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Nonlocal translationally invariant nuclear density

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In collaboration with

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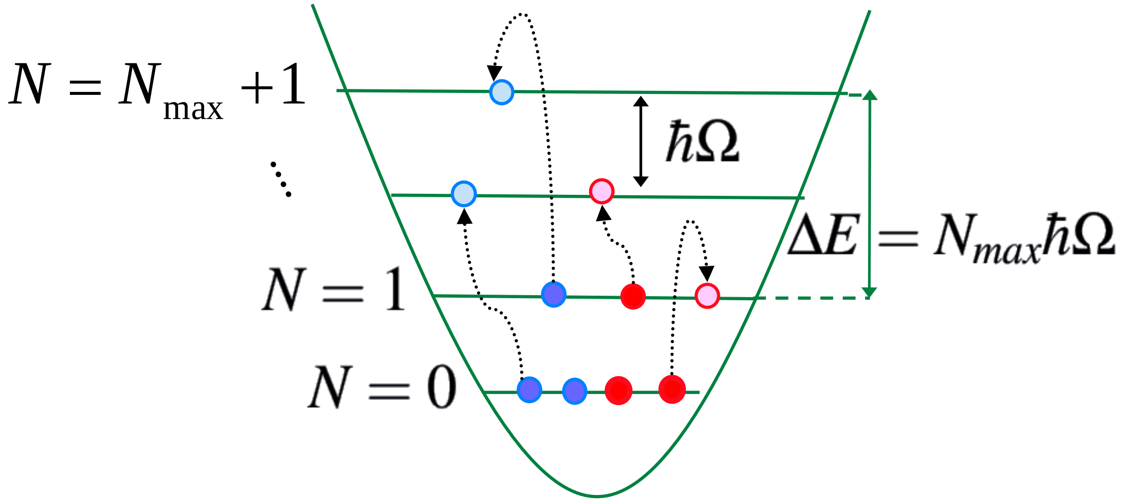
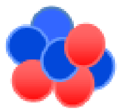
Discovery, accelerated

No-core shell model (NCSM)



- NCSM is an *ab initio* approach to solve the many-body Schrödinger equation for bound states (narrow resonances) starting from high-precision NN+NNN interactions
- Uses large (but finite!) expansions in HO many-body basis states

A

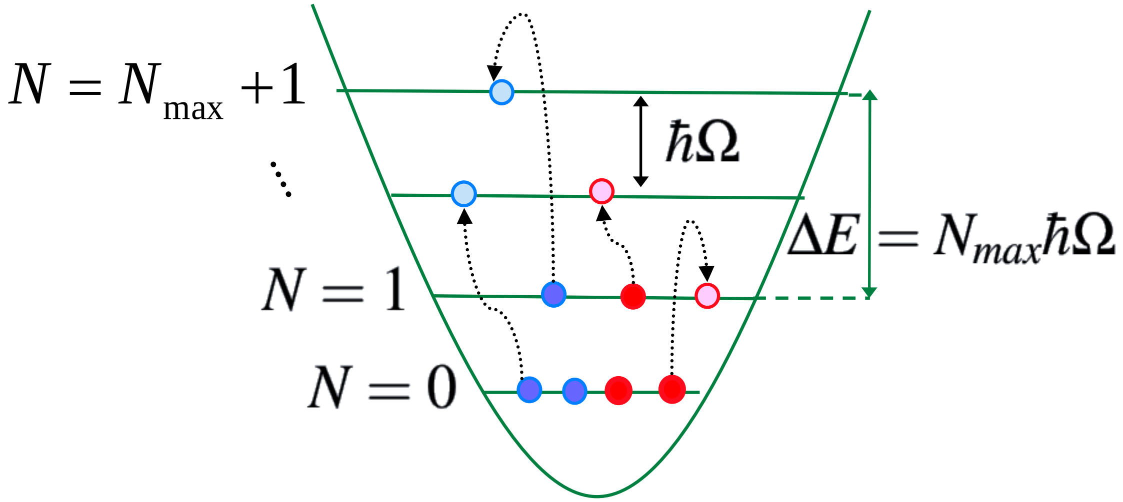


$$\Psi^A = \sum_{N=0}^{Nmax} \sum_i c_{Ni} \Phi_{Ni}^A$$

- Translational invariance of the internal wave function is preserved when single-particle Slater Determinant (SD) basis is used with N_{max} truncation

$$\langle \vec{r}_1 \cdots \vec{r}_A \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots \vec{\tau}_A | A\lambda JM \rangle_{SD} = \langle \vec{\xi}_1 \cdots \vec{\xi}_{A-1} \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots \vec{\tau}_A | A\lambda JM \rangle \varphi_{000}(\vec{\xi}_0)$$

No-core shell model (NCSM)



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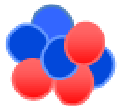


$$\Psi^A = \sum_{N=0}^{Nmax} \sum_i c_{Ni} \Phi^A_{Ni}$$

- Translational invariance of the internal wave function is preserved when single-particle Slater Determinant (SD) basis is used with $N_{\max}$ truncation

Intrinsic wavefunction

COM wavefunction

$$\langle \vec{r}_1 \cdots \vec{r}_A \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots \vec{\tau}_A | A\lambda JM \rangle_{SD} = \boxed{\langle \vec{\xi}_1 \cdots \vec{\xi}_{A-1} \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots \vec{\tau}_A | A\lambda JM \rangle} \boxed{\varphi_{000}(\vec{\xi}_0)}$$

Coordinate form of the density

Nonlocal translationally invariant density

- arXiv:1712.02879; Phys. Rev. C, in press.

$$\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r}-\vec{R}, \vec{r}' - \vec{R}) | A\lambda_i J_i M_i \rangle$$

$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f} (J_i M_i K k | J_f M_f) \left(Y_l^*\left(\widehat{\vec{r}-\vec{R}}\right) Y_{l'}^*\left(\widehat{\vec{r}'-\vec{R}}\right)\right)_k^{(K)}$$

$$\times R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}'-\vec{R}|\right)$$

$$\times (M^K)^{-1}_{n,l,n',l',n_1,l_1,n_2,l_2} (-1)^{l_1+l_2+K+j_2-\frac{1}{2}} \hat{j}_1 \hat{j}_2 \hat{K} \begin{Bmatrix} j_1 & j_2 & K \\ l_2 & l_1 & 1/2 \end{Bmatrix}$$

$$\times \frac{(-1)}{\hat{K}} {}_{SD}\langle A\lambda_f J_f \left\| \left(a^\dagger_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2}\right)^{(K)} \right\| A\lambda_i J_i \rangle_{SD}$$

Coordinate form of the density

Normalization

$$\int d\vec{x}\,\langle A\lambda JM|\rho_{op}^{phys}(\vec{x})|A\lambda JM\rangle = A$$

Nonlocal translationally invariant density

- arXiv:1712.02879; Phys. Rev. C, in press.

$$\begin{aligned}
&\langle A\lambda_f J_f M_f|\rho_{op}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})|A\lambda_i J_i M_i\rangle \\
&\quad = \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \sum \frac{1}{\hat{J}_f}(J_i M_i K k|J_f M_f)\,\boxed{\left(Y_l^*\left(\widehat{\vec{r}-\vec{R}}\right)Y_{l'}^*\left(\widehat{\vec{r}\,'-\vec{R}}\right)\right)_k^{(K)}} \\
&\quad \times R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}\,'-\vec{R}|\right) \\
&\quad \times (M^K)^{-1}_{n,l,n',l',n_1,l_1,n_2,l_2}(-1)^{l_1+l_2+K+j_2-\frac{1}{2}}\,\hat{j}_1\,\hat{j}_2\,\hat{K}\begin{Bmatrix} j_1 & j_2 & K \\ l_2 & l_1 & {}^1\!/_2 \end{Bmatrix} \\
&\quad \times \frac{(-1)}{\hat{K}}\,{}_{SD}\langle A\lambda_f J_f\,\|(a^\dagger_{n_1 l_1 j_1}\tilde{a}_{n_2 l_2 j_2})^{(K)}\|\,A\lambda_i J_i\rangle_{SD}
\end{aligned}$$

All angular dependence factorized out for plotting

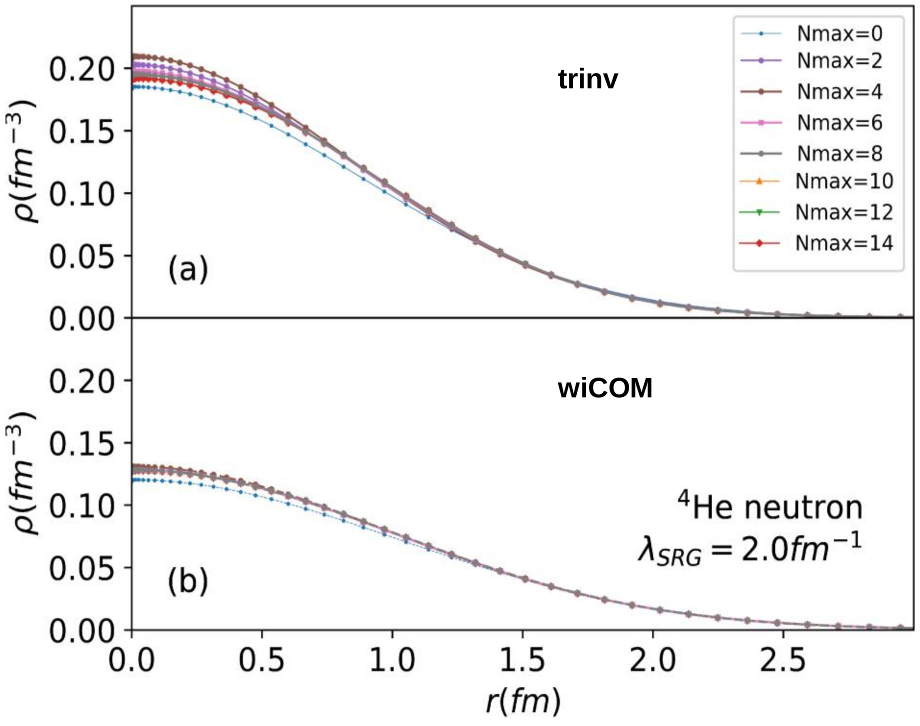
NN and 3N interactions – N^{4}LO(500)+3NlnI

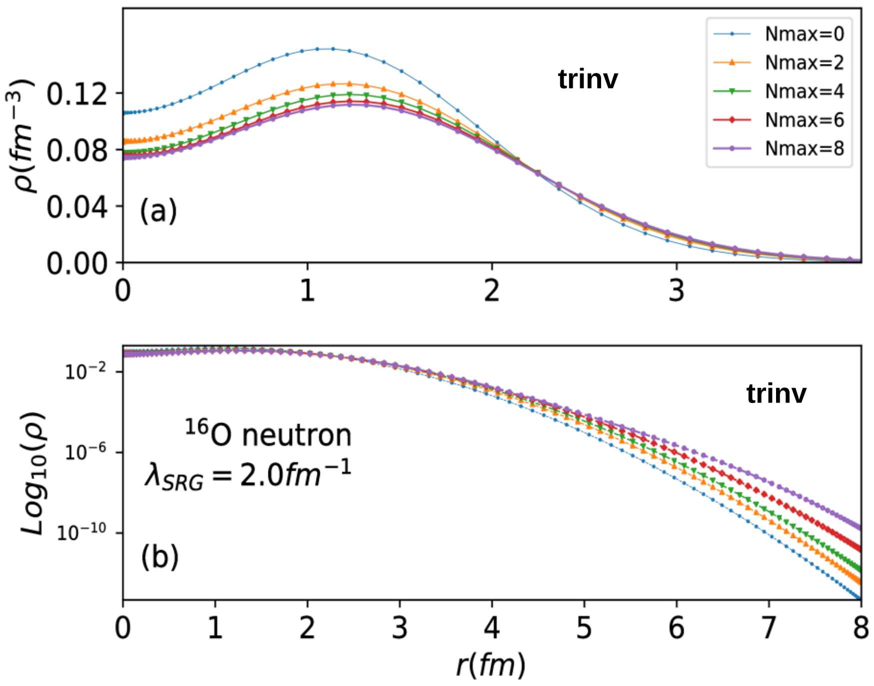
NN systematic from LO to N^{4}LO

- D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015)
- D. R. Entem, R. Machleidt, and Y. Nosyk, arXiv:1703.05454

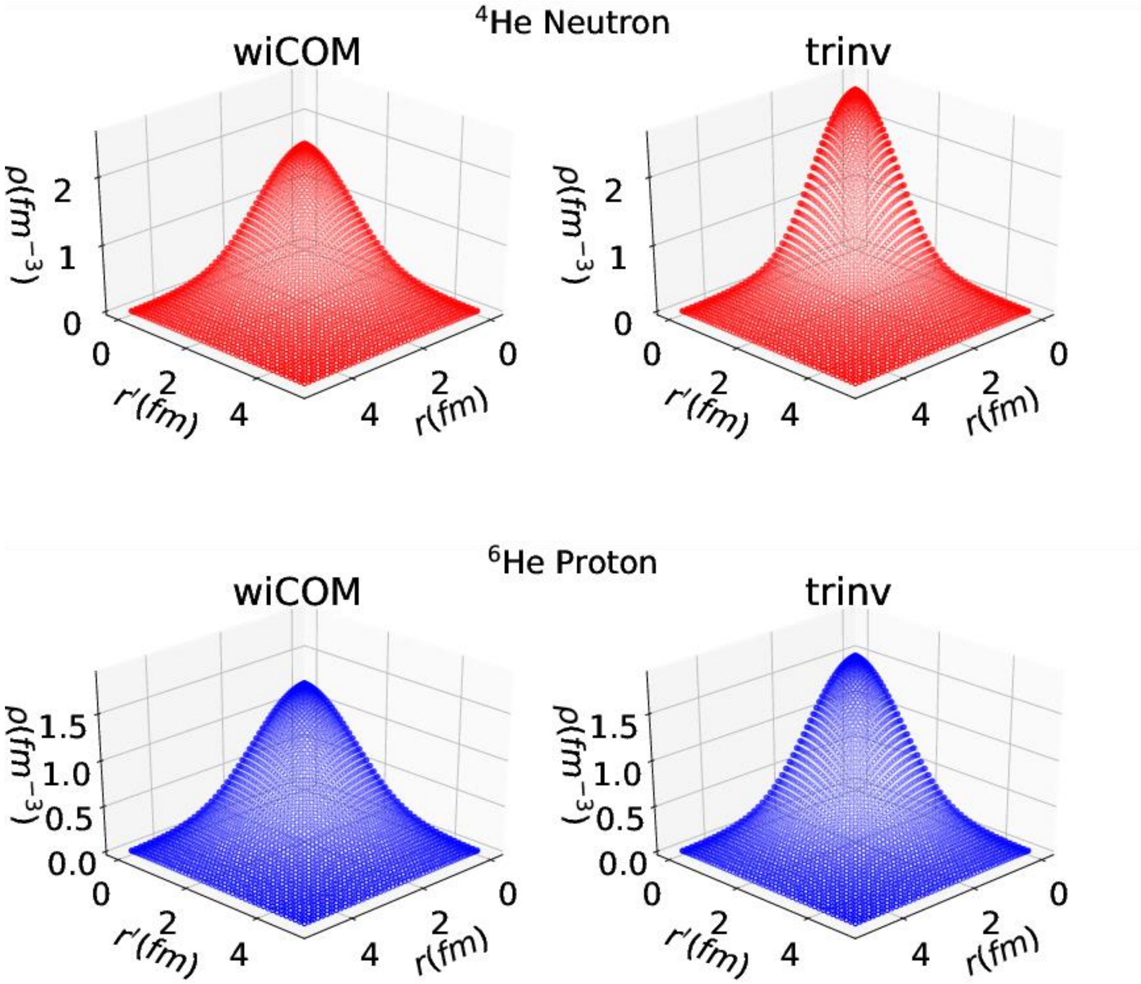
3N at N^{2}LO

- Navrátil, 650 MeV local cut-off and 500 MeV non-local cut-off

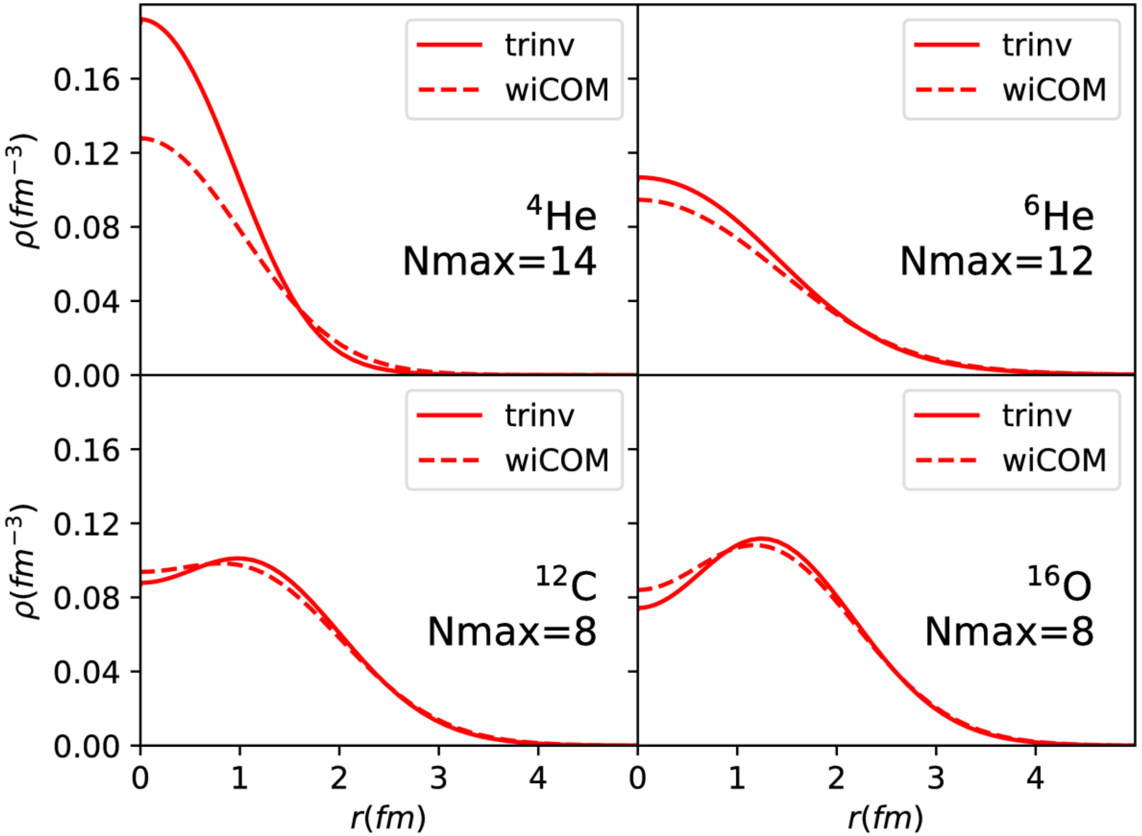




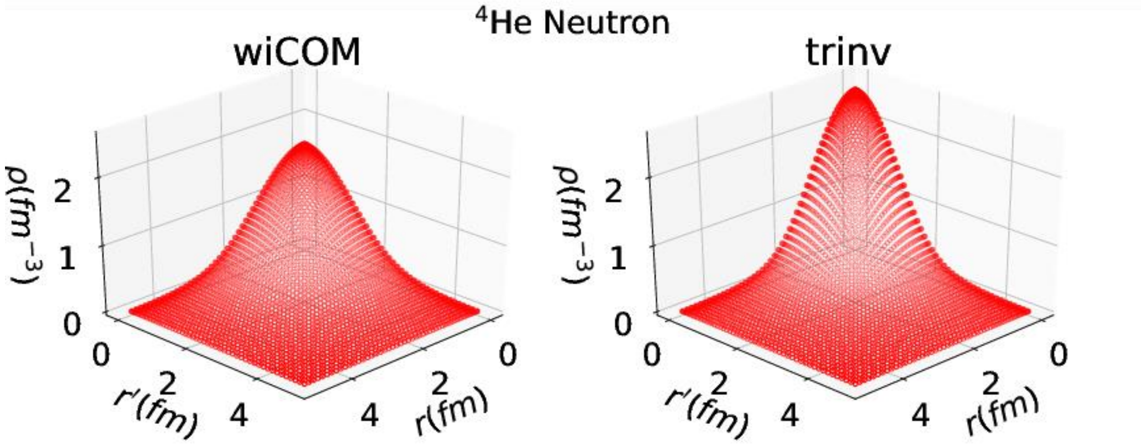
Density of ground state ^{4,6}He, ^{12}C, ^{16}O with NN-N^{4}LO(500)+3NlnI



Local density



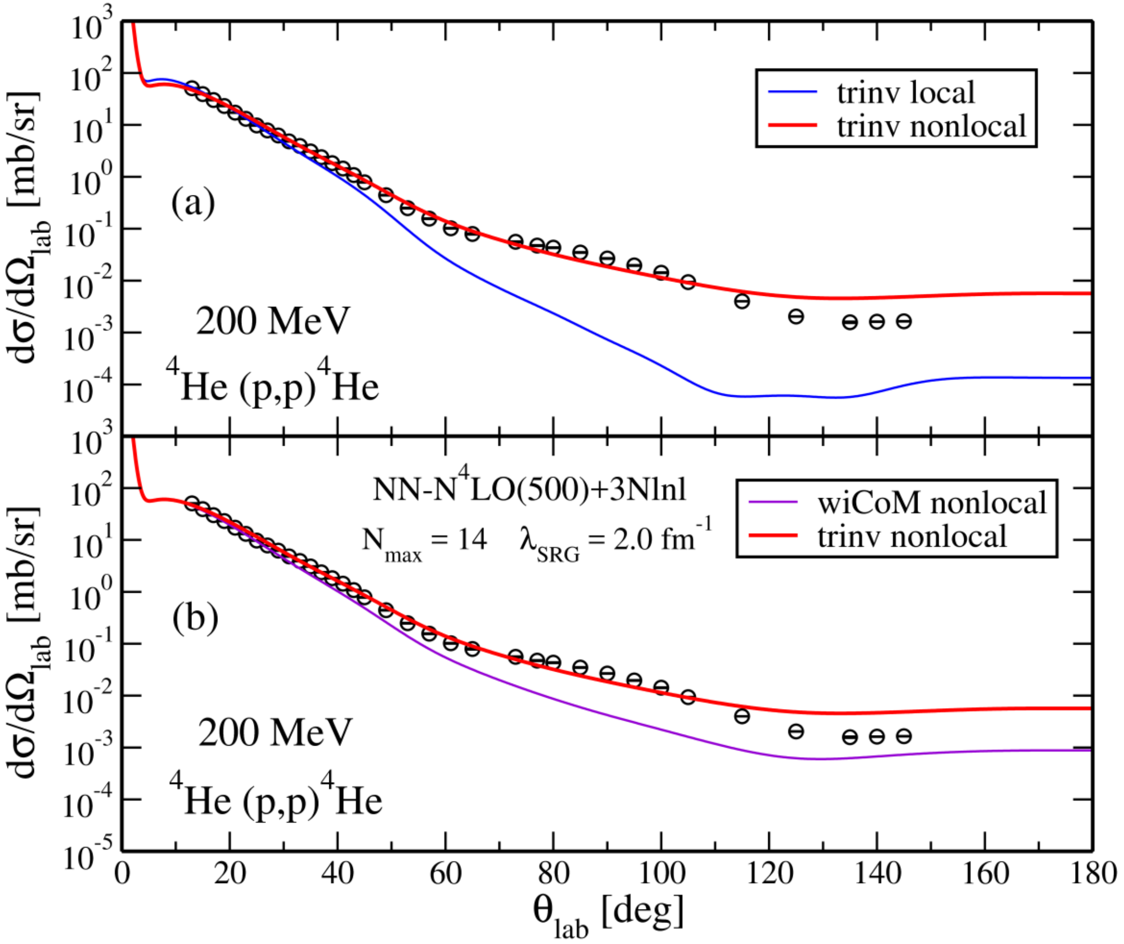
Applications to optical potentials



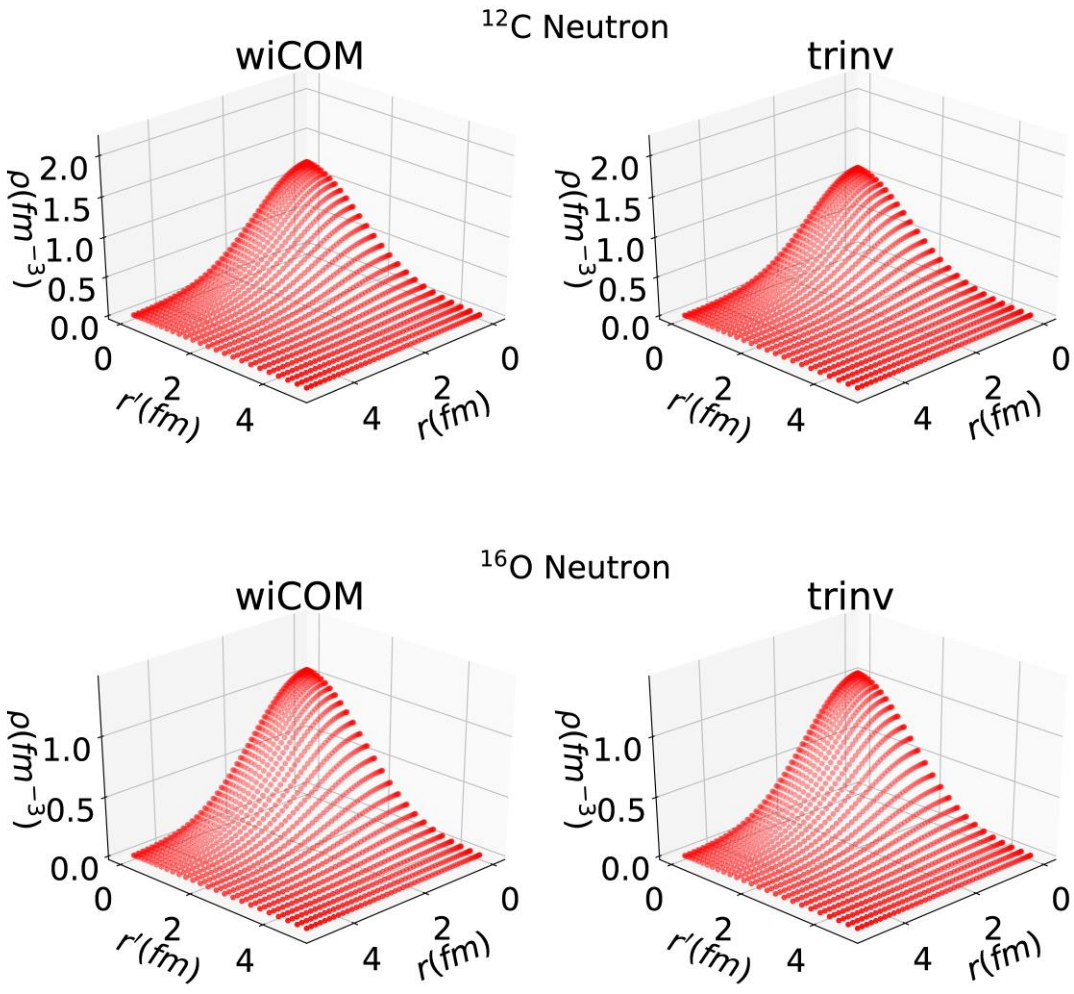
- We can achieve an additional step towards consistent optical potential calculations by using the nonlocal density

$$U(\vec{q},\vec{K}) = \sum_{N=n,p} \int d\vec{P} \;\; \eta(\vec{q},\vec{K},\vec{P})\, t_{pN}(\vec{q},\vec{K},\vec{P})\, \rho_N(\vec{q},\vec{P})$$

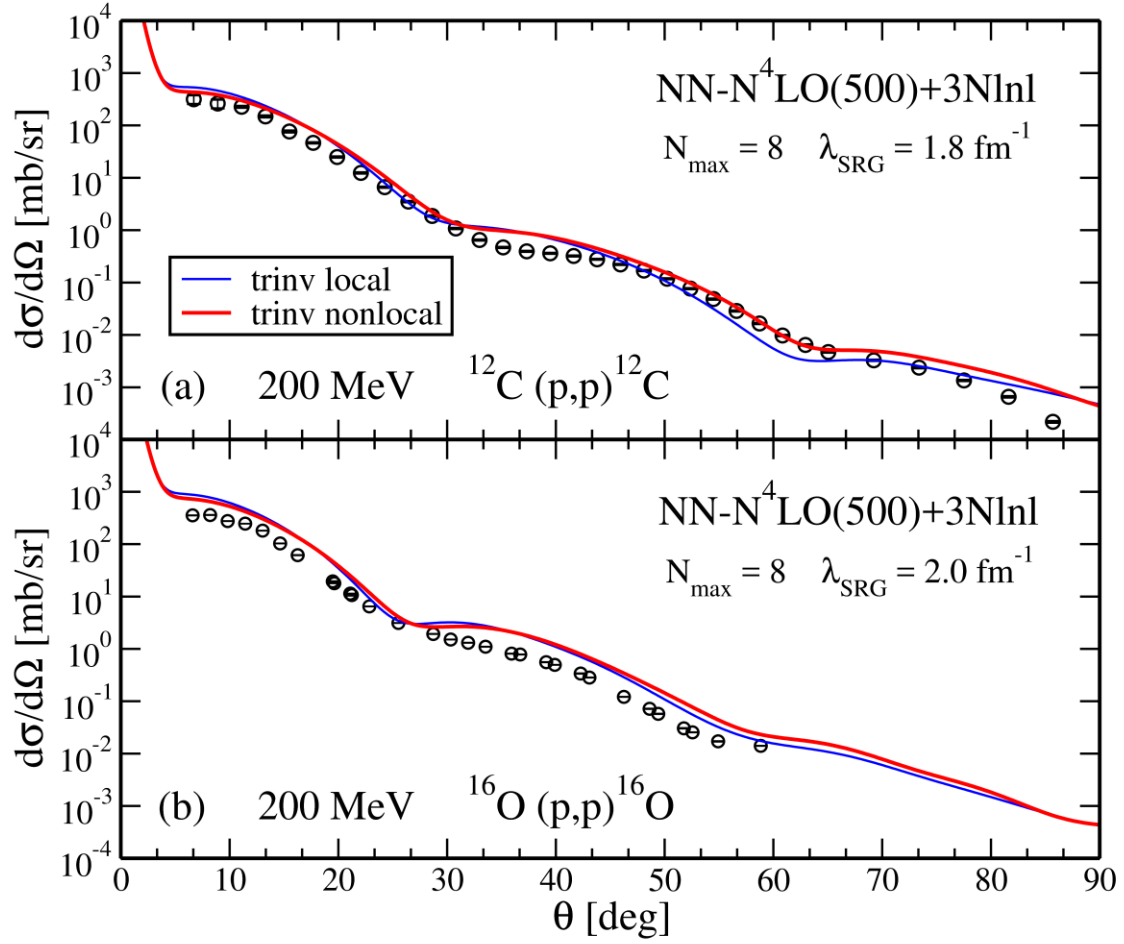
Differential cross sections



Applications to optical potentials



Differential cross sections



Applications to density functional theory

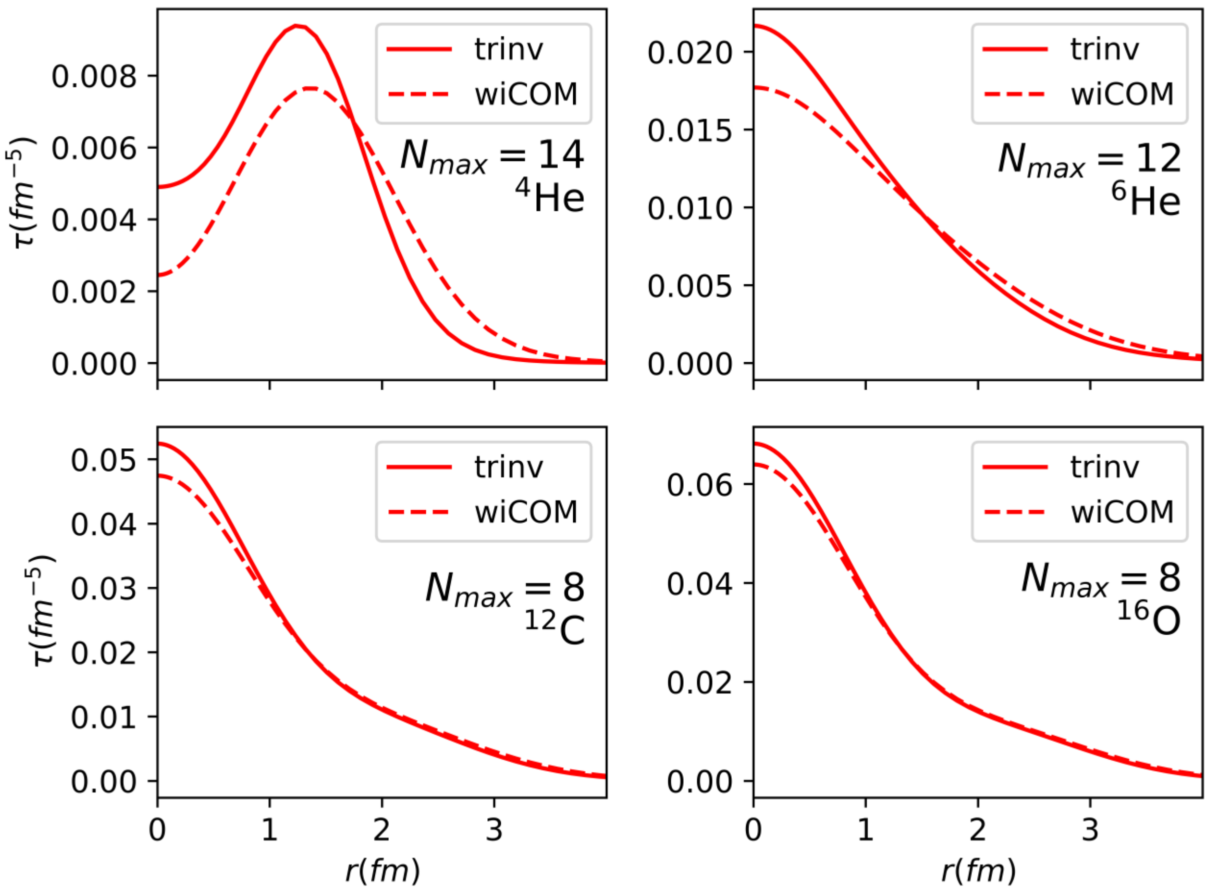
- Kinetic density (and other related densities) is a DFT quantity we are capable of calculating from *ab initio* wavefunctions according to

$$\tau_T(\vec{r}) = \left(\vec{\nabla}\cdot\vec{\nabla}'\,\rho_T(\vec{r},\vec{r}\,')\right)|_{\vec{r}=\vec{r}\,'}$$

$$\frac{d}{dr}R_{n,l}(r) = \frac{l}{r}R_{n,l}(r) - \frac{1}{b}\left[\sqrt{n+l+\frac{3}{2}}\cdot R_{n,l+1}(r) + \sqrt{n}\cdot R_{n-1,l+1}(r)\right]$$

- Effects of COM removal should be amplified in DFT quantities such as the kinetic density, due to the application of gradients on the nonlocal density

Kinetic density



Conclusions and outlook

- Conclusions
  - We observed significant differences in the nuclear density of light systems when the COM was removed
  - We can now use the more general, nonlocal density for optical potentials of nuclear reactions and *ab initio* calculations in DFT
  - More details on some of these results can be found in arXiv:1712.02879; Phys. Rev. C, in press.

- Outlook
  - We are now pursuing the use of these densities in calculations with natural orbitals (arxiv:1605.04976), reducing basis sizes and improving convergence
  - We will attempt to extend this to the translationally invariant one-body nuclear density matrix and further cut down basis sizes

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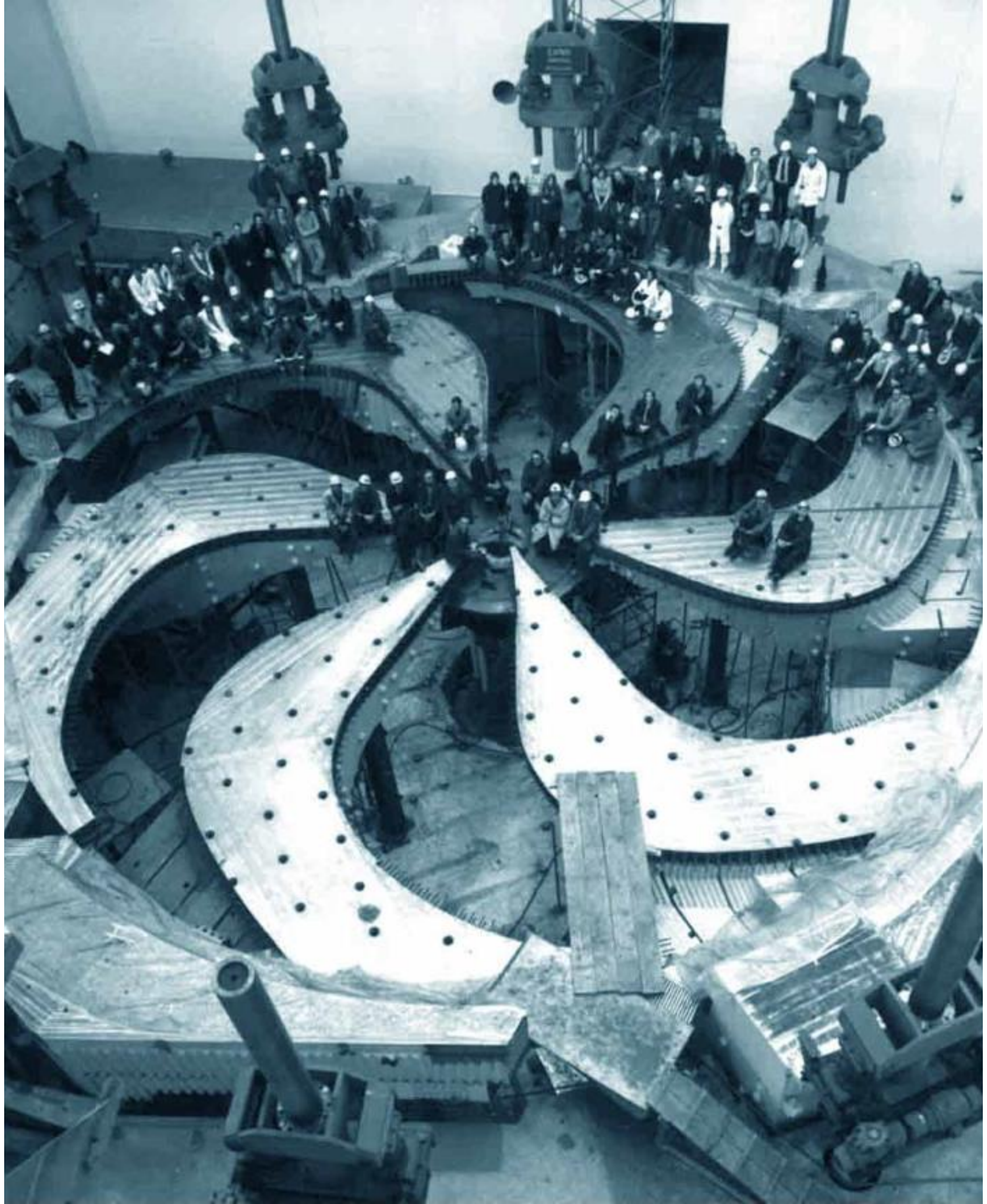
Thank you
Merci



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