Beyond the Harmonic Oscillator basis

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Outline

Beyond N_{max} truncation: Symmetry-Adapted No-Core Shell Model

Accelerating convergence: Laguerre basis

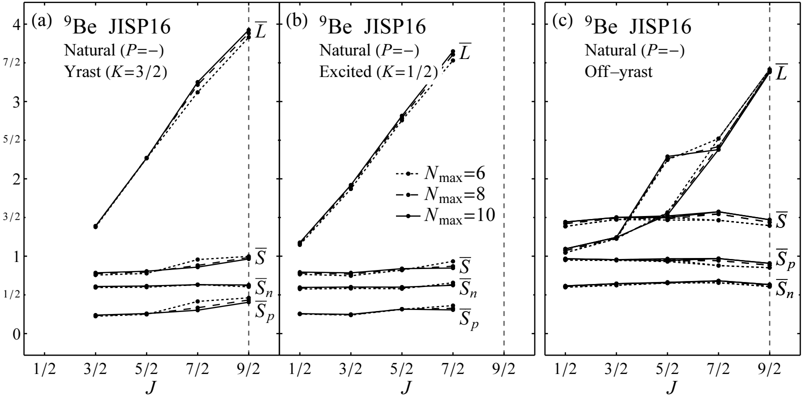
Accelerating convergence: Natural Orbitals

Orbital motion and intrinsic spin

Effective angular momenta $\bar{L}$, $\bar{S}_p$, $\bar{S}_n$, and $\bar{S}$ *"Root mean square"*

$$\bar{L}(\bar{L}+1) \equiv \langle \mathbf{L}\cdot\mathbf{L}\rangle \qquad \bar{S}(\bar{S}+1) \equiv \langle \mathbf{S}\cdot\mathbf{S}\rangle$$

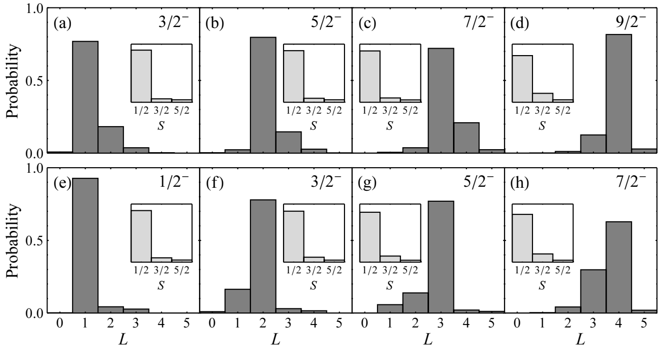
$$\bar{S}_p(\bar{S}_p+1) \equiv \langle \mathbf{S}_p\cdot\mathbf{S}_p\rangle \qquad \bar{S}_n(\bar{S}_n+1) \equiv \langle \mathbf{S}_n\cdot\mathbf{S}_n\rangle$$



Angular momentum decomposition

- CI calculations performed in M_j scheme:
  - single-particle states eigenstates of $\hat{\mathbf{J}}^2 = (\hat{\mathbf{L}} + \hat{\mathbf{S}})^2$
  - many-body basis states eigenstates of $\hat{\mathbf{J}}_\mathbf{z}$, with eigenvalye M_j
- Decomposition of wavefunction in terms of L^2 and S^2

C.W. Johnson, PRC91, 034313 (2015)

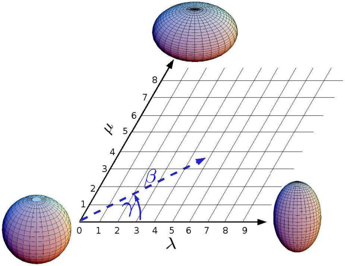


Approximate symmetries in nuclei

- Angular momentum plus quadrupole operators: SU(3)

Elliott, Proc. Roy. Soc. A245, 128 (1958)

- Quadrupole-quadrupole interaction $\hat{\mathbf{H}} \sim \hat{Q}\cdot, \hat{Q}$
- Intrinsic quadrupole deformations, characterized by $(\lambda\mu)$
- Successful in description rotational spectra of heavy deformed nuclei using nuclear shell model

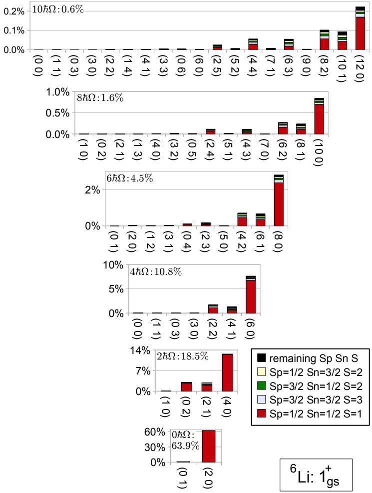


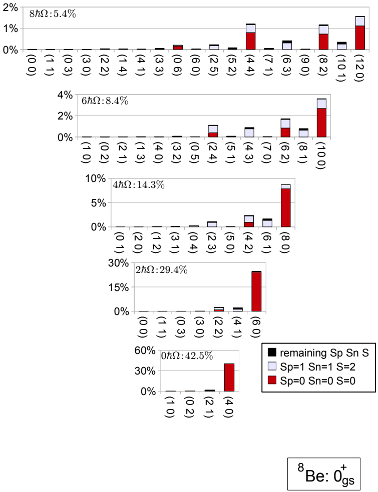
- Intrinsic spins $(S_p S_n S)$

Dytrych *et al*, J. Phy. G35, 123101 (2008)

SU(3) decomposition ^{6}Li and ^{8}Be gs wavefuntions

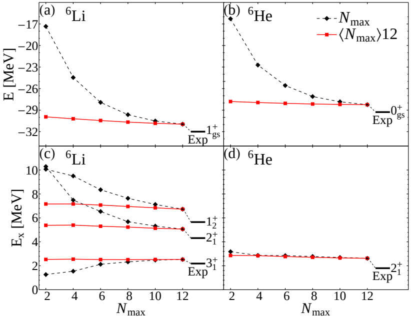
Dytrych *et al.* PRL 111, 252501 (2013)

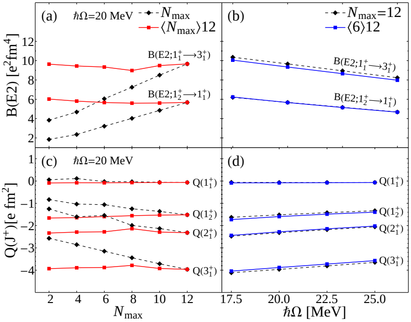




Truncated NCSM basis based on SU(3) decomposition

Dytrych *et al*, PRL111, 252501 (2013)





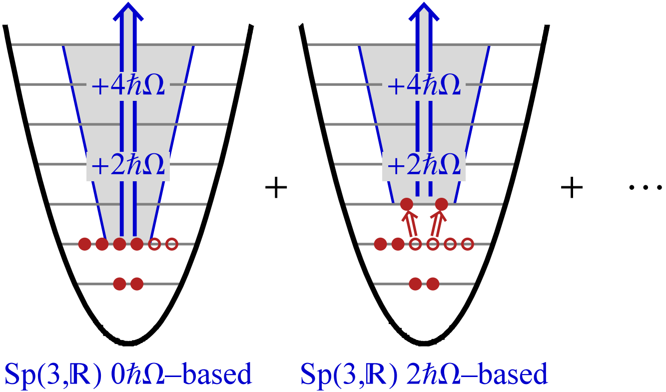
- Results obtained in reduced basis spaces $\langle N^{\perp}_{max}\rangle N^{\top}_{max}$
  - all configurations up to $N^{\perp}_{max}$
  - dominant SU(3) components up to $N^{\top}_{max}$
  - factorization of CM motion

Symplectic symmetry

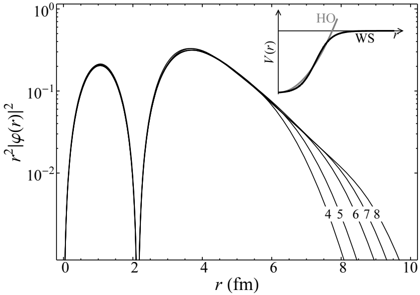
Sp(3, $\mathbb{R}$) symmetry

Dytrych, McCoy, Caprio, Draayer, Launey, Langr, ...

- relates SU(3) states with different number of oscillator quanta
- raising operators can be used to enlarge many-body basis



Harmonic Oscillator basis



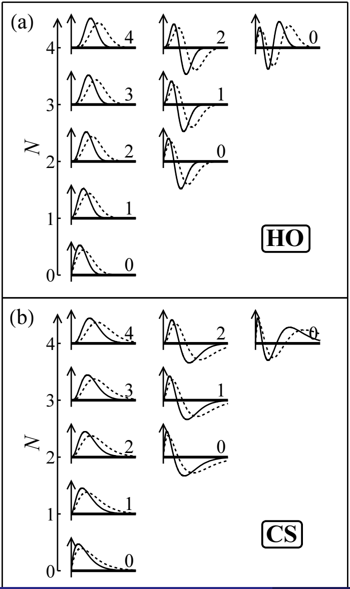
- Wood–Saxon potential
- Solved using H.O. basis functions
- Solution for $1s_{\frac{1}{2}}$

- Harmonic Oscillator radial wavefunction

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

- Wrong asymptotic behavior
  - need a lot of H.O. w.f. to build up asymptotic exponential tail
  - slow convergence for long-range operators

Laguerre basis (Coulomb–Sturmian basis)



Caprio, PM, Vary, PRC86, 034312 (2012); PRC90, 03405 (2014)

- Laguerre radial wavefunction

$$S_{nl}(b; r) = \left(\frac{2r}{b}\right)^{l+1} L_n^{2l+2}(2r/b)\, e^{-r/b}$$

- Length scale b_l choosen such that nodes of $n = 1$ Laguerre and $n = 1$ HO w.f. coincide
- Laguerre basis
  - truncation on $\sum(2n + l)$ for comparison with HO basis
  - no exact factorization of CM motion

Change of radial basis functions

- Talmi–Moshinsky brackets for H.O. basis functions, not for arbitrary radial wfns
- Transform NN potential in single-particle coordinates from H.O. to desired radial basis (i.e. Laguerre)
- 2-body matrix elements transfomation

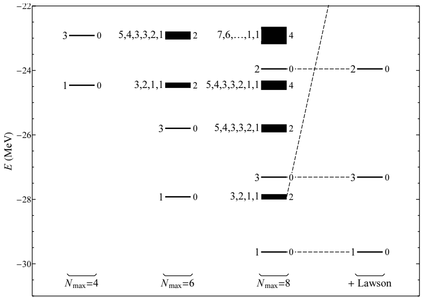
$$\langle \bar{a}\bar{b}; J|V|\bar{c}\bar{d}; J\rangle = \sum_{a,b,c,d} \langle a|\bar{a}\rangle\langle b|\bar{b}\rangle\langle c|\bar{c}\rangle\langle d|\bar{d}\rangle\langle ab; J|V|cd; J\rangle_{\text{H.O.}}$$

- Transformation coefficients for radial basis

$$\langle R^b_{nl}|S^{\bar{b}}_{\bar{n}l}\rangle = \int_0^\infty R^b_{nl}(b; r)\; S^{\bar{b}}_{\bar{n}l}(\bar{b}; r)dr$$

- Sum is in principle infinite sum
  - have to check convergence with truncation

Center of Mass motion – H.O. basis

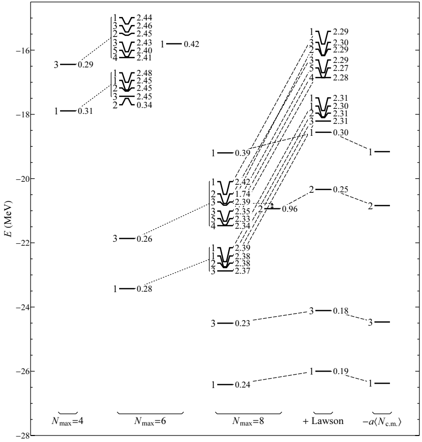


- Without Lagrange multiplier
  - at $N_{\mathrm{max}} = 6$
    - 4 degenerate states: $J^\pi = 1^+$ states at $N_{\mathrm{max}} = 4$ with 2 quanta CM excitations
    - 6 degenerate states: $J^\pi = 3^+$ states at $N_{\mathrm{max}} = 4$ with 2 quanta CM excitations
  - degenerate states at $N_{\mathrm{max}} = 8$:
    - 1^+ and 3^+ states at $N_{\mathrm{max}} = 6$ with 2 quanta CM excitations
    - 1^+ and 3^+ states at $N_{\mathrm{max}} = 4$ with 4 quanta CM excitations
- Adding Lagrange multiplier to Hamiltonian (Lawson term)

$$\hat{\mathbf{H}}_{\mathrm{rel}} \longrightarrow \hat{\mathbf{H}}_{\mathrm{rel}} + \Lambda_{\mathrm{CM}} \left(\hat{\mathbf{H}}_{\mathrm{CM}}^{\mathrm{H.O.}} - \frac{3}{2}\hbar\omega \right)$$

removes all states with CM excitations from low-lying spectrum

Center of Mass motion – Laguerre basis?



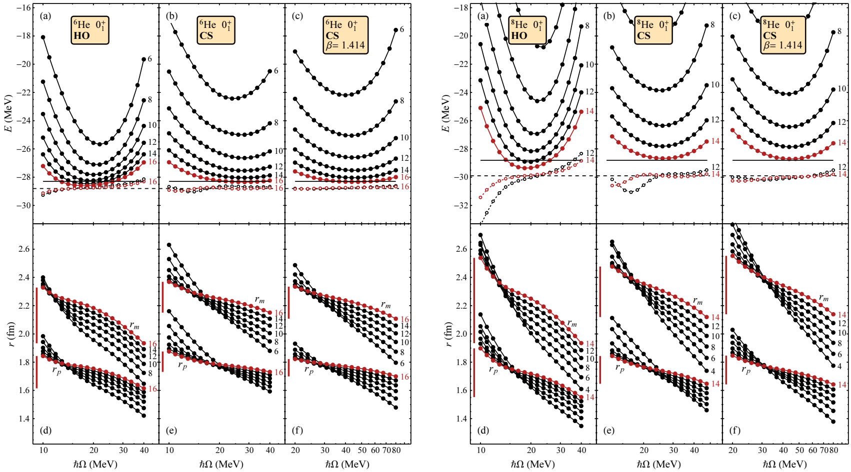
Caprio, PM, Vary, PRC86, 034312 (2012)

- Asymtotic behavior
  - H.O. basis $\exp(-a\,r^2)$
  - Laguerre basis $\exp(-c\,r)$
- Disadvantage
  - no exact factorization of Center-of-Mass motion
  - in practice, approximate factorization

    Hagen, Papenbrock, Dean, PRL103, 062503 (
  - can use Lawson term to remove spurious state
  - can correct for (most of) the effect of Lawson term on the intrinsic state

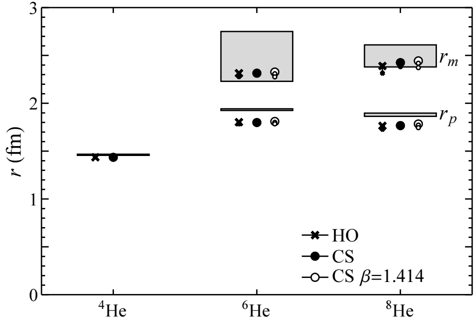
Laguerre basis for halo nuclei (Coulomb–Sturmian)

Caprio, Maris, Vary, PRC90, 03405 (2014)



- Different length parameters b_l for protons and neutrons

Radii of He isotopes with JISP16

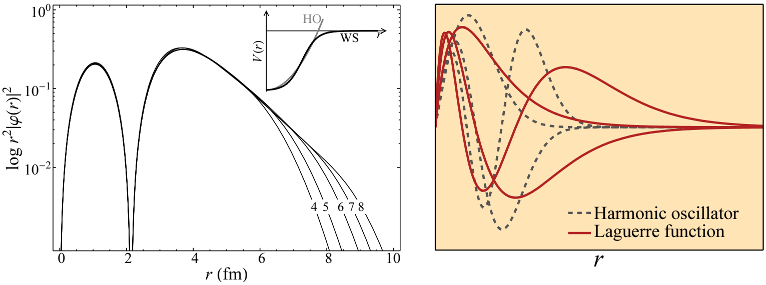


Caprio, Maris, Vary, PRC90, 03405 (2014)

- Radii exctracted from crossover point for three highest $N_{\max}$ values

- HO and Laguerre (CS) basis in good agreement with each other
- Qualitative agreement with data
- Note: matter radii in agreement with elastic scattering measurement/extraction of experimental radius

Choice of radial wavefunctions



- H.O. basis falls off like Gaussian, but asymptotic wavefunction falls of as an exponential
- Choose basis wavefunctions with explicit exponential falloff
  - Laguerre (Coulomb–Sturmian) basis
  - Wood–Saxon basis

Negoita, PhD thesis, ISU 2010

- Can we make the Hamiltonian construct the orbitals?
  - Natural orbitals

Constantinou, PhD thesis, Notre Dame 2016

Natural Orbitals

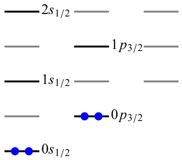
- Many-body basis: configurations of nucleons over (*nlj*) orbitals
- Scalar one-body density matrix

$$\rho^{(0)} = \langle \bar{\Psi} | [a^\dagger \tilde{b}]_{00} | \Psi \rangle$$

- Scalar OBDM is block diagonal

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

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

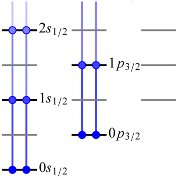


Natural Orbitals

- Many-body basis: configurations of nucleons over (*nlj*) orbitals
- Perform No-Core CI calculation in H.O. basis

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

$$\rho^{(0)} = \left(\begin{array}{ccc|cc|c} * & * & * & 0 & 0 & \cdots \\ * & * & * & 0 & 0 & \cdots \\ * & * & * & 0 & 0 & \cdots \\ \hline 0 & 0 & 0 & * & * & \cdots \\ 0 & 0 & 0 & * & * & \cdots \\ \hline \cdots & \cdots & \cdots & \cdots & \cdots & \end{array}\right) \begin{array}{l} 0s_{1/2} \\ 1s_{1/2} \\ 2s_{1/2} \\ 0p_{3/2} \\ 1p_{3/2} \\ \cdots \end{array}$$

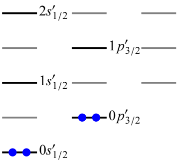


- Diagonalize block-diagonal scalar OBDM

Natural Orbitals

- Many-body basis: configurations of nucleons over (*nlj*) orbitals
- Perform No-Core CI calculation in H.O. basis
- Diagonalize block-diagonal scalar OBDM

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



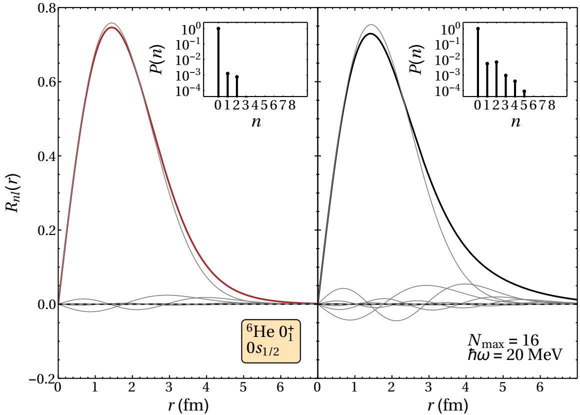
- Change basis on radial wavefunctions using eigenvectors of OBDM

Natural Orbitals for ^{6}He: $0s_{\frac{1}{2}}$

Initial NCCI calculation in harmonic oscillator basis

Scalar density matrix ⇒ natural orbitals

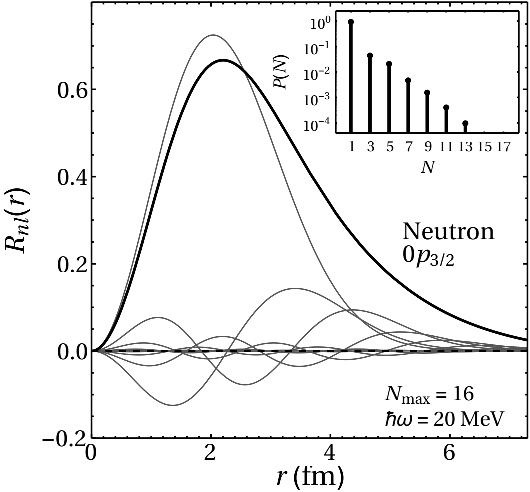
Accesses oscillator orbitals up to $N = N_{\max}$ (p) or $N_{\max} + 1$ (n) $\quad N = 2n + l$



JISP16 + Coulomb

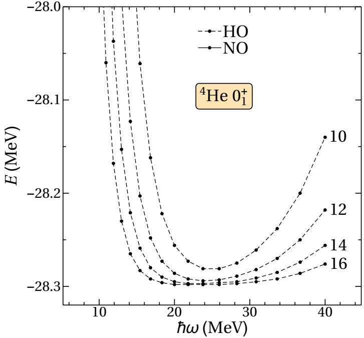
Natural Orbitals for ^{6}He: neutron $0p_{\frac{3}{2}}$

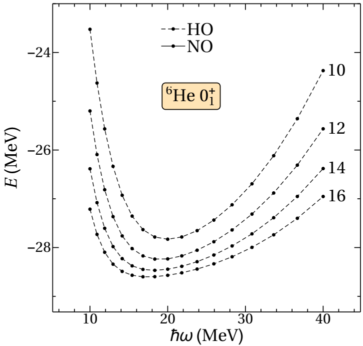
Constantinou, Caprio, Vary and Maris, arXiv:1605.04976 [nucl-th]



Ground state energies: H.O. basis

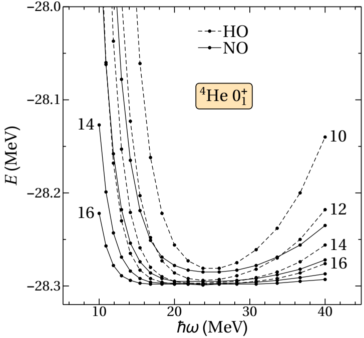
Constantinou, Caprio, Vary and Maris, arXiv:1605.04976 [nucl-th]

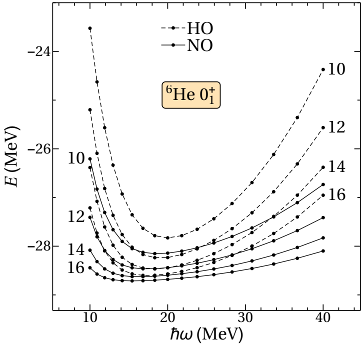




Ground state energies: Natural Orbitals

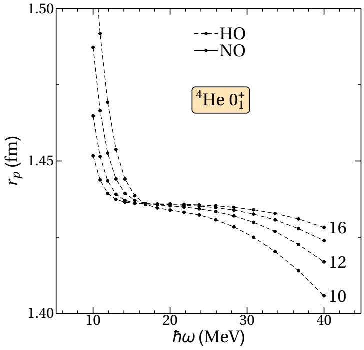
Constantinou, Caprio, Vary and Maris, arXiv:1605.04976 [nucl-th]

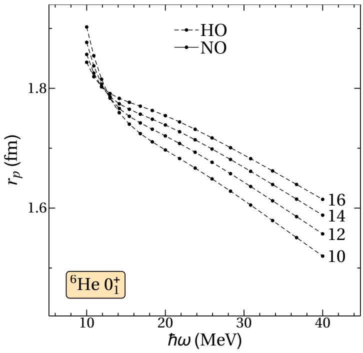




RMS radii: H.O. basis

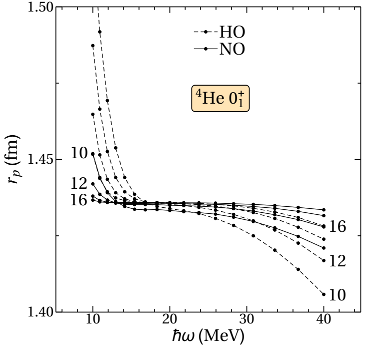
Constantinou, Caprio, Vary and Maris, arXiv:1605.04976 [nucl-th]

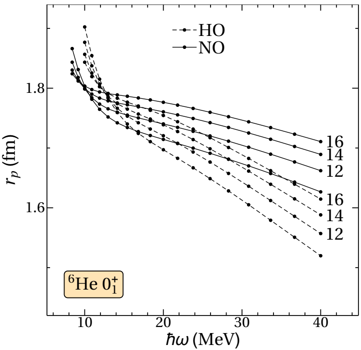




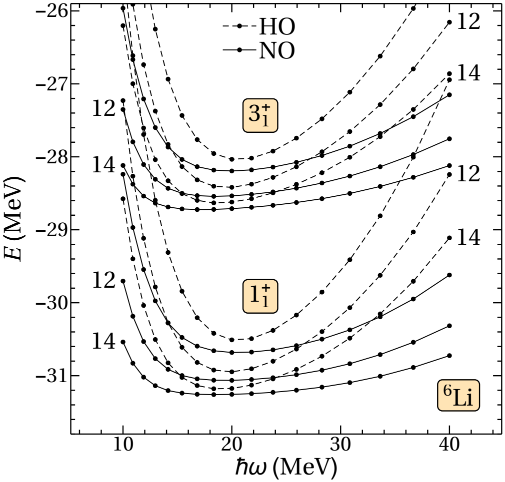
RMS radii: Natural Orbitals

Constantinou, Caprio, Vary and Maris, arXiv:1605.04976 [nucl-th]





Also works for excited states: ^{6}Li



- More calculations underway
- Next step: iterate
  - self-consistent natural orbitals
- To be continued . . .

Resonances: need to include continuum

For further reading

- Berggren basis / Gamow Shell Model
  - incorporate continuum into basis
    Berggren, Nucl. Phys. A109 265 (1968)
  - diagonalize complex symmetrix matrix
    Michel, Nazarewicz, Ploszajczak, Vertse
    J. Phys. G36, 013101 (2009) arXiv:0810.2728 [nucl-th]
- No-Core CI calculations with Berggren basis
  - Papadimitriou, Rotureau, Michel, Ploszajczak and Barrett,
    Phys. Rev. C88 044318 (2013), arXiv:1301.7140 [nucl-th]
  - Shin, Kim, PM, Vary, Forssén, Rotureau and Michel,
    arXiv:1605.02819 [nucl-th]