Natural orbitals for *ab initio* calculations

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Progress in *Ab Initio* Techniques in Nuclear Physics
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Natural orbitals for nuclear no-core calculations?

Valentino Constantinou, Mark Caprio, James Vary, Pieter Maris

Change of basis to orbitals which diagonalize the density matrix

> *"If the system has exactly N spin-orbitals which are fully occupied, the total wave function may be reduced to a single Slater determinant. However, due to the mutual interaction between the particles, this limiting case is never physically realized, but the introduction of natural spin-orbitals leads then instead to a configurational expansion of most rapid convergence."* P.-O. Löwdin, Phys. Rev. 97, 1474 (1955).

Will this approach accelerate convergence in the nuclear problem?

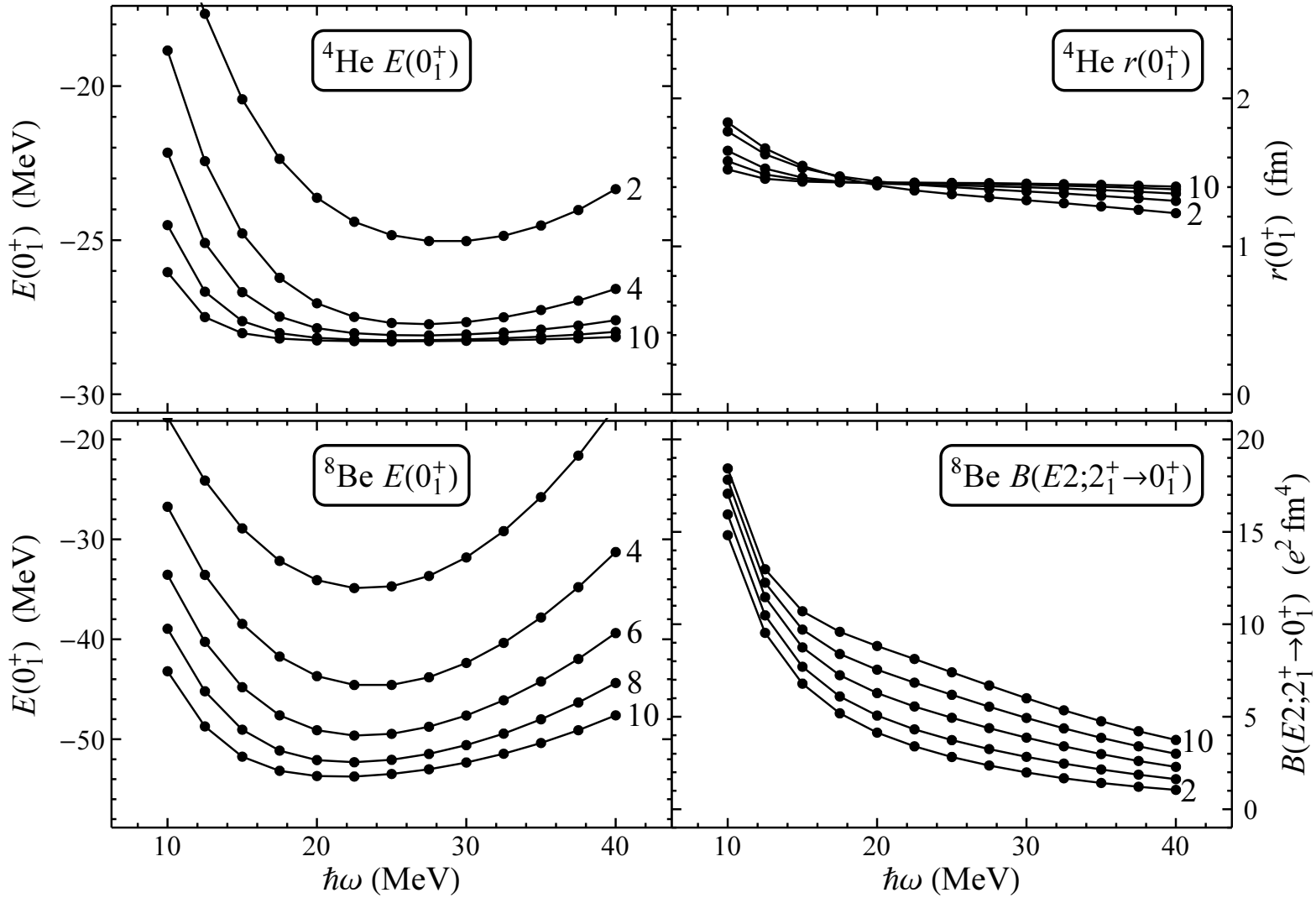
How to adapt idea to translationally-invariant, spherical *j*-shell scheme?

No-core configuration interaction (NCCI) approach

- Basis of antisymmetrized product states (Slater determinants)
- Represent many-body Hamiltonian as matrix in this basis
- No inert core; systematic expansion towards full many-body space

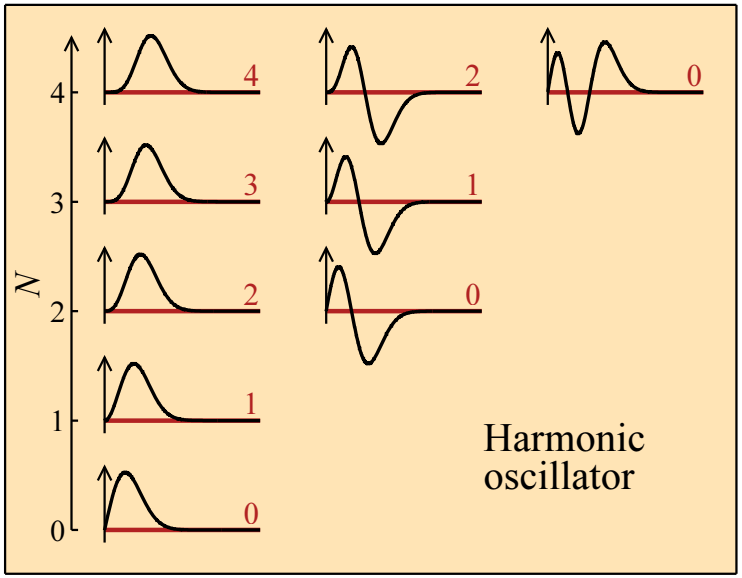
OUTLINE (1) convergence challenge (2) natural orbitals (3) illustration ^{6}He

Convergence in NCCI calculations?



M. A. Caprio, P. Maris, J. P. Vary, and R. Smith, Int. J. Mod. Phys. E 24, 1541002 (2015). JISP16 + Coulomb.

Oscillator basis for NCCI calculations



$$R_{nl}(r) \propto \left(\frac{r}{b}\right)^{l+1} L_n^{(l+1/2)}\left[\left(\frac{r}{b}\right)^2\right] e^{-(r/b)^2/2}$$

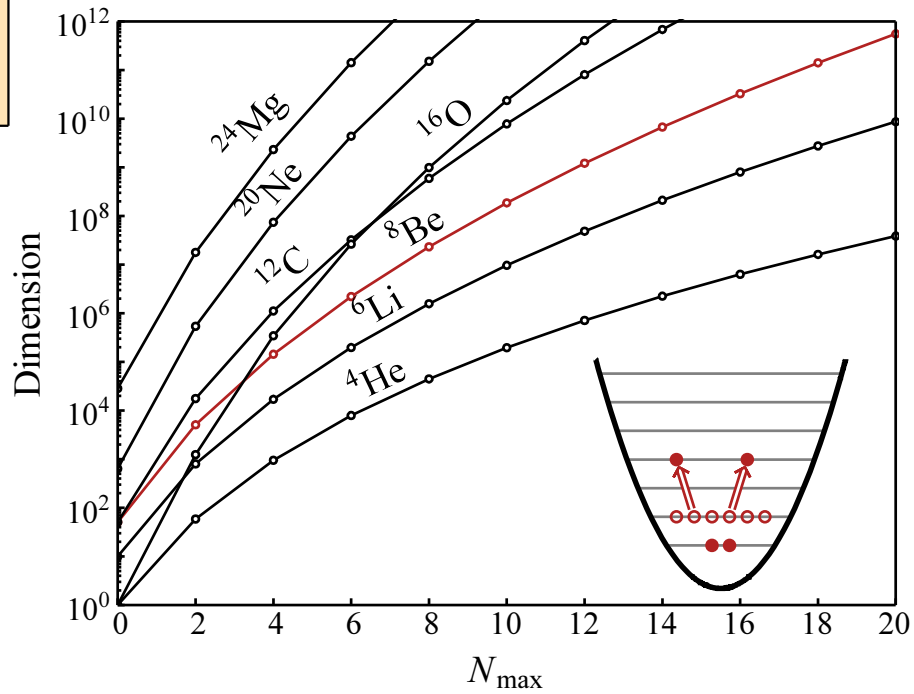
$$b(\hbar\omega) = \frac{(\hbar c)}{[(m_N c^2)(\hbar\omega)]^{1/2}}$$

$N = 2n + l$ *major shell*

Truncation by excitation quanta

$$N_{\text{tot}} = \sum_i N_i = N_0 + N_{\text{ex}}$$

$$N_{\text{ex}} \leq N_{\text{max}}$$

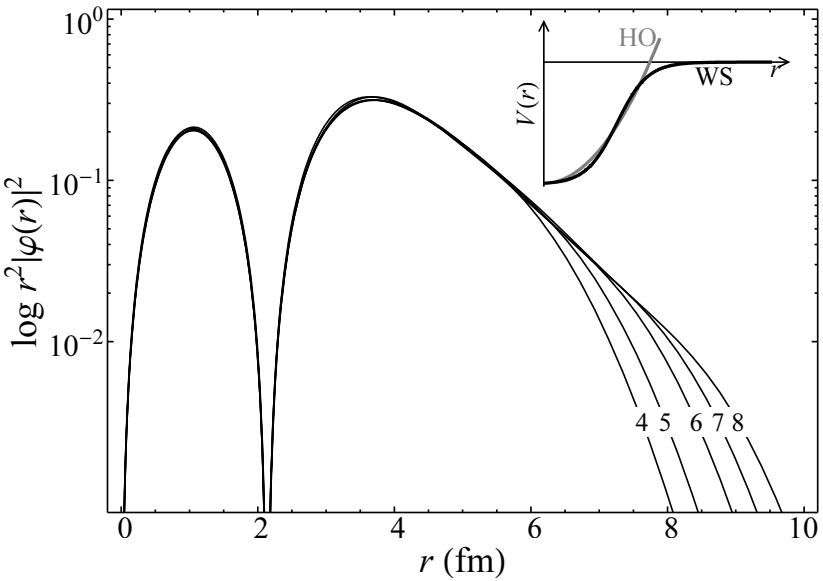


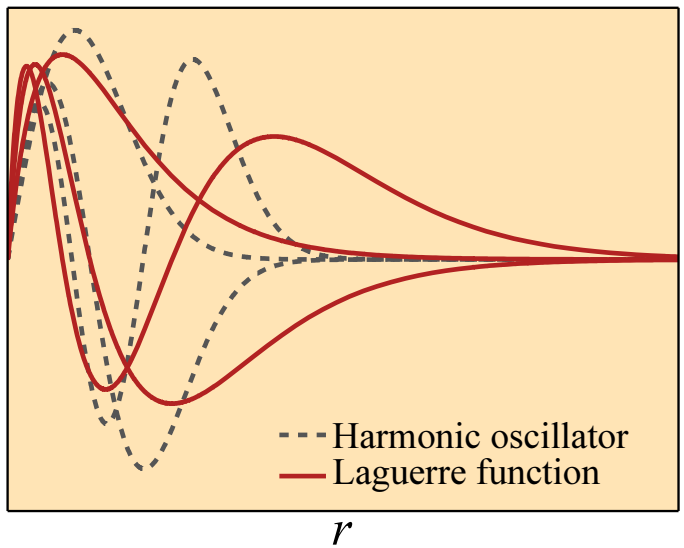
Radial functions in NCCI calculations

Harmonic oscillator basis is convenient...

- Matrix elements of *NN* interaction easily transformed from *relative* basis $[\Psi_{nl}(\mathbf{r}_1 - \mathbf{r}_2)]$ to *two-body* basis $[\Psi_{n_1 l_1}(\mathbf{r}_1)\Psi_{n_2 l_2}(\mathbf{r}_2)]$ by *Moshinsky transformation*
- Exact *separation of center-of-mass motion* in $N_{\max}$ truncation

Reproducing exponential asymptotics ($\propto e^{-\beta r}$) in basis with Gaussian asymptotics ($\propto e^{-\alpha r^2}$)...





Try to extrapolate the problem away? *Box size $L \to \infty$*

R. J. Furnstahl, G. Hagen, and T. Papenbrock, Phys. Rev. C **86**, 031301 (2012).

Pick a specific alternative form for the radial functions? *Laguerre ($\approx$"Coulomb-Sturmian")*

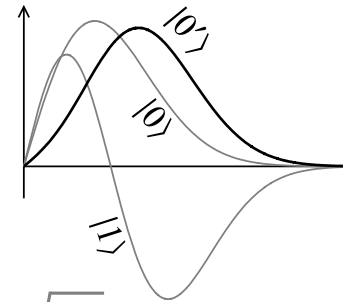
M. A. Caprio, P. Maris, and J. P. Vary, Phys. Rev. C **86**, 034312 (2012); Phys. Rev. C **90**, 034305 (2014).

Or let the Hamiltonian pick the orbitals for you? *Natural orbitals*

Illustration with two-level system

EXAMPLE: Many-body wave function is simple in terms of $|0'\rangle$ orbital

$$|0'\rangle = \sqrt{\tfrac{3}{4}}\,|0\rangle - \sqrt{\tfrac{1}{4}}\,|1\rangle$$



But we are working in the $|0\rangle$, $|1\rangle$ basis...

$$|\Psi\rangle = \sqrt{\tfrac{9}{16}}\,|0\rangle|0\rangle - \sqrt{\tfrac{3}{16}}\,|0\rangle|1\rangle - \sqrt{\tfrac{3}{16}}\,|1\rangle|0\rangle + \sqrt{\tfrac{1}{16}}\,|1\rangle|1\rangle$$

$$= \left[\sqrt{\tfrac{3}{4}}\,|0\rangle - \sqrt{\tfrac{1}{4}}\,|1\rangle\right]\left[\sqrt{\tfrac{3}{4}}\,|0\rangle - \sqrt{\tfrac{1}{4}}\,|1\rangle\right]$$

$$\sqrt{\tfrac{9}{16}}\underbrace{|00\rangle}_{N_{ex}=0} - \sqrt{\tfrac{6}{16}}\underbrace{|01\rangle}_{N_{ex}=2} + \sqrt{\tfrac{1}{16}}\underbrace{|11\rangle}_{N_{ex}=4} = \underbrace{|0'0'\rangle}_{N_{ex}=0}$$

The superposition of Slater determinants* here serves, not to build up correlations, but simply to reconstruct the single-particle wave functions (painfully, using the many-body basis!).

*Well, actually, Slater *permanents* in this simple illustration, to obtain a meaningful two-level example with nontrivial occupations... But think of Slater determinants of two fermions in opposite spin states.

Illustration with two-level system

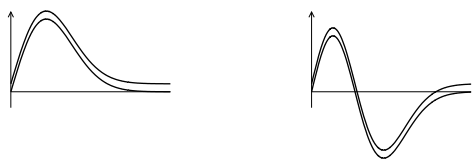
Why do we need so many Slater determinants for convergence?

- Single-particle mismatch?
- Genuine correlations?

EXAMPLE: Many-body wave function can also be genuinely correlated

$$|\Psi\rangle = \sqrt{\tfrac{3}{4}}\,|0\rangle|0\rangle + \sqrt{\tfrac{1}{4}}\,|1\rangle|1\rangle$$

Same mean occupations as before



Building correlations into the nuclear many-body basis...

Importance truncation (IT-NCSM), Monte Carlo (NC-MCSM) *Abe*

Clustering correlations (NCSM/RGM, NCSMC) *Romero-Redondo*

Correlations from many-body symmetries *Baker, Dreyfuss, McCoy*

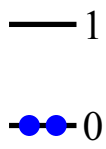
Can we undo the damage?

Density matrix for a Slater determinant*

$$\rho_{\alpha\beta} = \langle \Psi | c_\beta^\dagger c_\alpha | \Psi \rangle$$

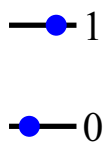
EXAMPLE: $|\Psi\rangle = |00\rangle$

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



EXAMPLE: $|\Psi\rangle = |01\rangle$

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



If $|\Psi\rangle$ is a Slater determinant *in some basis*, its density matrix is diagonal *in that basis*. The diagonal entries are the occupations. $\mathcal{N}_\alpha = \rho_{\alpha\alpha}$

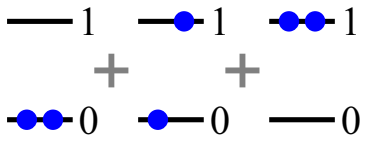
If we stumble across this $|\Psi\rangle$ expressed in any other basis, we can recover the "natural" basis by finding the change of single-particle basis which returns the density matrix to diagonal form. *Diagonalize* ρ

* Again, we will actually use Slater *permanents* in this example, to allow nontrivial occupations...

Can we undo the damage?

EXAMPLE: Deciphering an uncorrelated state

$$|\Psi\rangle = \sqrt{\tfrac{9}{16}}\,|00\rangle - \sqrt{\tfrac{6}{16}}\,|01\rangle + \sqrt{\tfrac{1}{16}}\,|11\rangle$$



$$\rho_{00} = \langle\Psi|c_0^\dagger c_0|\Psi\rangle = \sqrt{\tfrac{9}{16}}^2(2) + \sqrt{\tfrac{6}{16}}^2(1) + \sqrt{\tfrac{1}{16}}^2(0) = \tfrac{3}{2}$$

$$\rho_{01} = \langle\Psi|c_1^\dagger c_0|\Psi\rangle = -\sqrt{\tfrac{6}{16}}\sqrt{\tfrac{9}{16}}\langle 01|c_1^\dagger c_0|00\rangle + \cdots = -\sqrt{\tfrac{3}{4}}$$

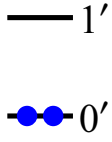
Natural orbitals (one-body transformation)

$$\rho = \begin{pmatrix} \frac{3}{2} & -\sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & \frac{1}{2} \end{pmatrix} \Rightarrow \underset{2}{\begin{pmatrix} \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{1}{4}} \end{pmatrix}}\ |0'\rangle\ ,\ \underset{0}{\begin{pmatrix} \sqrt{\frac{1}{4}} \\ \sqrt{\frac{3}{4}} \end{pmatrix}}\ |1'\rangle \quad \therefore \quad \rho' = \begin{pmatrix} 2 & \\ & 0 \end{pmatrix}$$

Order by decreasing eigenvalue

Many-body wave function in new basis

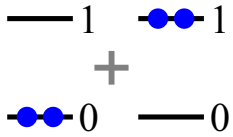
$$|\Psi\rangle = |0'0'\rangle$$



Can we undo the damage?

EXAMPLE: Attempting natural orbitals for a correlated superposition

$$|\Psi\rangle = \sqrt{\tfrac{3}{4}}\,|00\rangle + \sqrt{\tfrac{1}{4}}\,|11\rangle$$

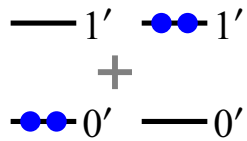


$$\rho_{00} = \langle\Psi|c_0^\dagger c_0|\Psi\rangle = \sqrt{\tfrac{3}{4}}^{\,2}(2) + \sqrt{\tfrac{1}{4}}^{\,2}(0) = \tfrac{3}{2}$$

$$\rho_{01} = \langle\Psi|c_1^\dagger c_0|\Psi\rangle = 0$$

$$\rho = \begin{pmatrix} \frac{3}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad \Rightarrow \quad \underset{3/2}{\begin{pmatrix} 1 \\ 0 \end{pmatrix}} \;,\; \underset{1/2}{\begin{pmatrix} 0 \\ 1 \end{pmatrix}} \qquad \begin{matrix} |0'\rangle & |1'\rangle \end{matrix}$$

$$|\Psi\rangle = \sqrt{\tfrac{3}{4}}\,|0'0'\rangle + \sqrt{\tfrac{1}{4}}\,|1'1'\rangle$$



We cannot do anything to simplify this genuinely correlated state.

Beware the converse... A diagonal density matrix does not necessarily mean that $|\Psi\rangle$ is a Slater determinant![*]

[*] Yes, yes, a Slater *permanent* in this example, but the point is the same...

Natural orbitals for a "spherical shell model"

Many-body basis is based on configurations of nucleons over nlj orbitals

Single Slater determinant ⇒ Single configuration

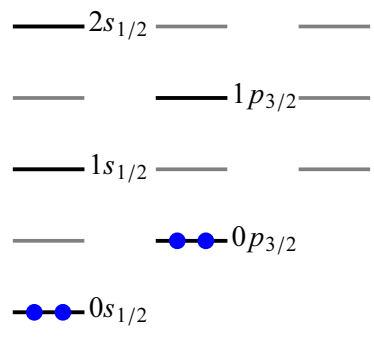
Many M-scheme Slater determinants contribute to good total-J states

A pure configuration has diagonal *scalar densities*

$$\rho^{(0)}_{ab} \equiv \langle \Psi | [c^\dagger_b \tilde{c}_a]_{00} | \Psi \rangle \qquad \mathcal{N}_a = \sqrt{2\hat{j}_a + 1}\,\rho^{(0)}_{aa}$$

EXAMPLE $(s_{1/2})^2 (p_{3/2})^2$ *e.g.*, ^{6}He neutrons

$$\rho^{(0)} = \left(\begin{array}{ccc:ccc:c} \frac{1}{\sqrt{2}}2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \hdashline 0 & 0 & 0 & \frac{1}{\sqrt{4}}2 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & \cdots \\ \hdashline \cdots & \cdots & \cdots & \cdots & \cdots & \end{array}\right) \begin{array}{l} 0s_{1/2} \\ 1s_{1/2} \\ 2s_{1/2} \\ 0p_{3/2} \\ 1p_{3/2} \\ \cdots \end{array}$$



Scalar density matrix only connects orbitals $(n'lj) \leftrightarrow (nlj)$ of same (lj)

Natural orbitals defined by diagonalizing scalar density

Change of basis on *radial* functions within (lj) space $\quad |n'lj\rangle = \sum_n a^{(lj)}_{n',n} |nlj\rangle$

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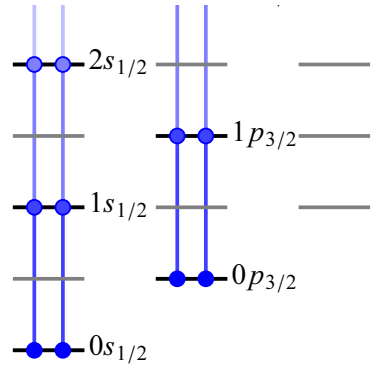

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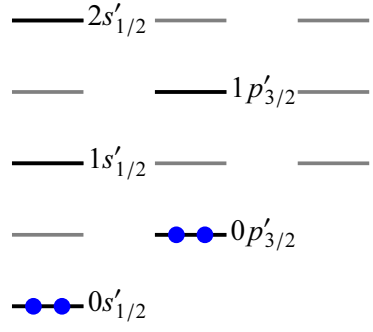
EXAMPLE $(s_{1/2})^2 (p_{3/2})^2$ *e.g.*, ^{6}He neutrons

$$\rho^{(0)\prime} = \left(\begin{array}{ccc:ccc:c} * & 0 & 0 & 0 & 0 & \cdots \\ 0 & * & 0 & 0 & 0 & \cdots \\ 0 & 0 & * & 0 & 0 & \cdots \\ \hdashline 0 & 0 & 0 & * & 0 & \cdots \\ 0 & 0 & 0 & 0 & * & \cdots \\ \hdashline \cdots & \cdots & \cdots & \cdots & \cdots & \end{array}\right) \begin{array}{c} 0s'_{1/2} \\ 1s'_{1/2} \\ 2s'_{1/2} \\ \\ 0p'_{3/2} \\ 1p'_{3/2} \\ \\ \cdots \end{array}$$



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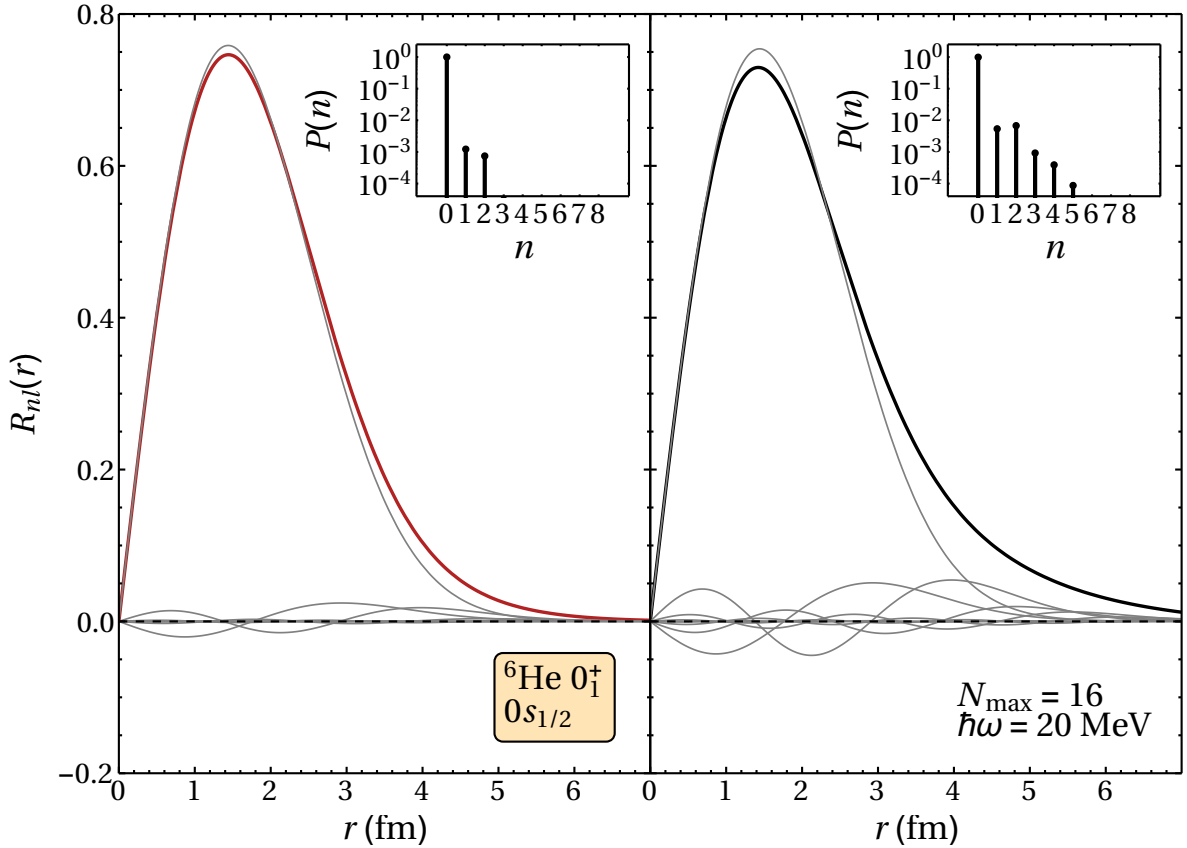
Change of basis on *radial* functions within (lj) space $\quad |n'lj\rangle = \sum_n a^{(lj)}_{n',n} |nlj\rangle$

Natural orbitals from initial NCCI calculation

Initial NCCI calculation in harmonic oscillator basis

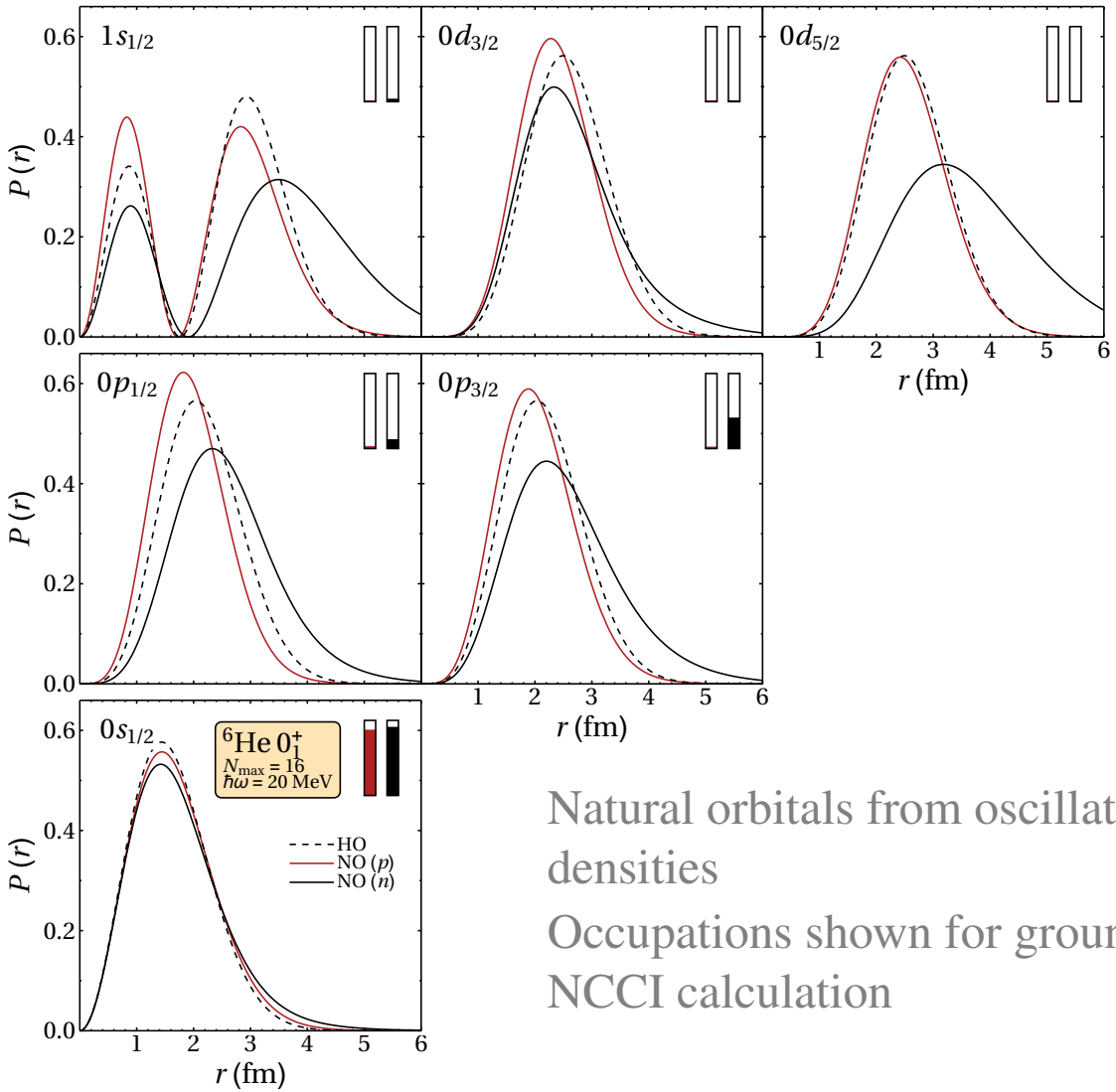
Scalar density matrix ⇒ natural orbitals

Accesses oscillator orbitals up to $N = N_{\max}$ (p) or $N_{\max} + 1$ (n) $N = 2n + l$



JISP16 + Coulomb

Natural orbitals in an NCCI calculation for ^{6}He

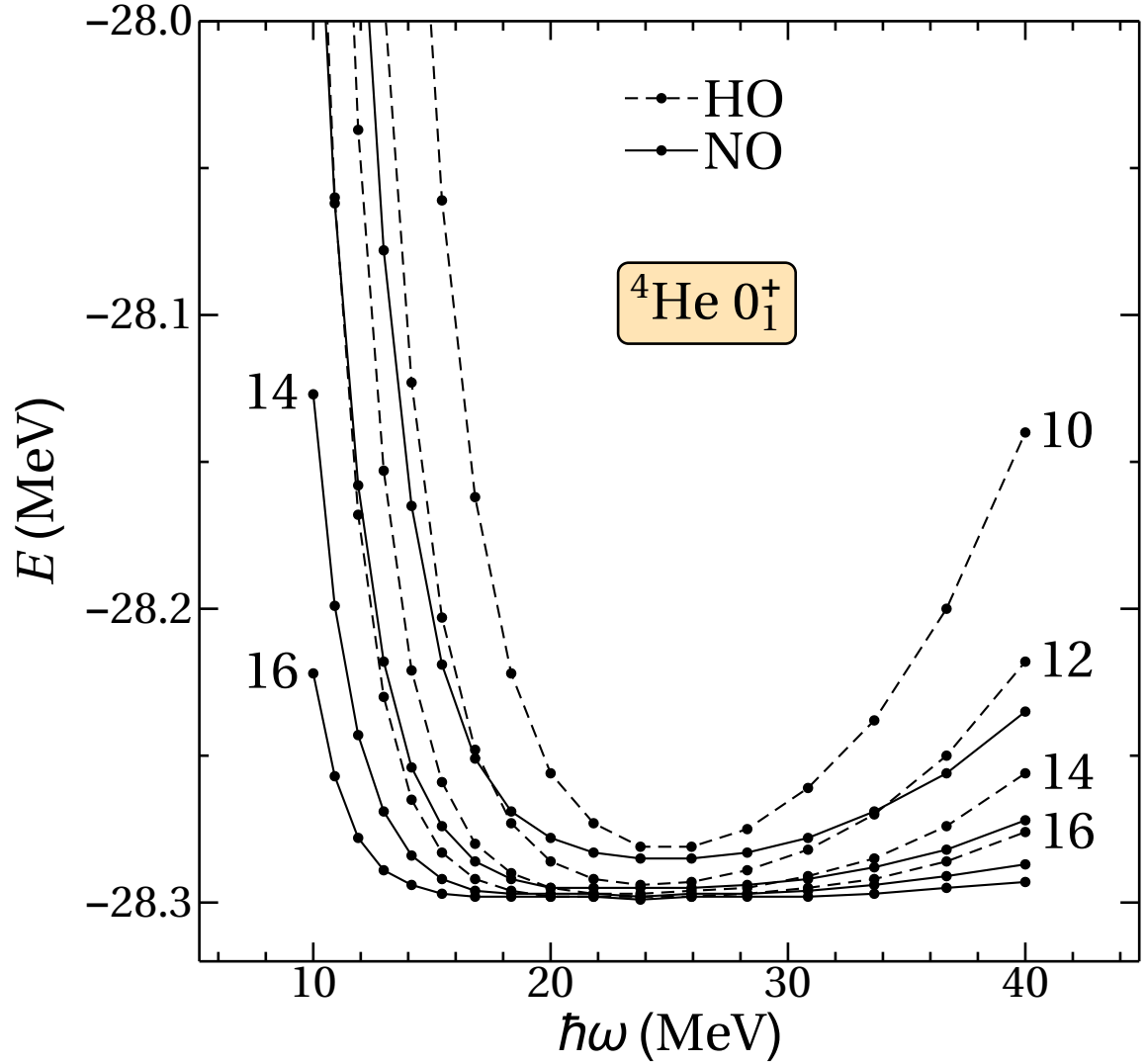


JISP16 + Coulomb

Natural orbitals from oscillator basis ground state densities

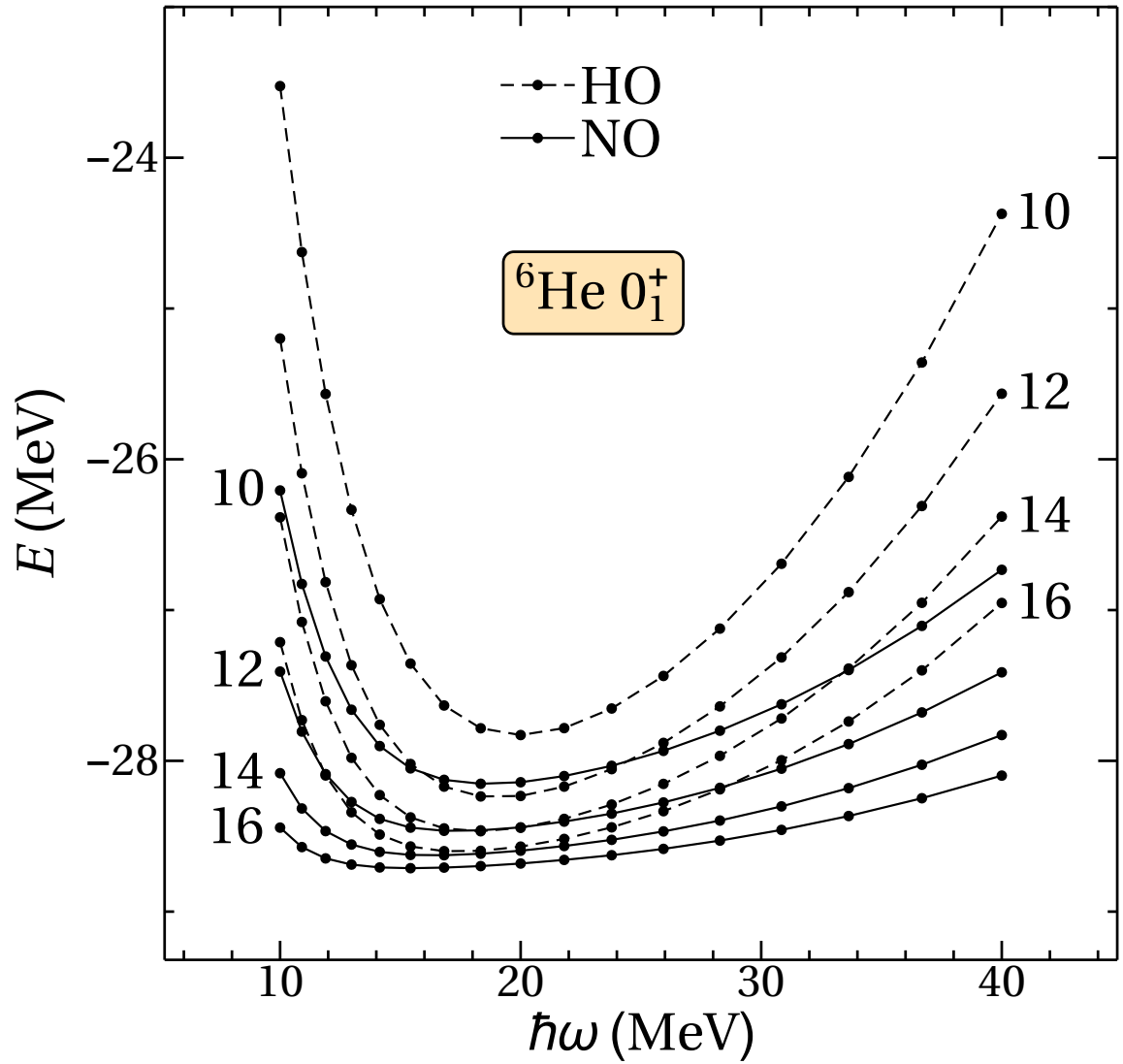
Occupations shown for ground state in subsequent NCCI calculation

Calculations with natural orbitals: Energies



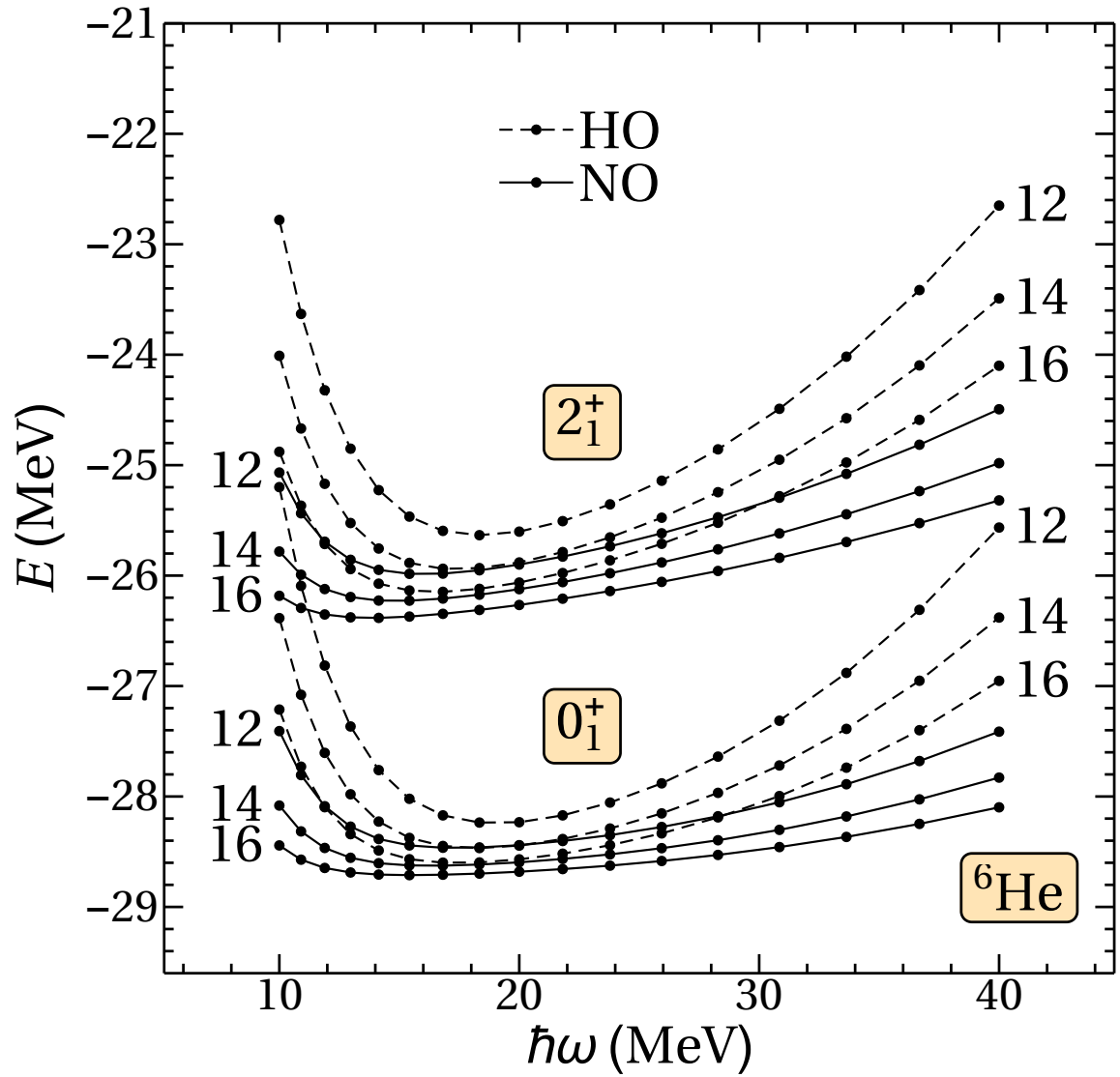
JISP16 + Coulomb

Calculations with natural orbitals: Energies



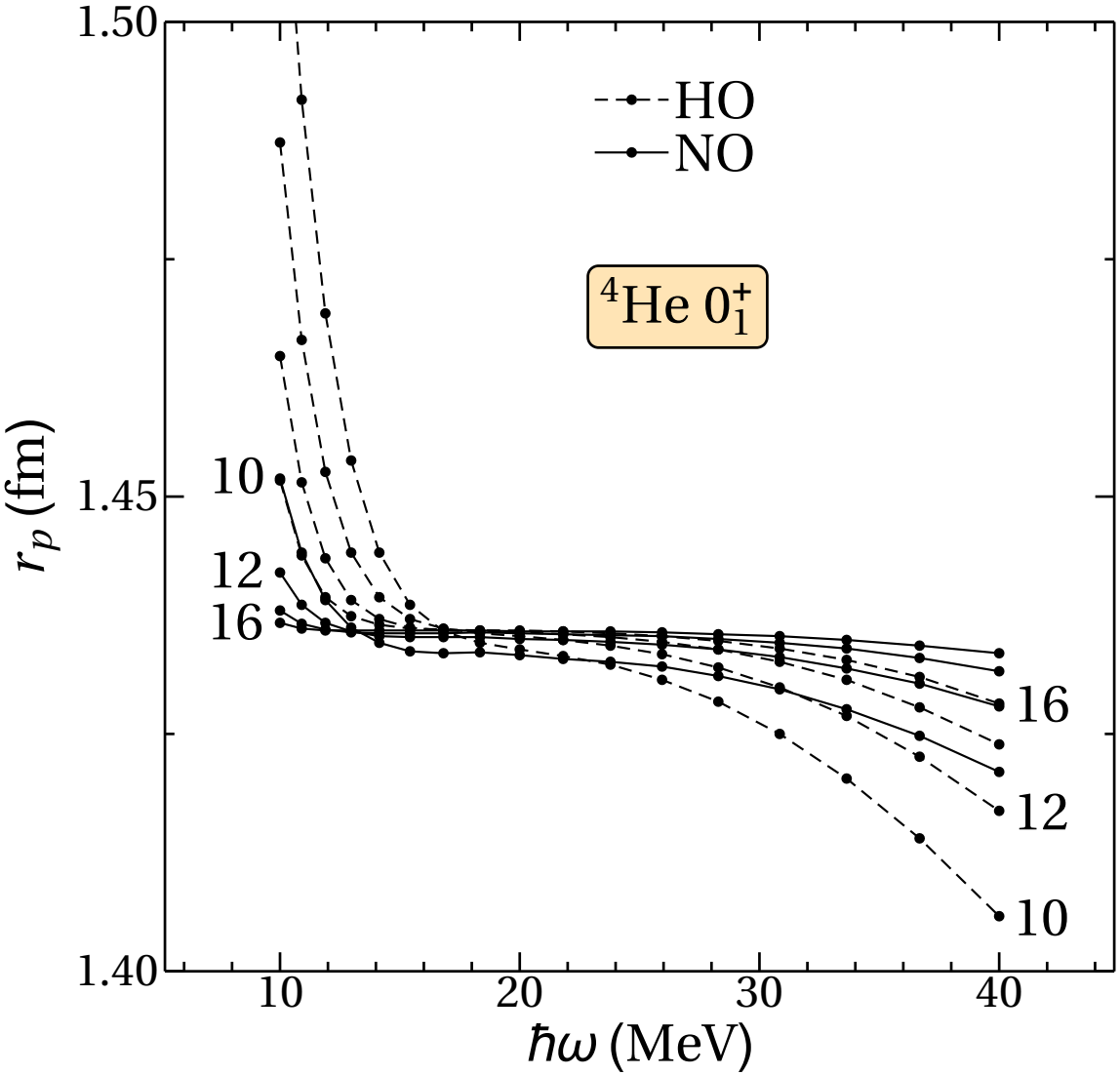
JISP16 + Coulomb

Calculations with natural orbitals: Excited states



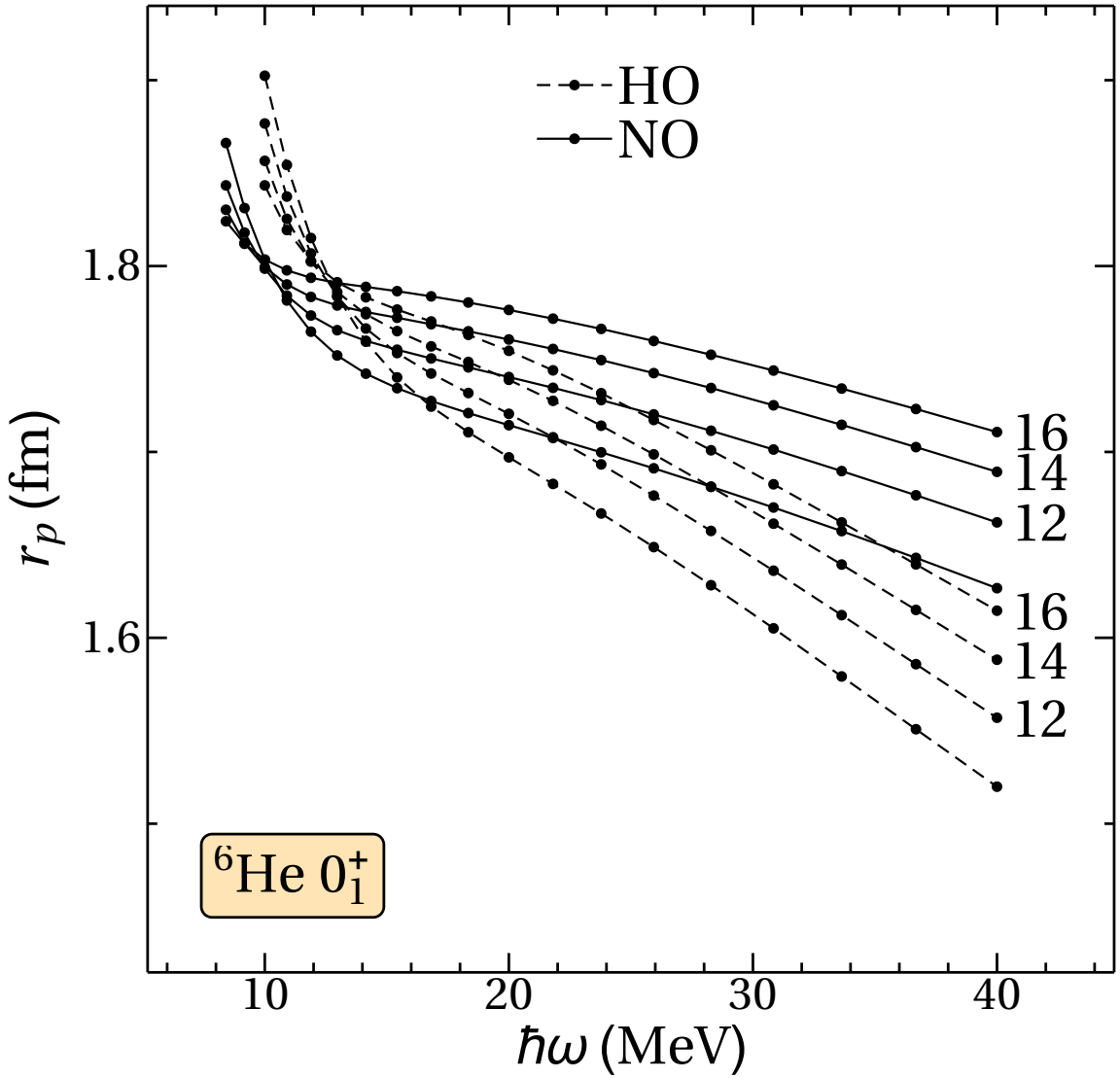
JISP16 + Coulomb

Calculations with natural orbitals: Radii



JISP16 + Coulomb

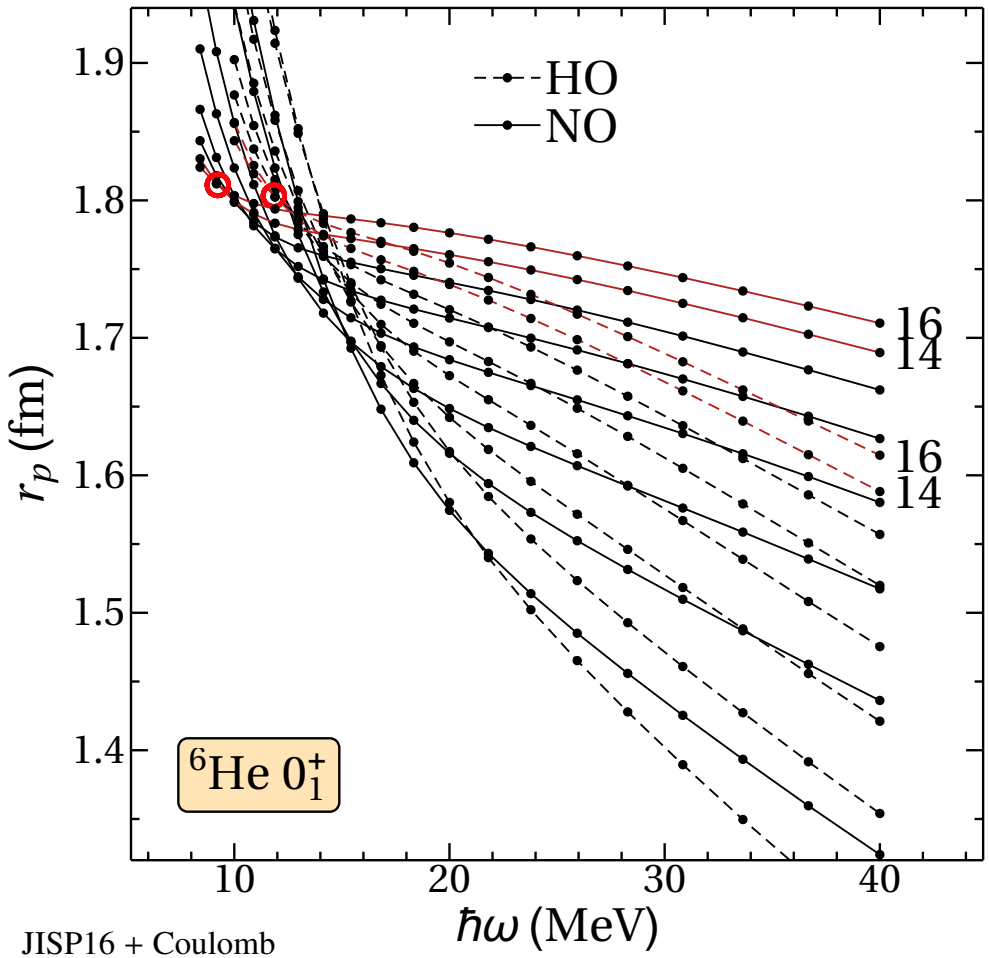
Calculations with natural orbitals: Radii



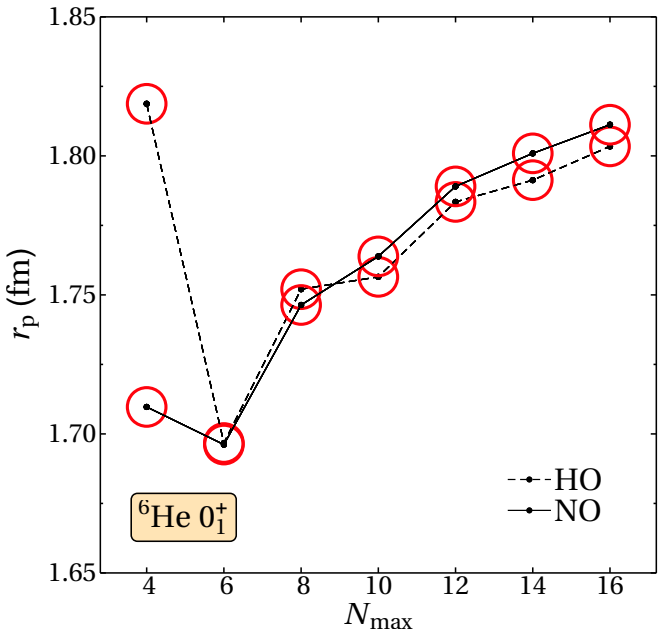
JISP16 + Coulomb

Extracting radius by crossover?

S. K. Bogner, R. J. Furnstahl, P. Maris, R. J. Perry, A. Schwenk, and J. Vary, Nucl. Phys. A **801**, 21 (2008).
C. Cockrell, J. P. Vary, and P. Maris, Phys. Rev. C **86**, 034325 (2012).



JISP16 + Coulomb



Infrared basis extrapolation

R. J. Furnstahl, G. Hagen, and T. Papenbrock, Phys. Rev. C **86**, 031301(R) (2012).

Basis only provides "support" in limited region of phase space

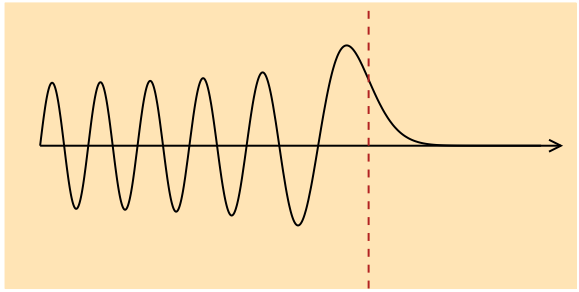
Tail of true wave function is "cut off" at some...

- Cutoff L in coordinate space *i.e., box size* *(IR cutoff)*
- Cutoff $\Lambda \equiv \hbar K$ in momentum space *(UV cutoff)*

HO classical turning point...

$$L(N,\hbar\Omega) \approx \sqrt{2(N+3/2)}\,b$$

$$K(N,\hbar\Omega) \approx \sqrt{2(N+3/2)}\,b^{-1}$$



Reparametrize *basis* dependence as *cutoff* dependence

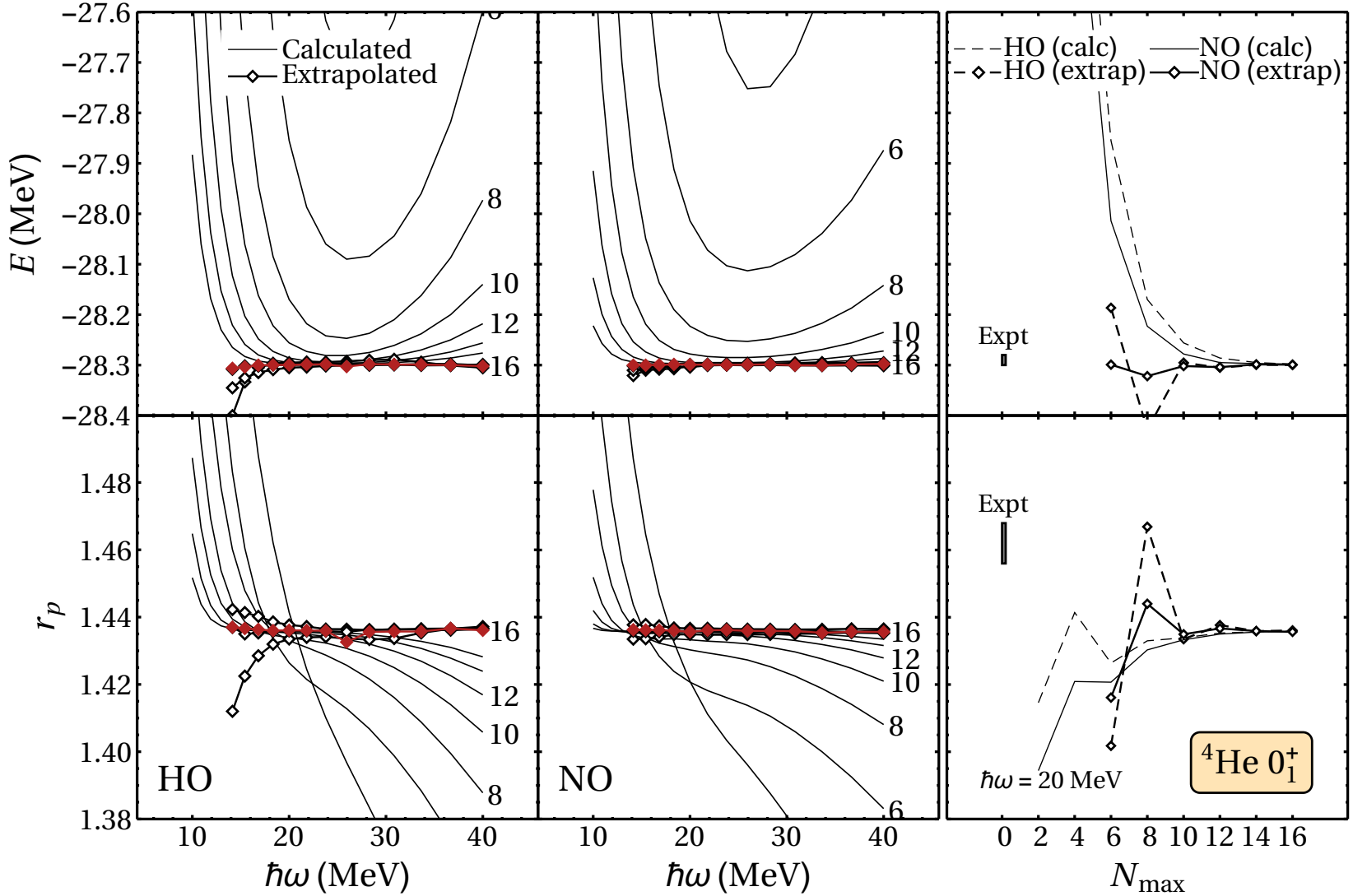
$$E(N,\hbar\Omega) \;\Rightarrow\; E(L,K)$$

At large K, expect *UV convergence* and *IR correction dominance*

$$E(N,\hbar\Omega) \overset{?}{\Rightarrow} E(L) \approx E_\infty + a_0 e^{-2k_\infty L}$$

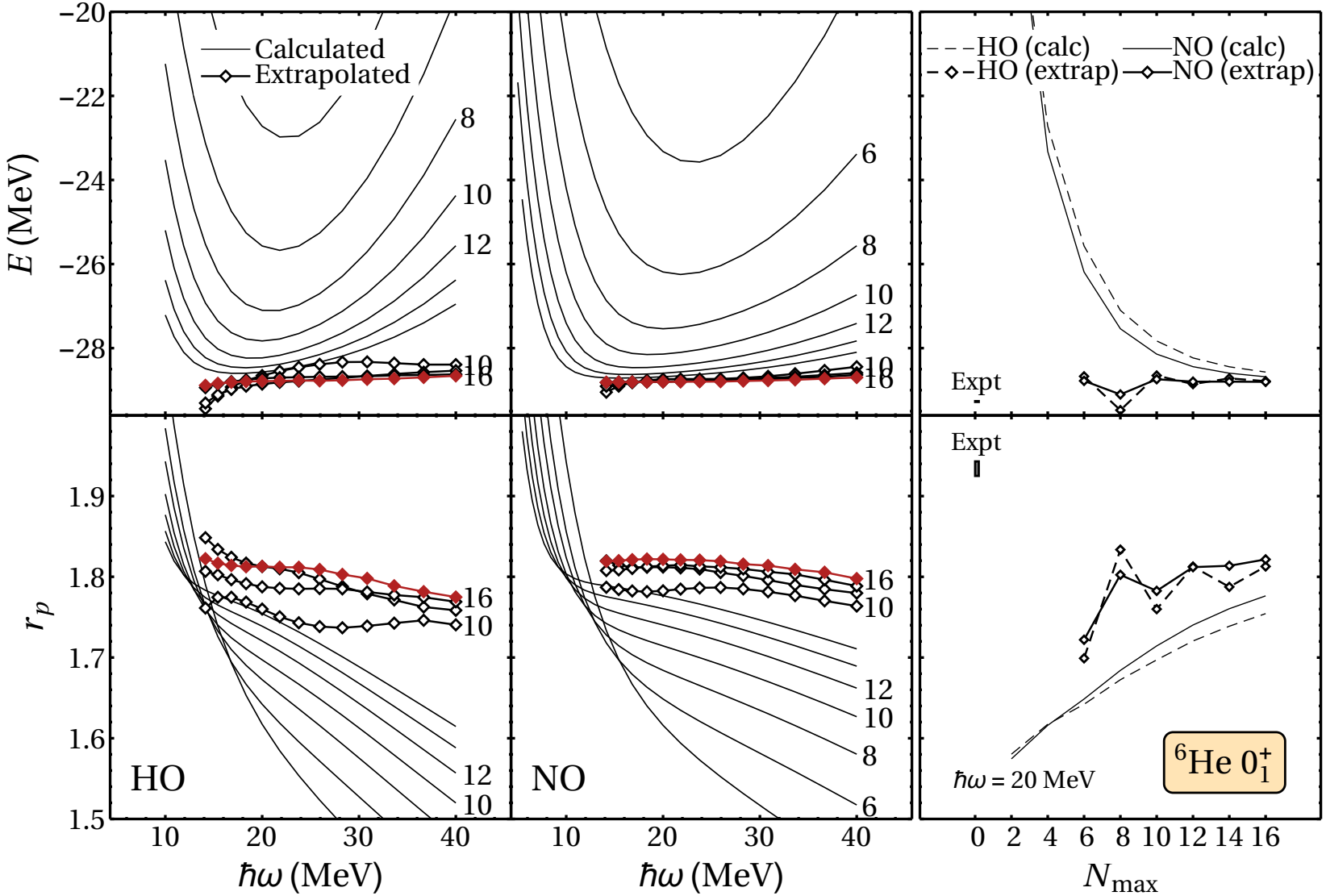
$$r^2(N,\hbar\Omega) \overset{?}{\Rightarrow} r^2(L) \approx r_\infty^2[1-(c_0+c_1\beta^{-2})\beta^3 e^{-\beta}] \qquad \beta \equiv 2k_\infty L$$

Infrared extrapolation of natural orbital calculations



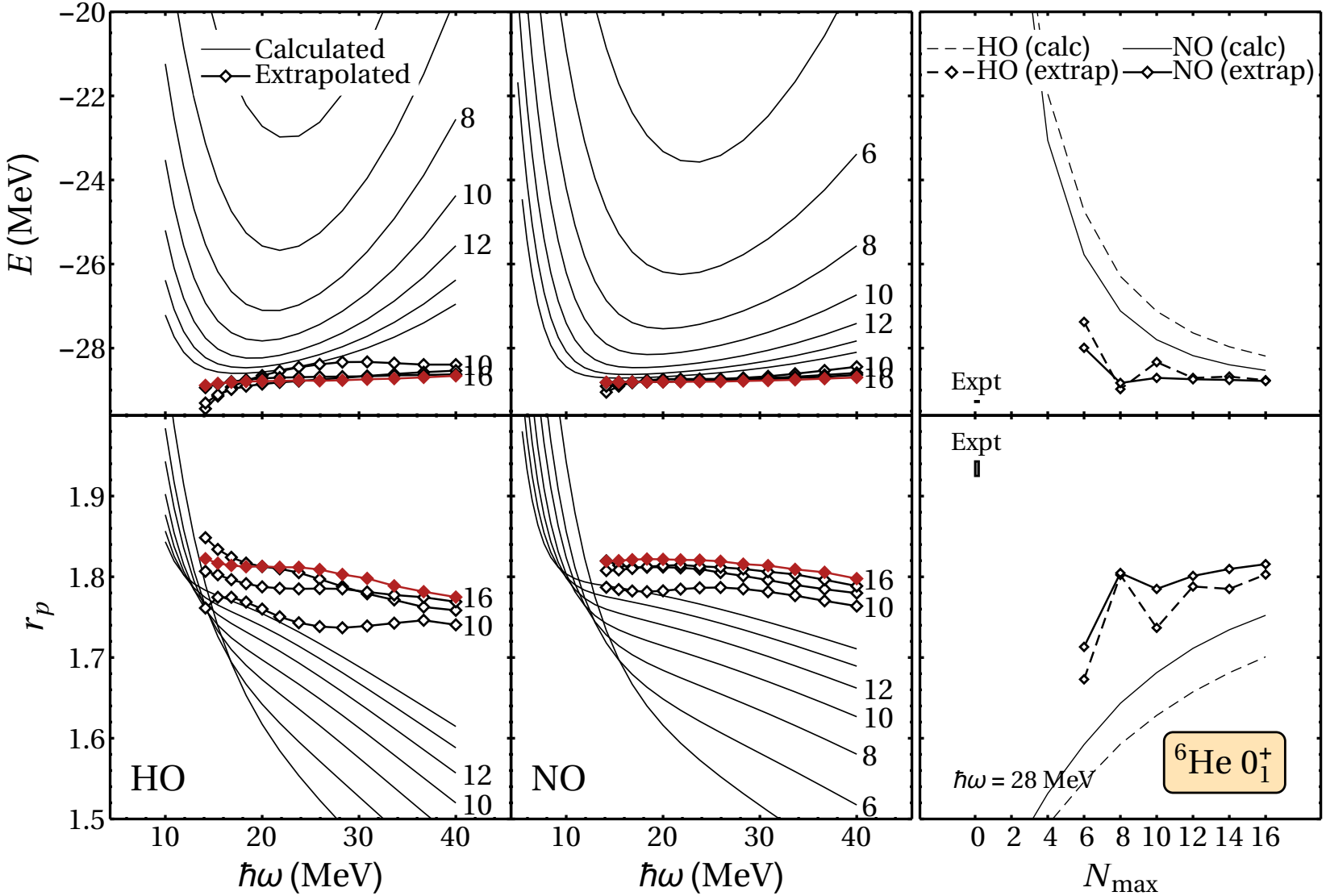
JISP16 + Coulomb

Infrared extrapolation of natural orbital calculations



JISP16 + Coulomb

Infrared extrapolation of natural orbital calculations



JISP16 + Coulomb

Summary and outlook

Change of basis to orbitals which diagonalize the density matrix

Deduced (so far) from initial calculation in harmonic oscillator basis

Improvement in convergence (energies and radii)

- About one step in $N_{\max}$ near variational minimum, more at high $\hbar\omega$
- Stability of IR extrapolation

Natural orbitals from excited state densities

Matching basis to excited state structure

Iterated natural orbitals *More effectively mix in contributions from high-lying orbitals which are poorly represented in initial many-body calculation*

Starting from an initial basis with natural asymptotics

Laguerre function basis

Natural many-body truncation scheme based on expected occupations *Potentially much more efficient than conventional oscillator $N_{\max}$ scheme*

Valentino Constantinou