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Canadian Institute of Nuclear Physics

Institut canadien de physique nucléaire

Nuclear density from *ab initio* theory

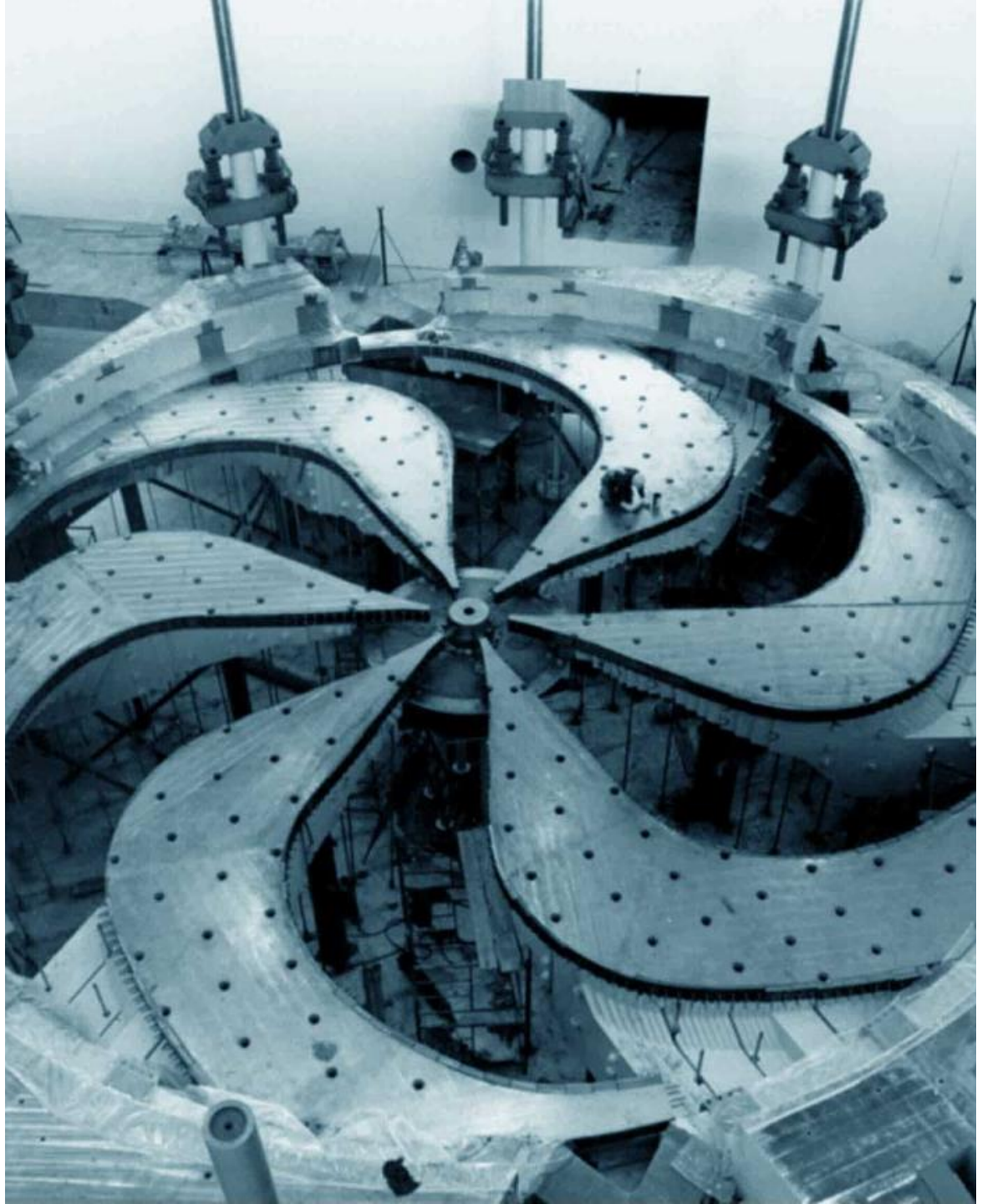
Michael Gennari

TRIUMF – Undergraduate researcher from University of Waterloo

In collaboration with

Petr Navrátil and Matteo Vorabbi

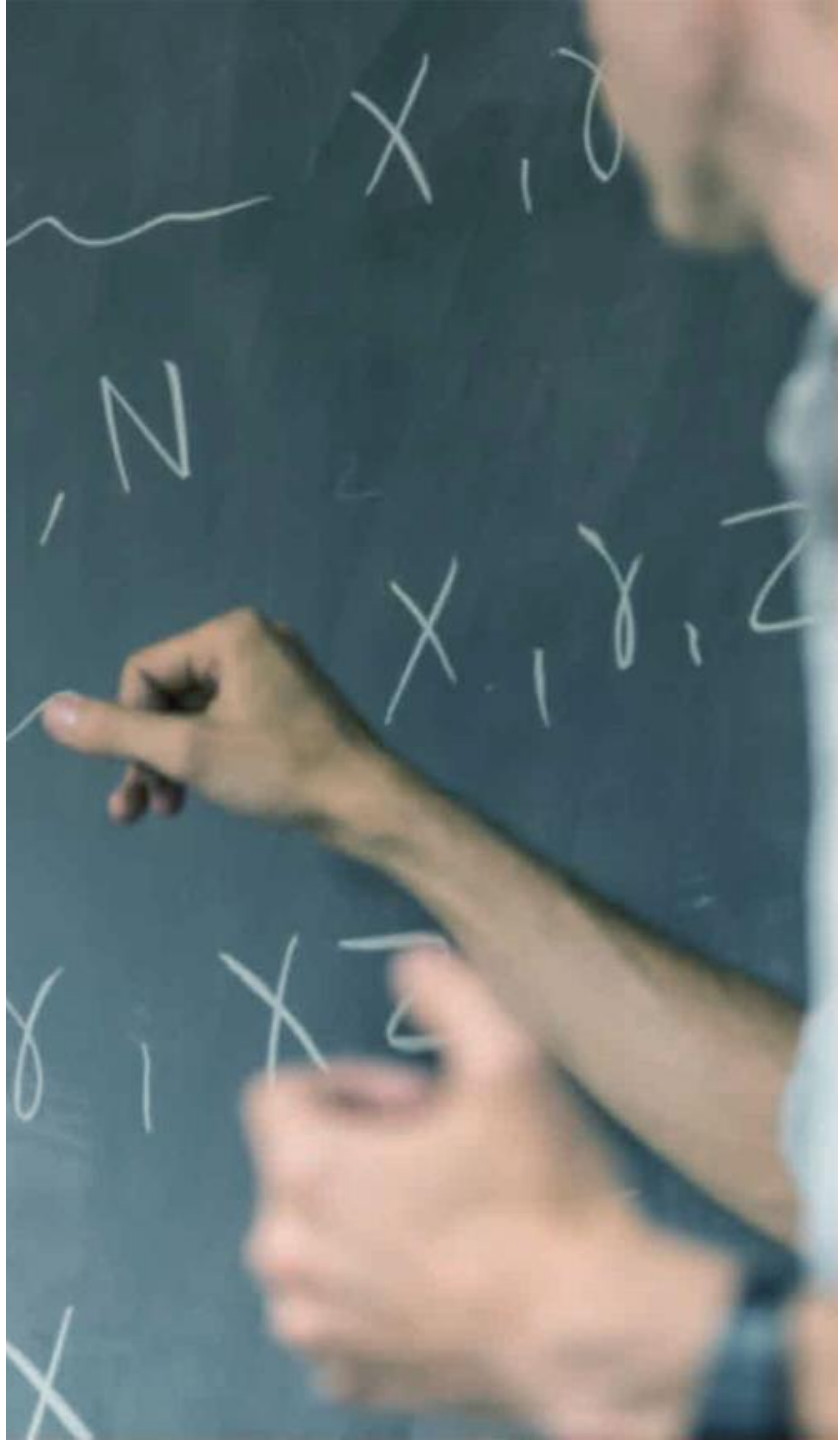
2018-08-11



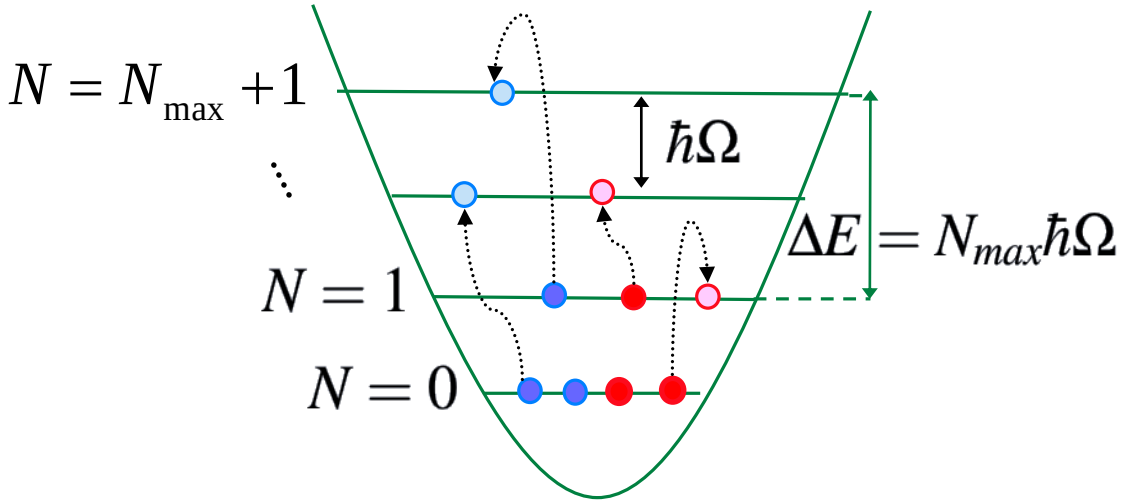
Discovery, accelerated

Outline

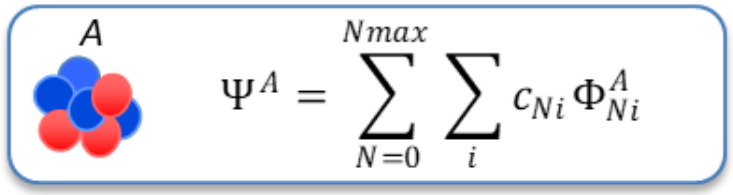
1. **Ab Initio No-Core Shell Model (NCSM)**
   a) Introduction to NCSM
   b) Factorization of spurious COM motion
   c) Coordinate space nonlocal density
2. **Chiral Effective Field Theory Interactions (EFT)**
   a) Chiral expansion in many-body interactions
   b) Convergence
3. **Results**
   a) Nonlocal density
   b) Applications to optical potentials
   c) Applications to density functional theory



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



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

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

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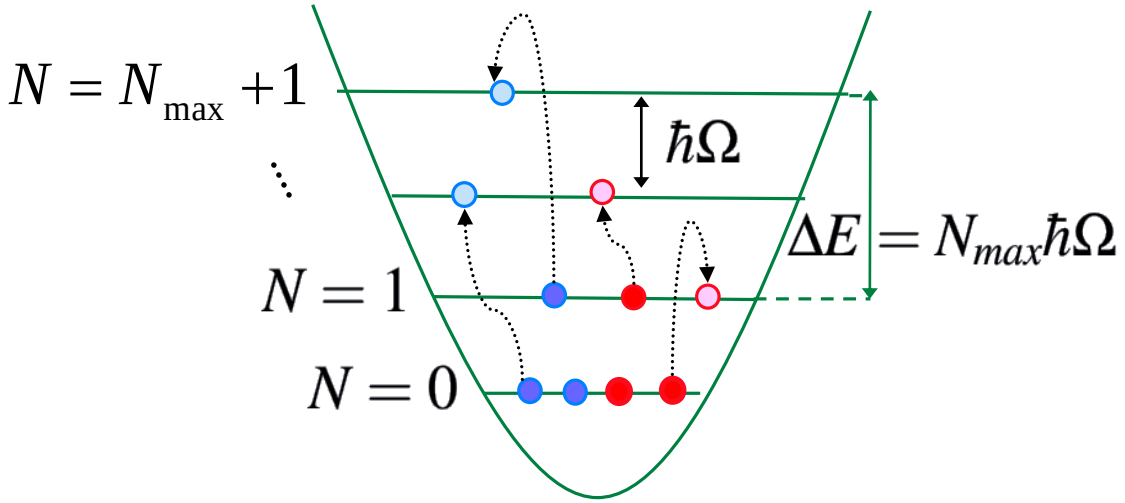

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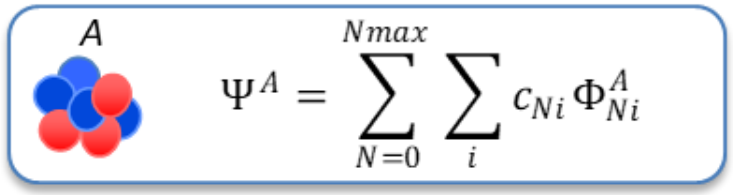

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Intrinsic wavefunction

COM wavefunction

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Coordinate form of the density

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

PHYSICAL REVIEW C **97**, 034619 (2018)

Microscopic optical potentials derived from *ab initio* translationally invariant nonlocal one-body densities

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University of Waterloo, 200 University Avenue West Waterloo, Ontario N2L 3G1, Canada and TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia V6T 2A3, Canada

Matteo Vorabbi,† Angelo Calci, and Petr Navrátil‡
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Nonlocal translationally invariant density

- Translationally invariant nuclear density is obtained from intrinsic wavefunction
- Slater determinant description is advantageous for A > 4
- When slater determinant description is used, there is a spurious COM contribution
- It is possible to exactly remove this contamination

Normalization

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

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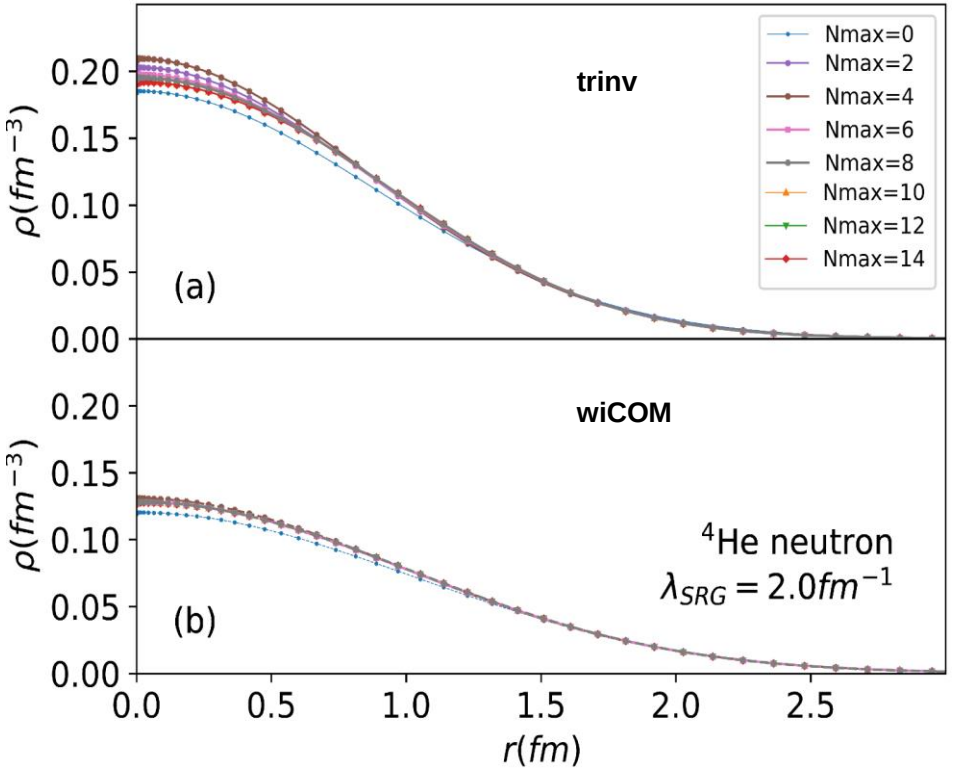
NN and 3N interactions – N^{4}LO(500)+3Nlnl

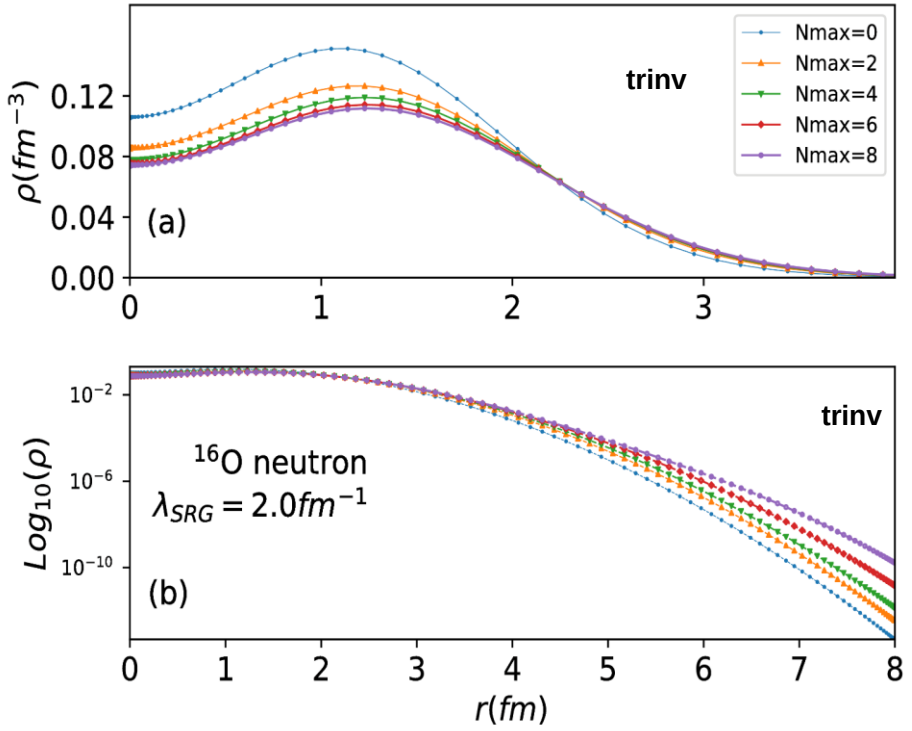
NN systematic from LO to N^{4}LO

- D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015)
- D. R. Entem, R. Machleidt, and Y. Nosyk, Phys. Rev. C 96, 024004 (2017)

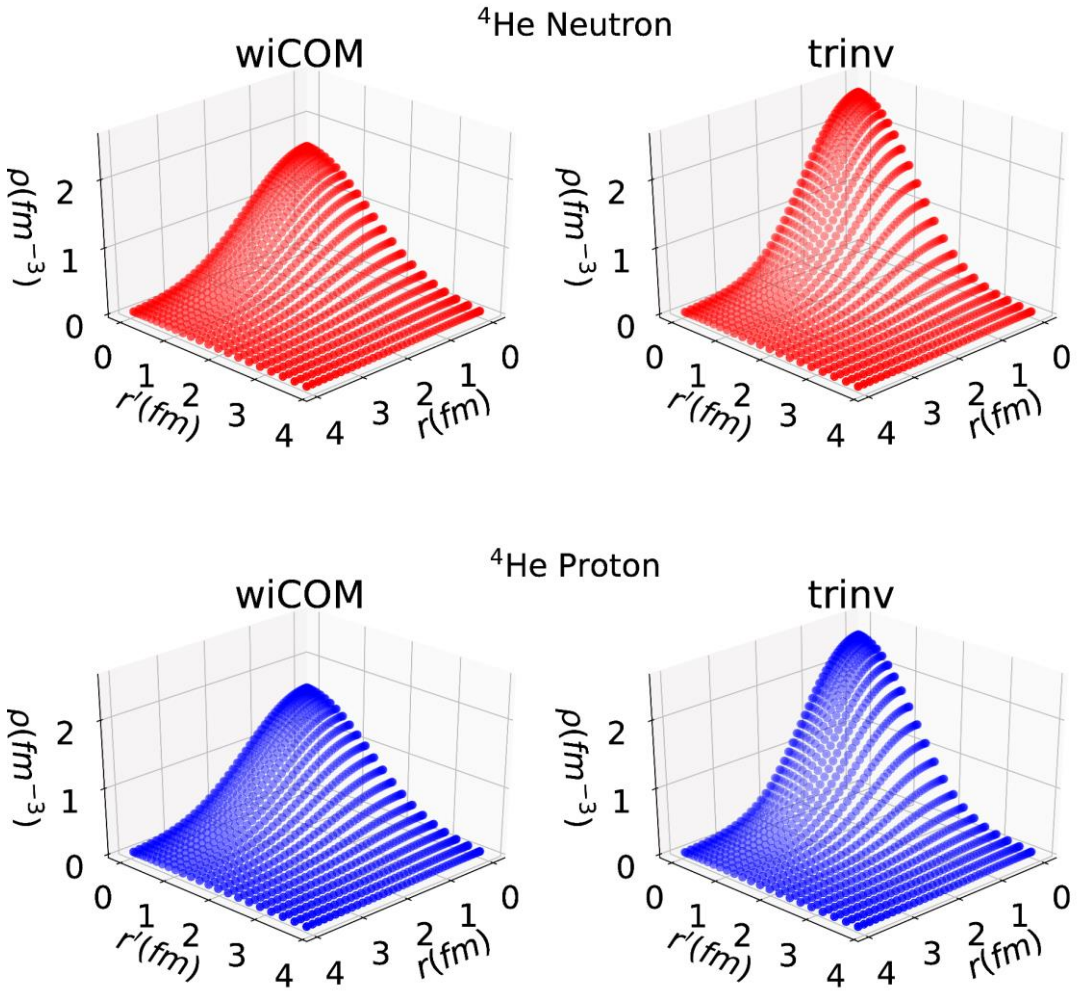
3N at N^{2}LO

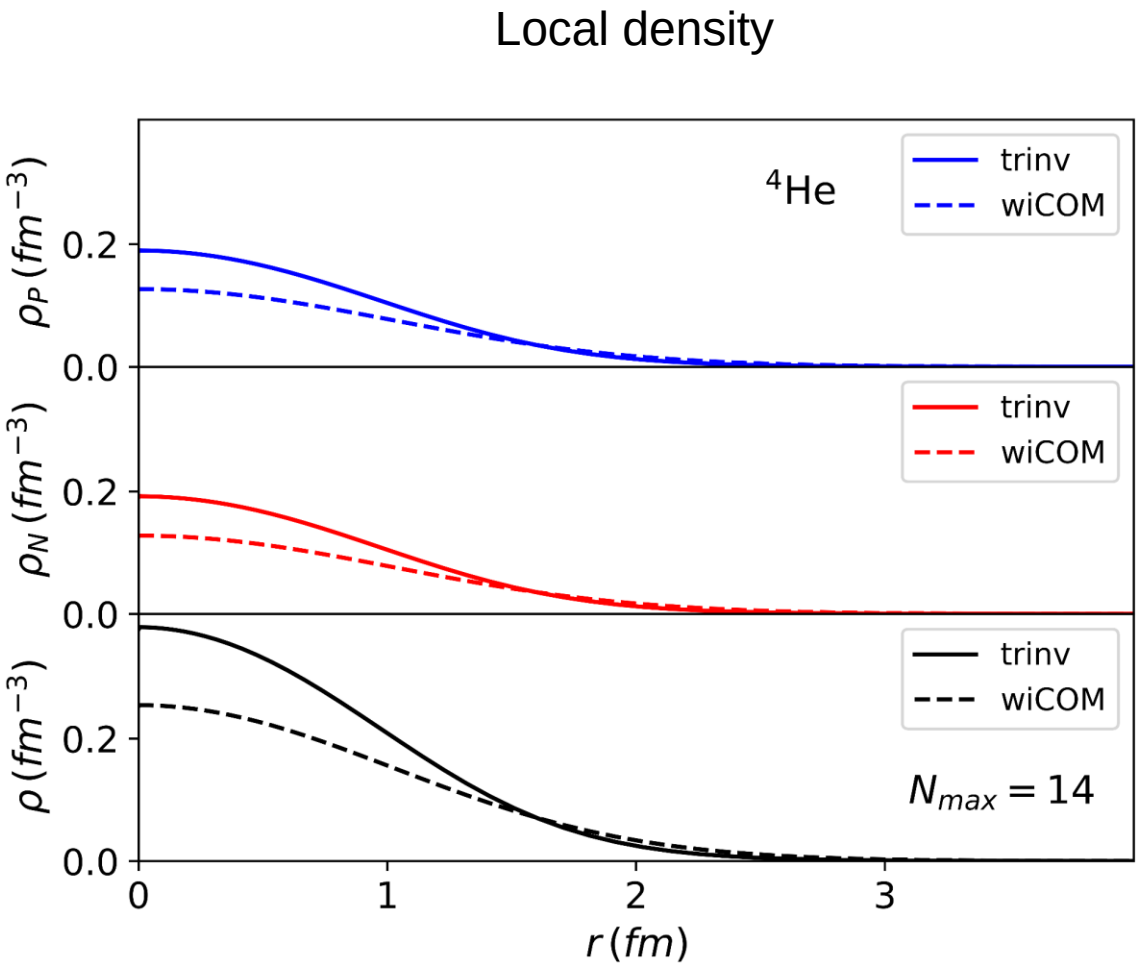
- Navrátil, 650 MeV local cut-off and 500 MeV nonlocal cut-off





Density of ground state ^{4,6,8}He, ^{12}C, ^{16}O with NN-N^{4}LO(500)+3Nlnl





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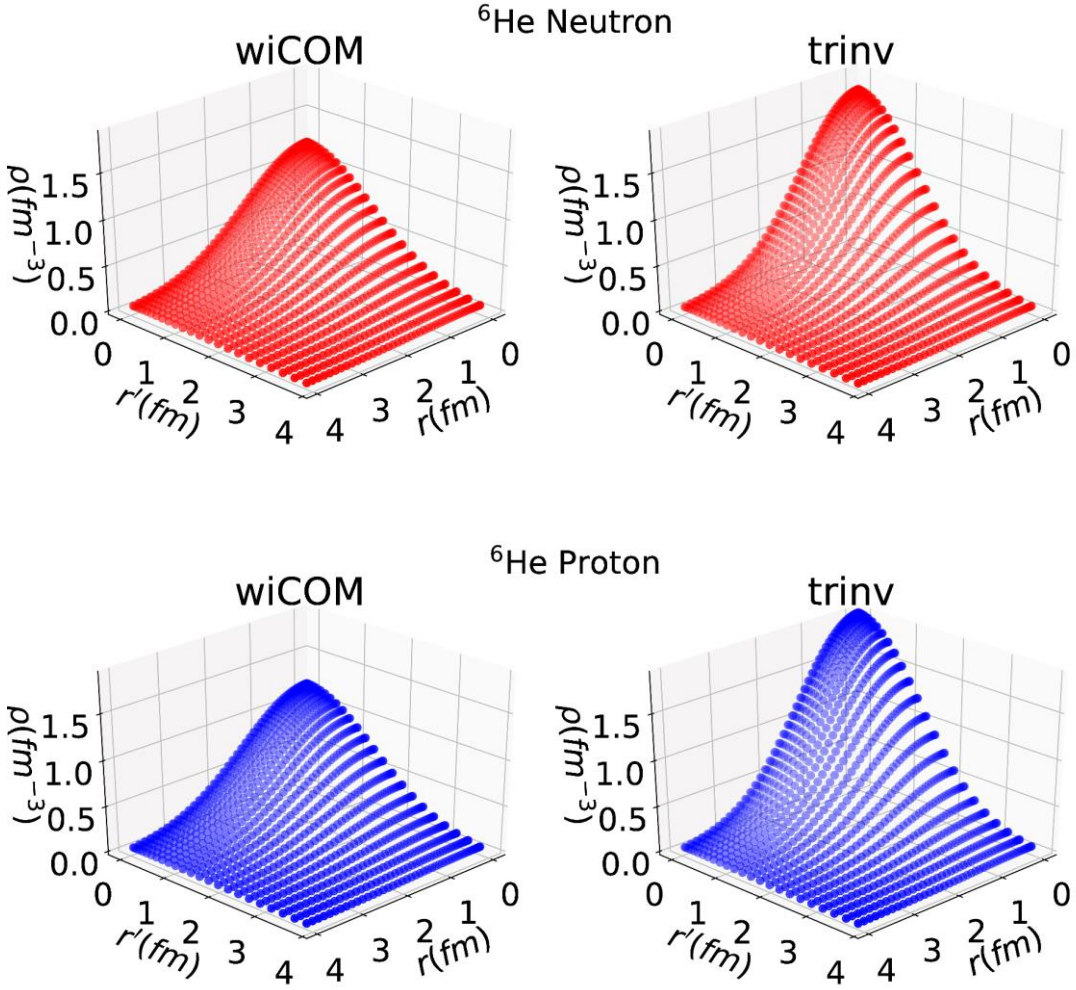

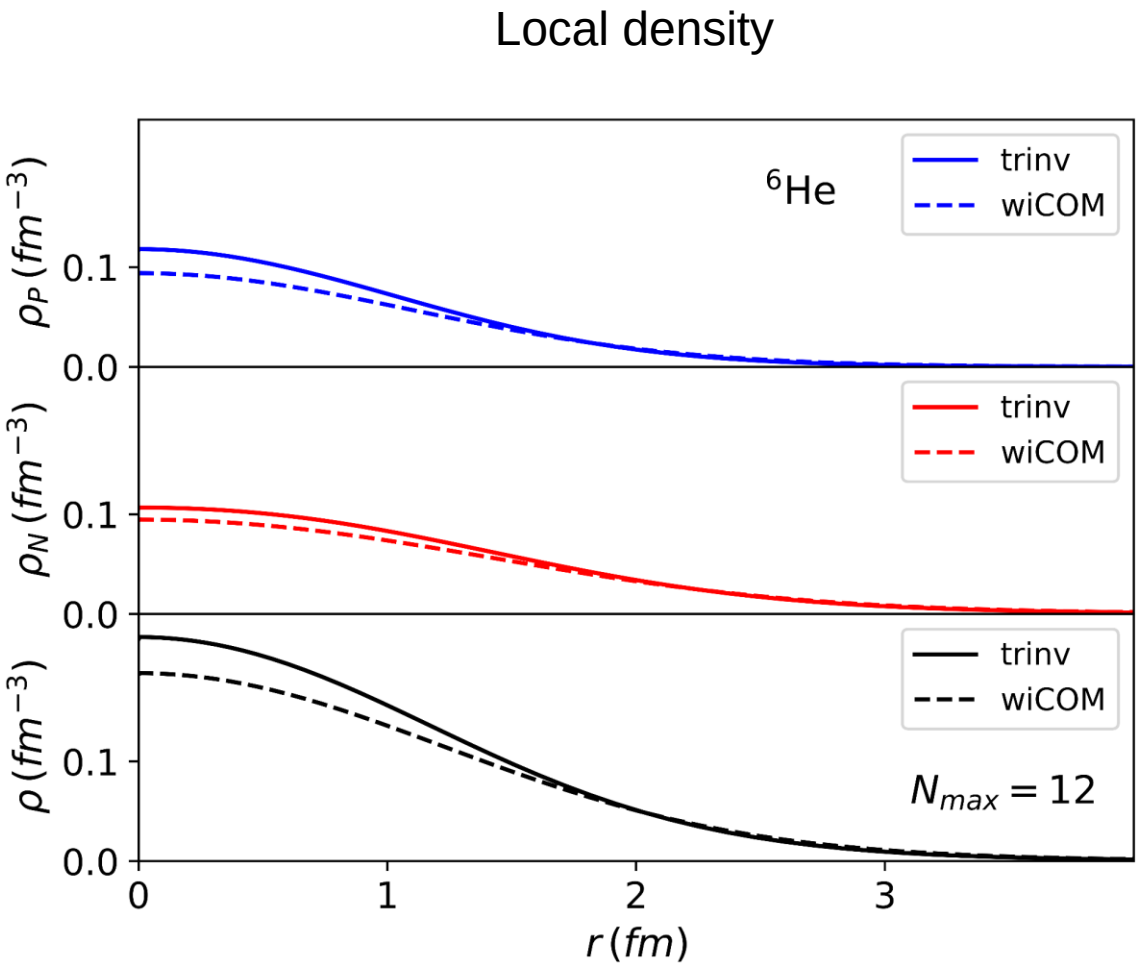

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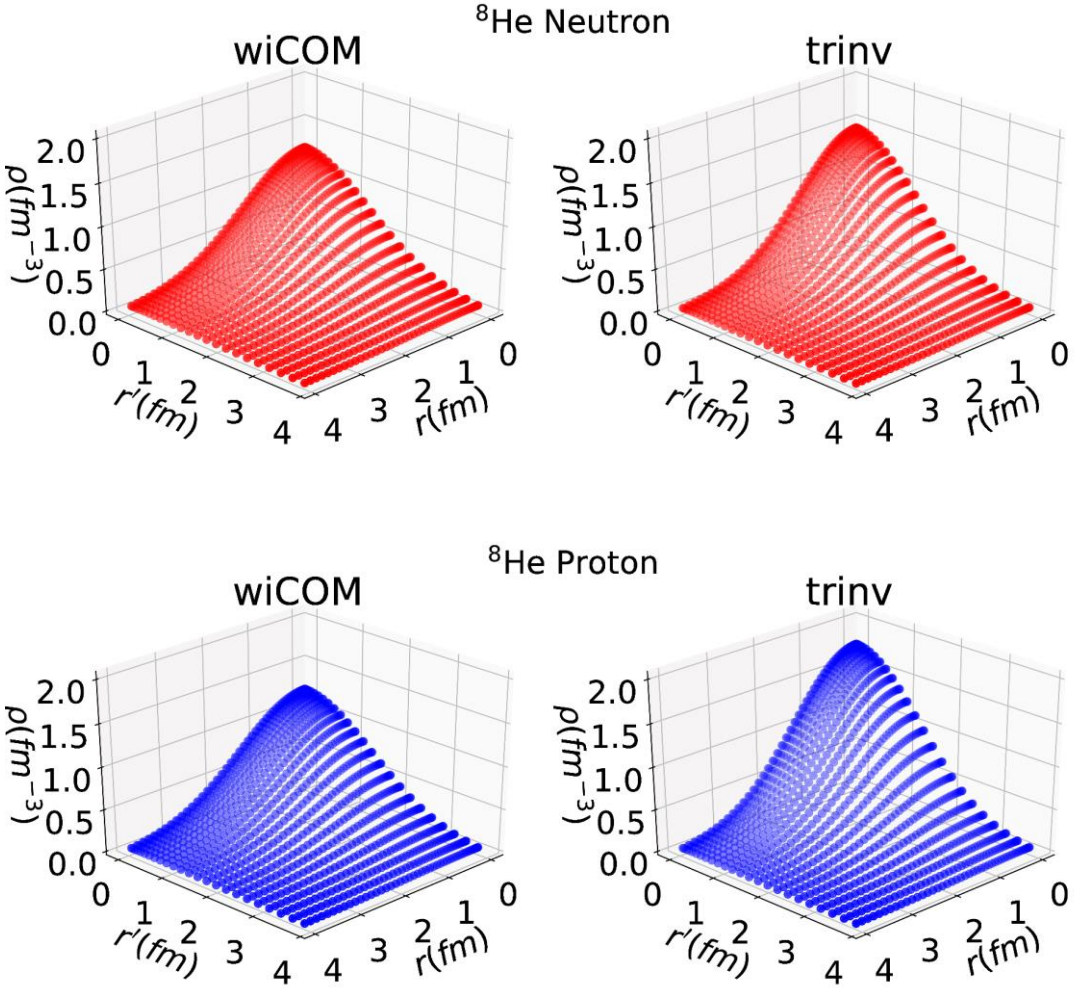

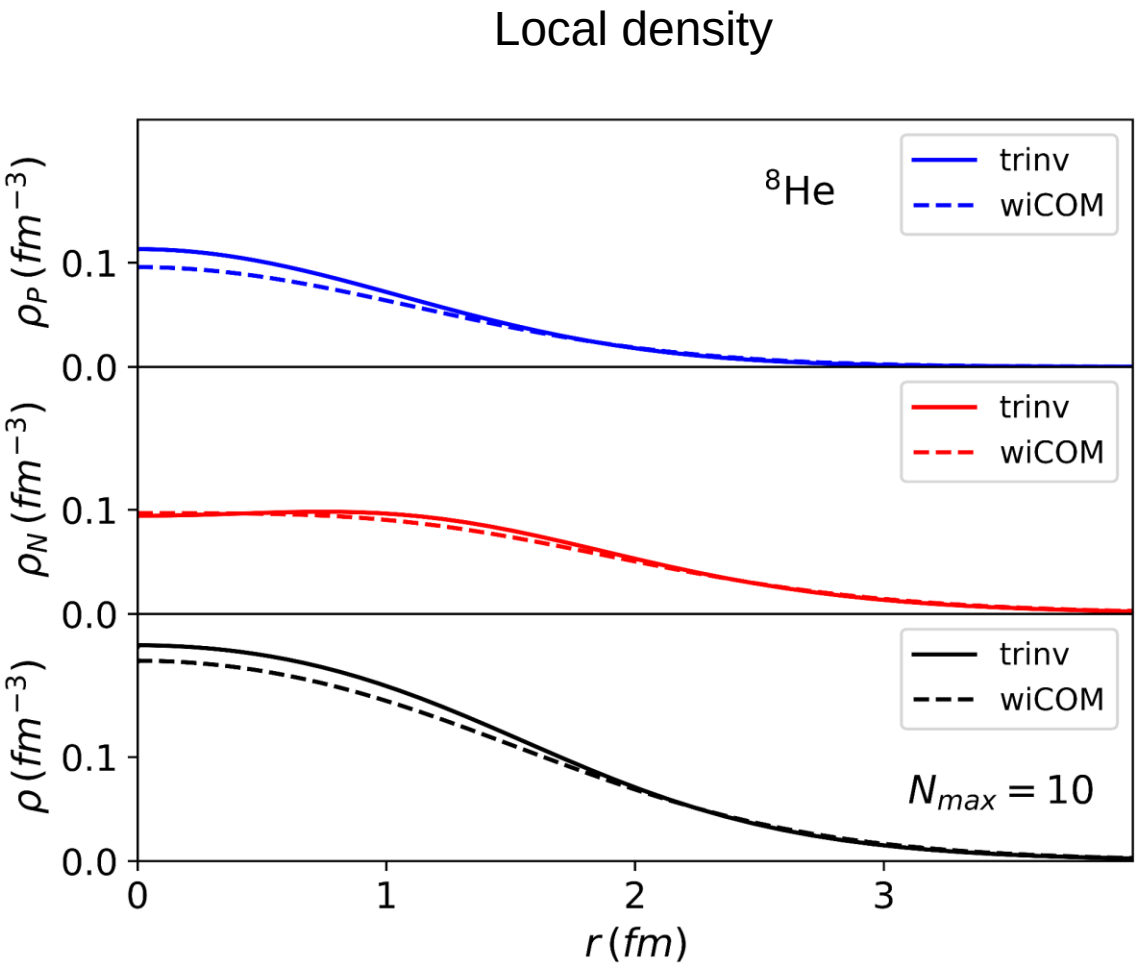

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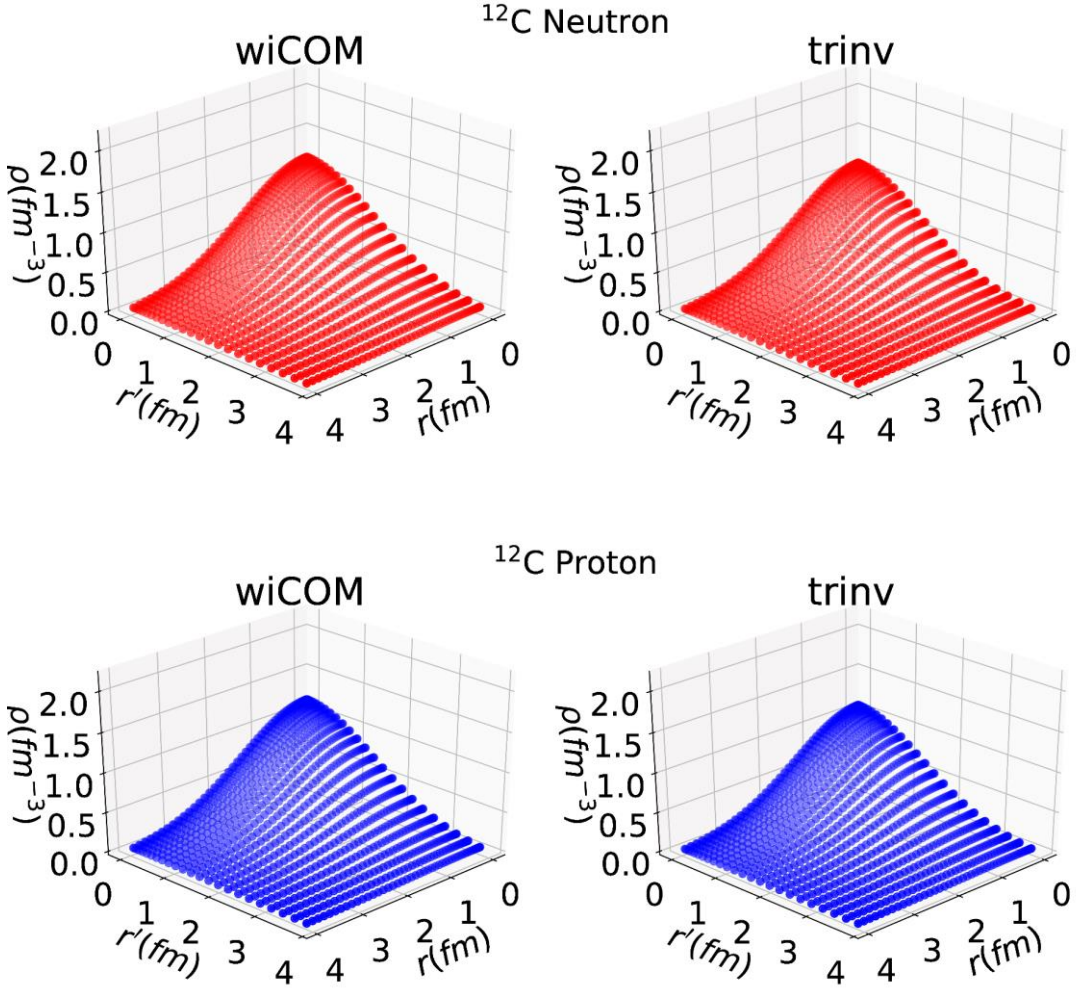

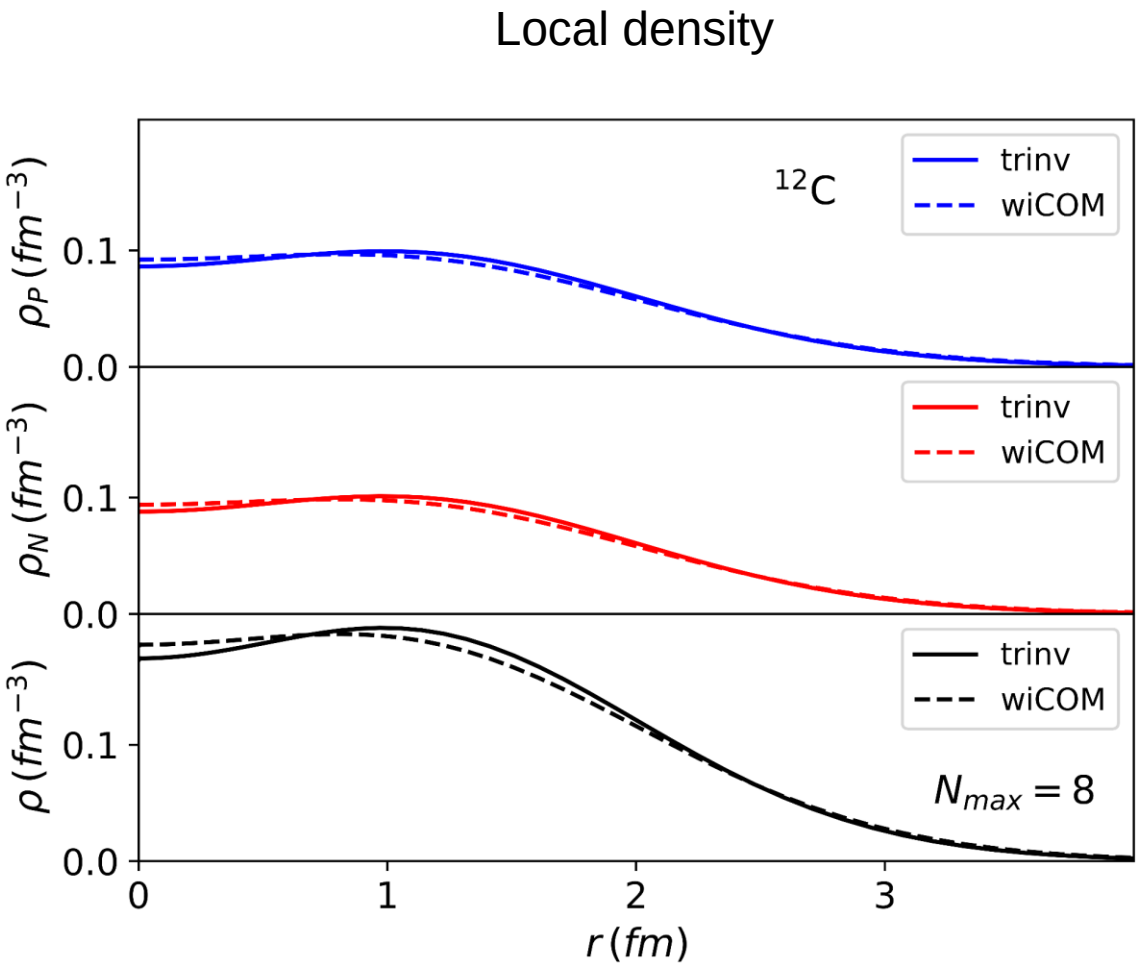

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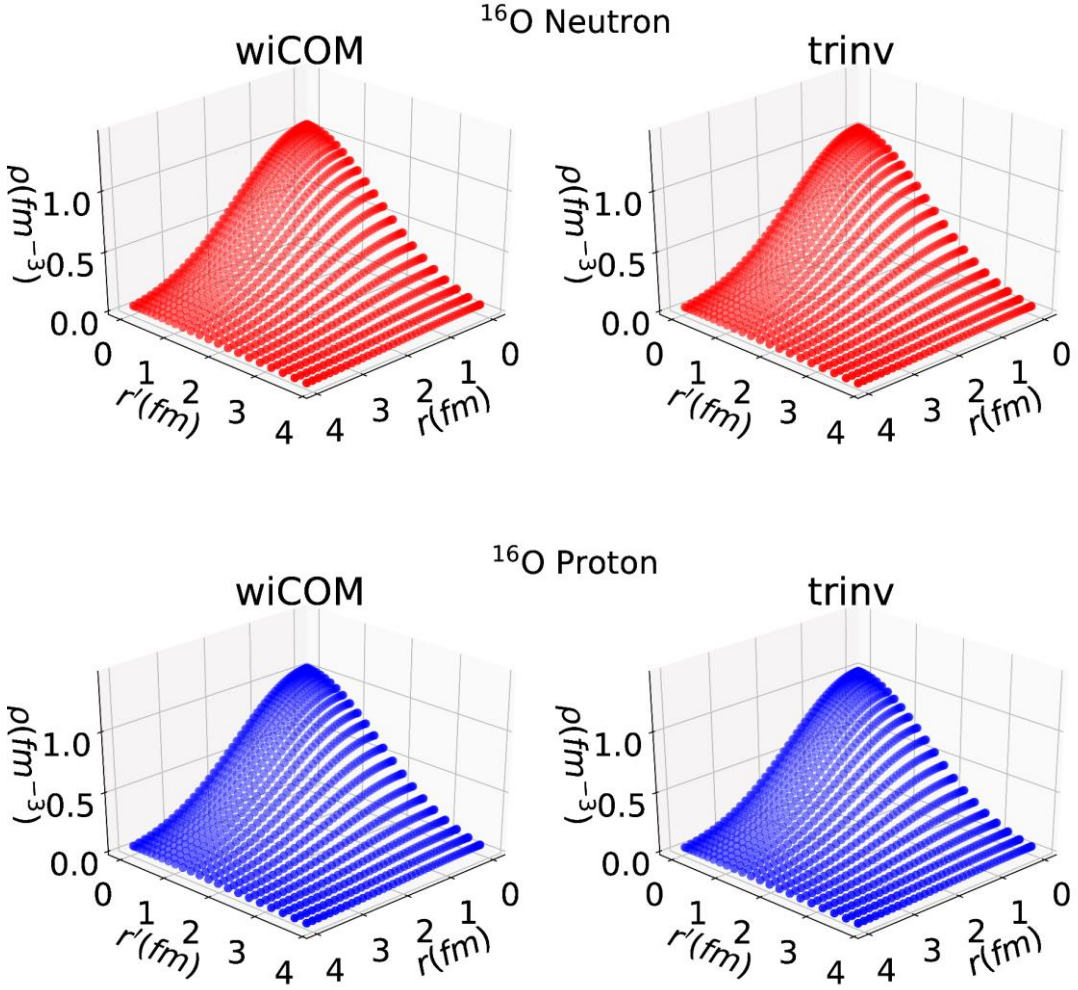
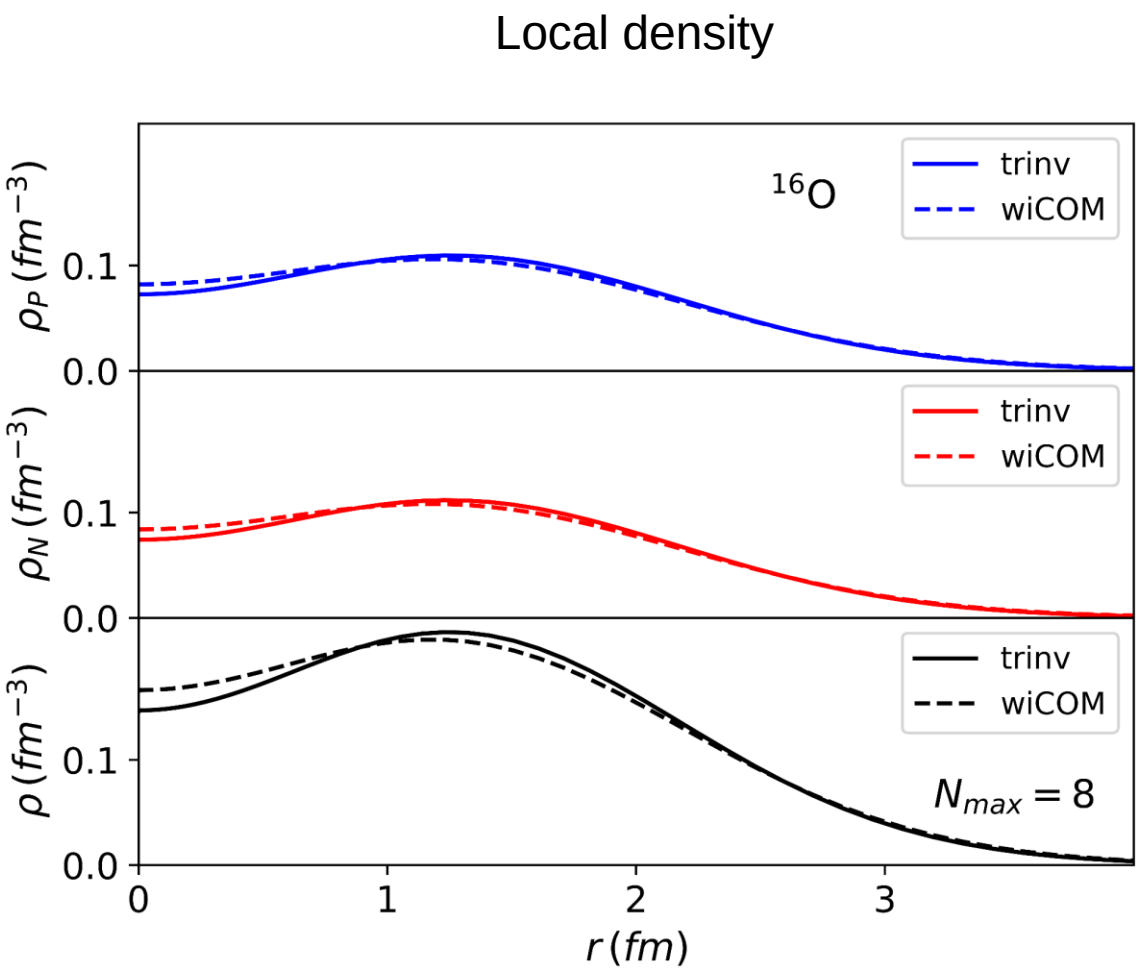
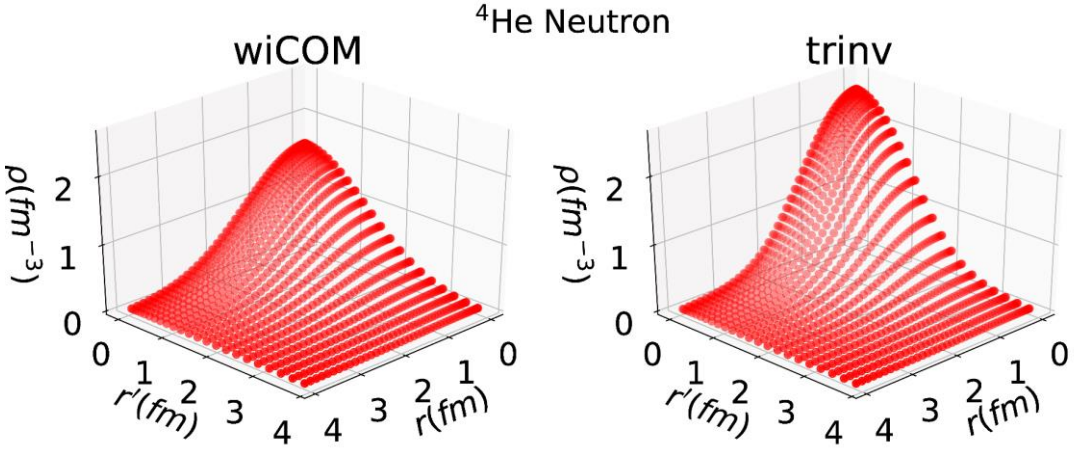




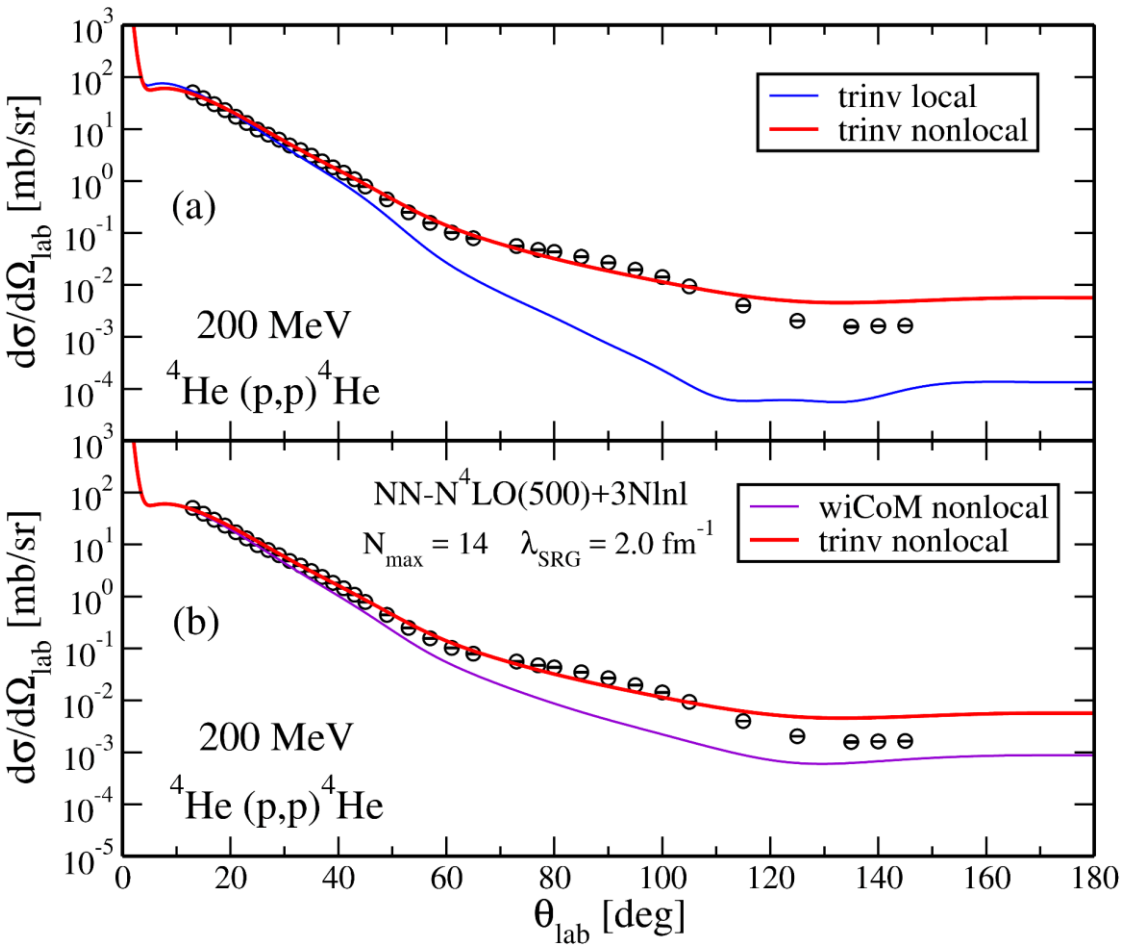
Applications to optical potentials



- 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



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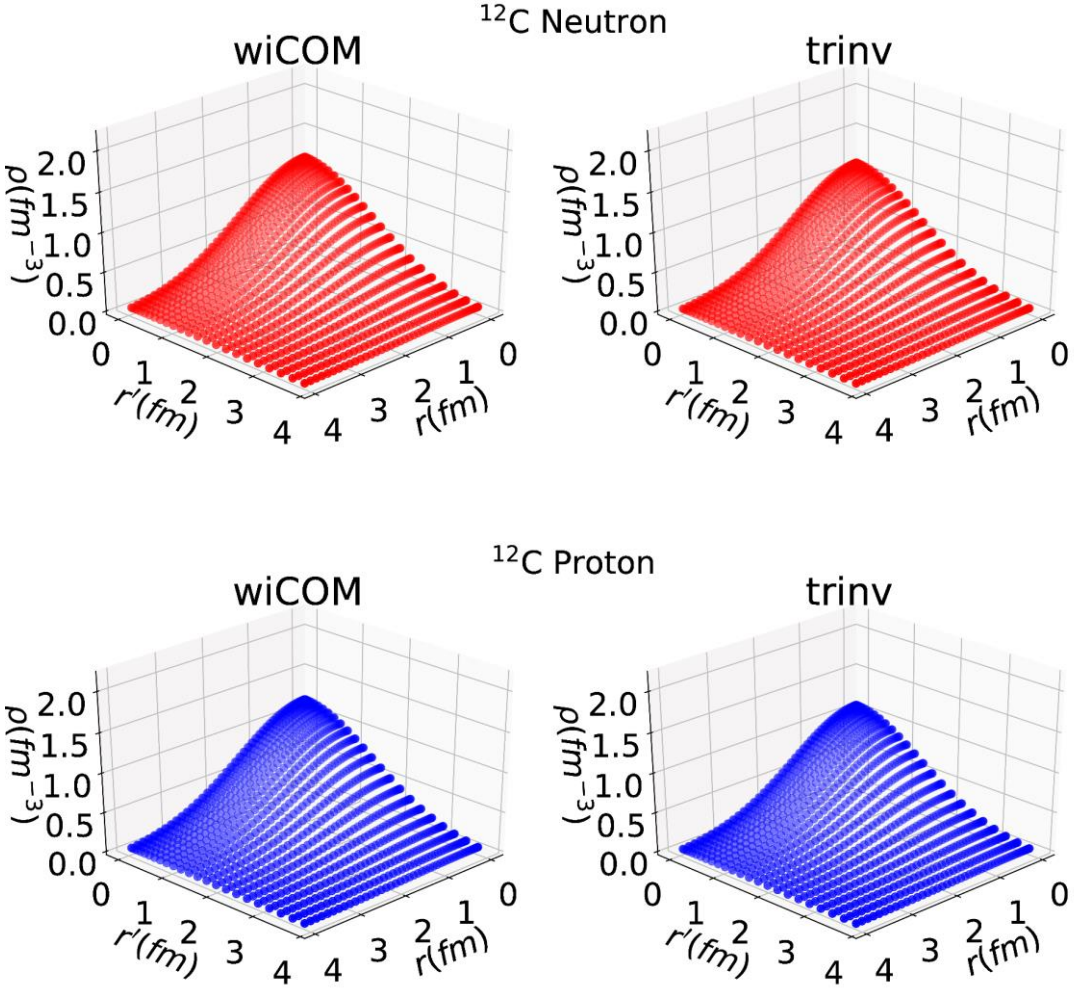

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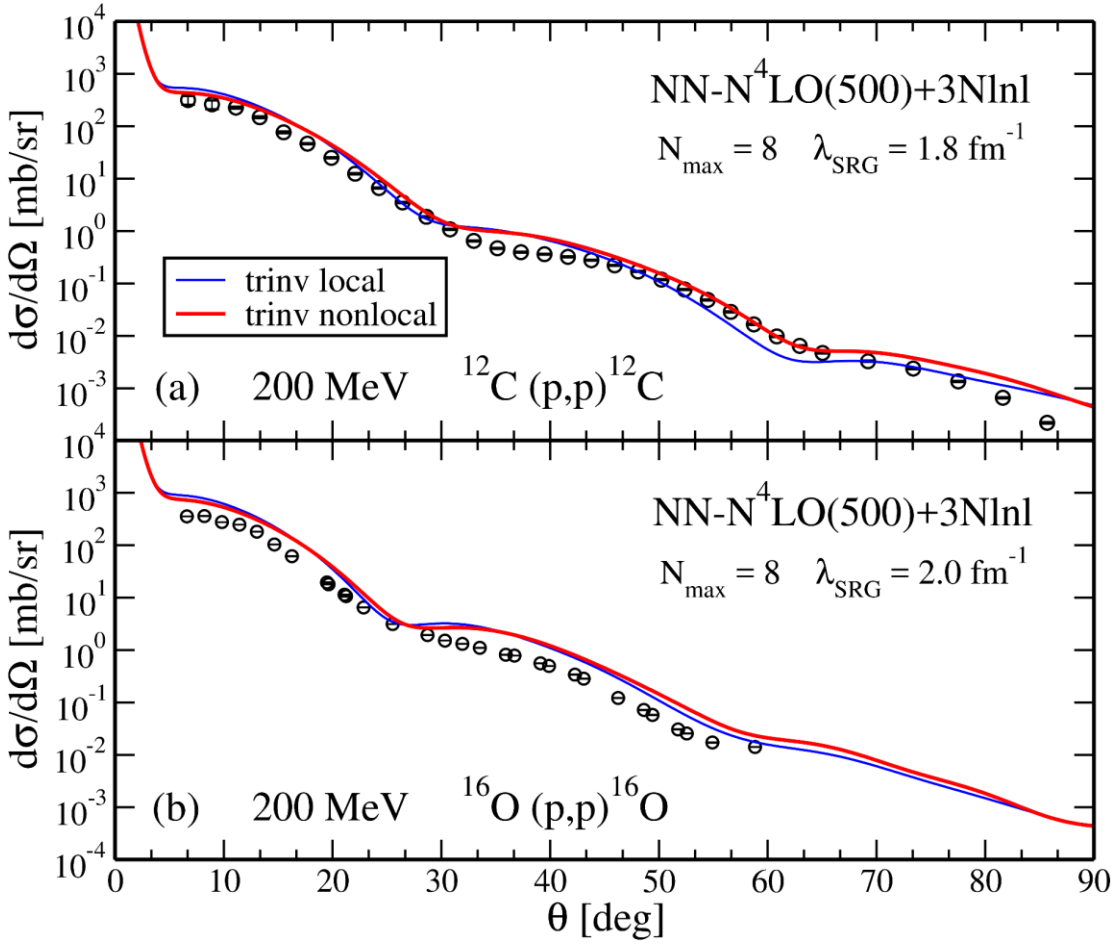


Applications to density functional theory (DFT)

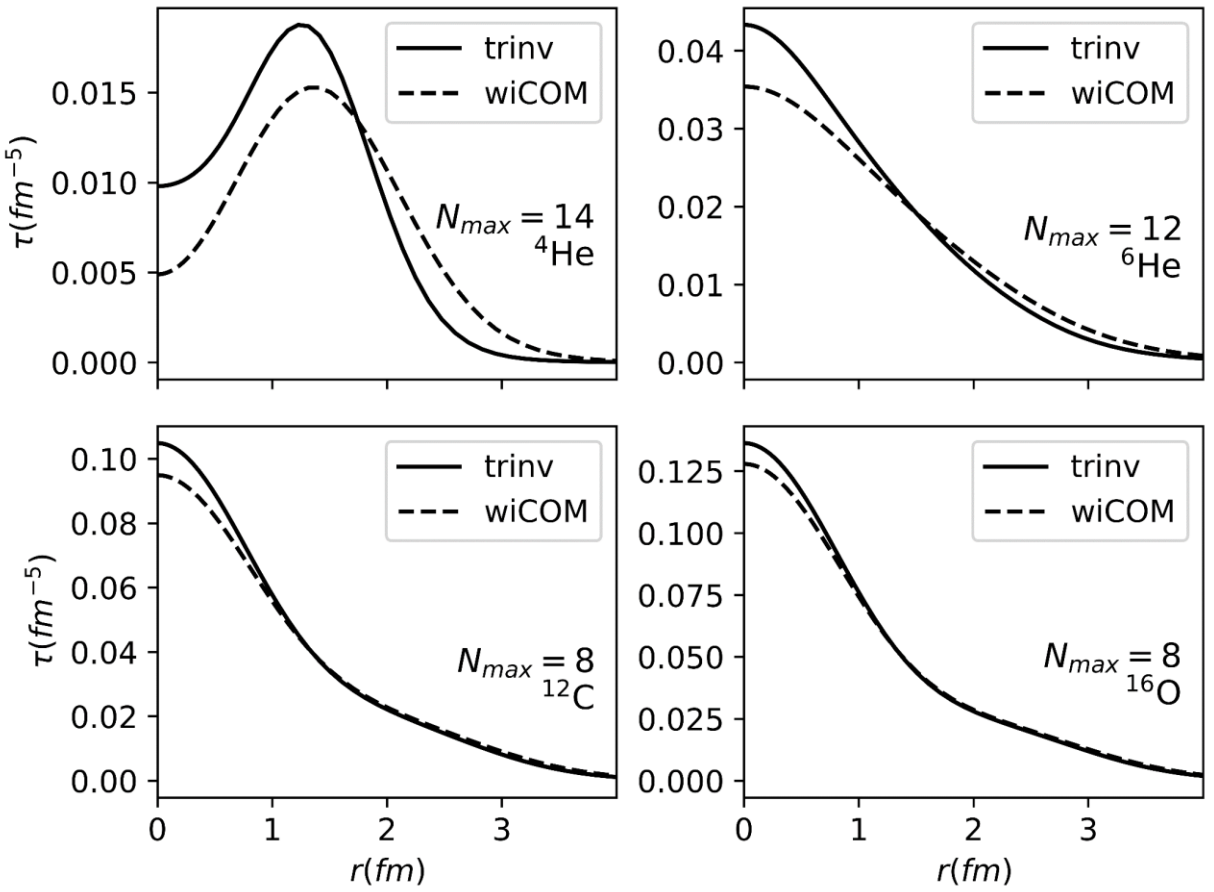
- The kinetic density, a DFT quantity used in energy density functionals, is calculable from *ab initio* wavefunctions by making use of the relations,

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

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

- 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
  - When the spurious COM contamination was removed, we observed significant differences in the nuclear structure of light systems
  - 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 Phys. Rev. C 97, 034619 (2018)

- Outlook
  - We are now pursuing the use of these densities in calculations with natural orbitals, reducing necessary 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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