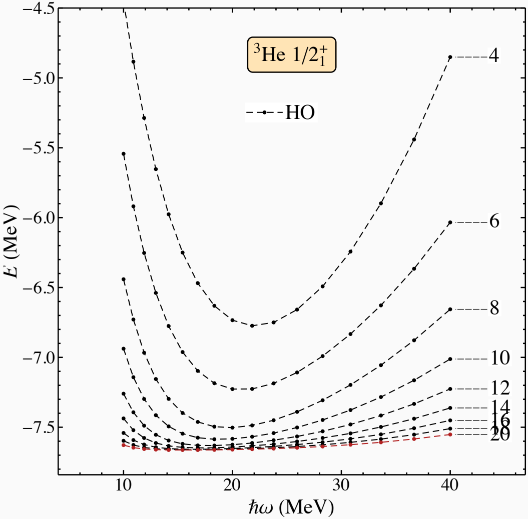

Ch. Constantinou *et al.*, in preparation

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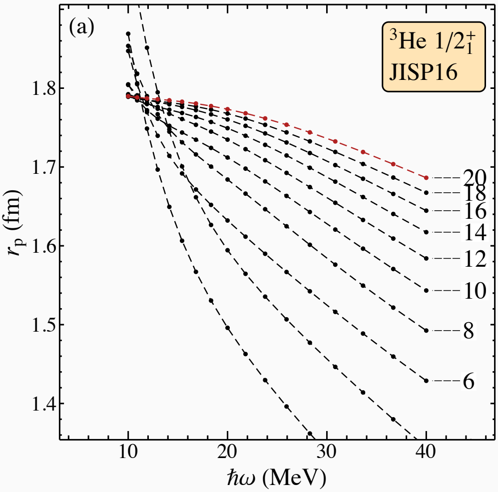

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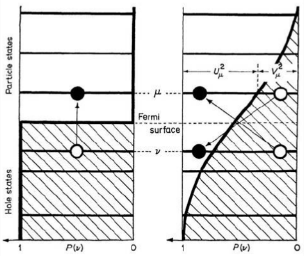
Natural Orbitals for Nuclear Physics

- Attempt to formulate a "natural" basis for performing NCCI calculations.
- Define "natural" $\rightarrow$ minimum depletion of the Fermi sea.
- Run many-body calculation, diagonalize one-body static density matrix, use eigenvectors as similarity transformation on single-particle space.
- Minimizing depletion of Fermi sea, not minimizing energy!
- Built from many-body calculation, so "aware" of correlations.



D. J. Rowe, *Nuclear collective motion: models and theory*, (World Scientific, Singapore, 2010)

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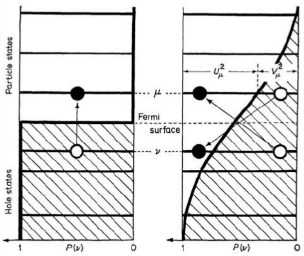

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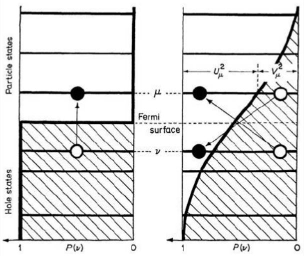

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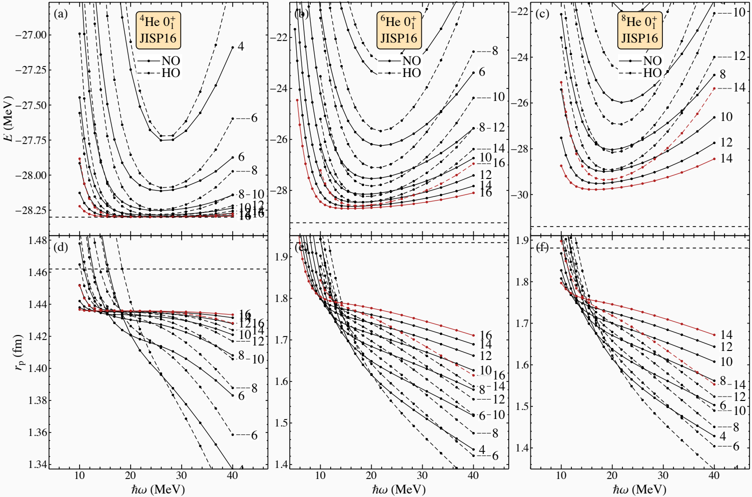

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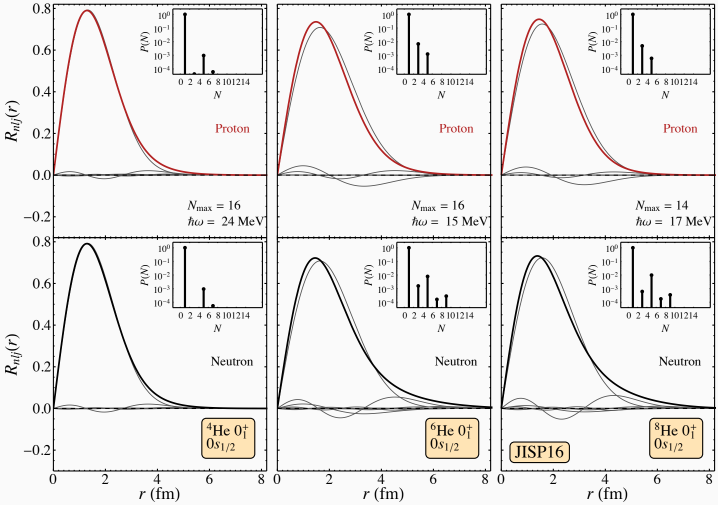

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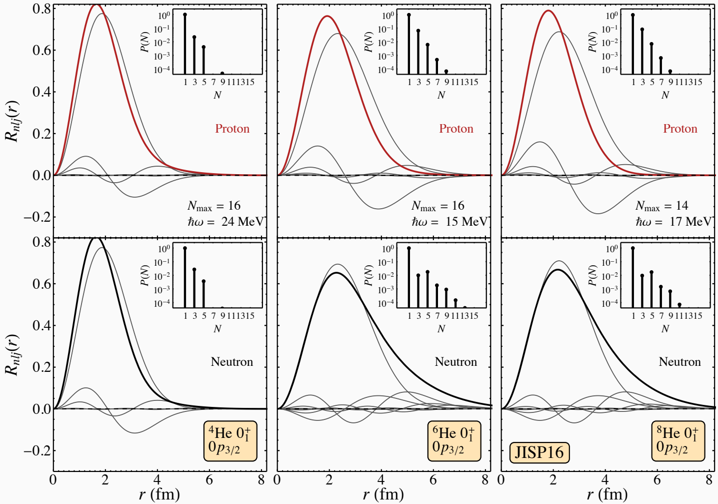

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Summary

- Goal: Try to solve the many-body problem starting with a realistic NN (and 3N) interaction.
- Treat all nucleons on an equal footing; all nucleons in the “valence space”. Truncate basis based on general weighting scheme.
- Convergence assessed based on independence from single-particle basis and many-body truncation.
- Picking better basis functions leads to better convergence!