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for particle and nuclear physics
and accelerator-based science

Non-Local Translationally Invariant Nuclear Density

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April 21st, 2017

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Motivation

- Substantial advancements in developments of *ab initio* approaches to nuclear physics
- Can calculate **nuclear densities**, a quantity crucial to nuclear physics
  - Provide insight into nuclear structure
  - Input to construct optical potentials for nuclear reactions at high energy
  - Central object for density functional theory (DFT)

Typically, two major issues are not taken care of:

Locality: Local densities used as approximation, need to generalize to non-local densities

$$\rho_{op}(\vec{r}) = \sum_{i=1}^{A} \{|\vec{r}\rangle\langle\vec{r}|\}^{i} = \sum_{i=1}^{A} \delta(\vec{r}-\vec{r}_i) \qquad \rho_{op}(\vec{r},\vec{r}\,') = \sum_{i=1}^{A} \{|\vec{r}\rangle\langle\vec{r}\,'|\}^{i} = \sum_{i=1}^{A} \delta(\vec{r}-\vec{r}_i)\delta(\vec{r}\,'-\vec{r}_i)$$

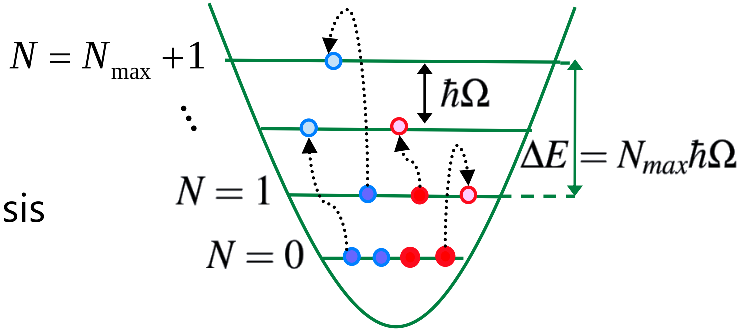
Centre of Mass (COM) Contamination: Spurious COM component often not addressed properly, causing unphysical densities

$$\rho_{op}(\vec{r}) \to \rho_{op}^{trinv}(\vec{r}-\vec{R}) \qquad \rho_{op}(\vec{r},\vec{r}\,') \to \rho_{op}^{trinv}(\vec{r}-\vec{R},\vec{r}\,'-\vec{R})$$

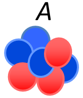
No-core shell model

- 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



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

  - 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

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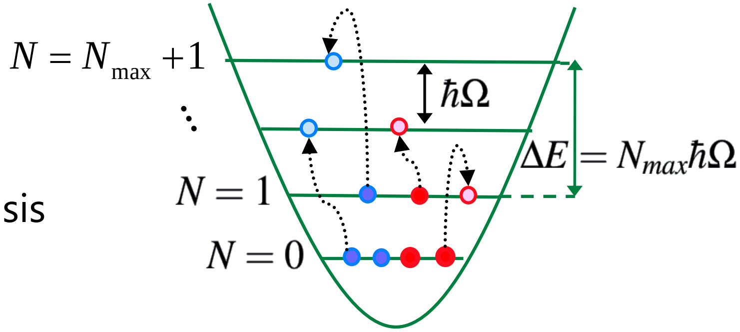

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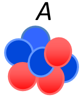

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Nuclear Density with COM

$$
{}_{SD}\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r}) | A\lambda_i J_i M_i \rangle_{SD}
= \frac{1}{\hat{J}_f} \sum (J_i M_i K k | J_f M_f)\, R_{n_1,l_1}(r)\, R_{n_2,l_2}(r)\, \langle l_1, \tfrac{1}{2}, j_1 \| Y_K \| l_2, \tfrac{1}{2}, j_2 \rangle
\times \frac{(-1)}{\hat{K}}\, {}_{SD}\langle A\lambda_f J_f \left\| \left(a^{\dagger}_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2} \right)^{(K)} \right\| A\lambda_i J_i \rangle_{SD}\, Y^{*}_{Kk}(\theta, \phi)
$$

Local Nuclear Density with COM

- Navrátil, PRC 70, 014317 (2004)

$$
\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r}, \vec{r}') | A\lambda_i J_i M_i \rangle
= \frac{1}{\hat{J}_f} \sum (J_i M_i K k | J_f M_f)\, R_{n_1,l_1}(r)\, R_{n_2,l_2}(r')\, (-1)^{j_2 + \frac{1}{2}} (-1)^{l_1 + l_2 + K}\, \hat{j}_1 \hat{j}_2 \hat{K} \begin{Bmatrix} j_2 & l_2 & \frac{1}{2} \\ l_1 & j_1 & K \end{Bmatrix}
\times \frac{(-1)}{\hat{K}}\, {}_{SD}\langle A\lambda_f J_f \left\| \left(a^{\dagger}_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2} \right)^{(K)} \right\| A\lambda_i J_i \rangle_{SD} \left(Y^{*}_{l_1}(\theta, \phi) Y^{*}_{l_2}(\theta', \phi') \right)^{(K)}_{k}
$$

Non-Local Nuclear Density with COM

- Densities are normalized via this condition:

$$
\int d\vec{x}\, \langle A\lambda J M | \rho_{op}(\vec{x}) | A\lambda J M \rangle = A
$$

Nuclear Density with COM

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$$

Local Nuclear Density with COM

- Navrátil, PRC 70, 014317 (2004)

Angular dependence factorized out for plotting

$$
\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r},\vec{r}') | A\lambda_i J_i M_i \rangle
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Non-Local Nuclear Density with COM

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Translationally Invariant (TRINV) Nuclear Density

Local TRINV Nuclear Density
- Navrátil, PRC 70, 014317 (2004)

$$\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r}-\vec{R}) | A\lambda_i J_i M_i \rangle$$
$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \frac{1}{\hat{J}_f} \sum (J_i M_i K k | J_f M_f)\, R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right)$$
$$\times (M^K)^{-1}_{n,l,n',l',n_1,l_1,n_2,l_2} \frac{(-1)^K \cdot \hat{l}\hat{l}'(l0l'0|K0)}{\hat{l}_1\hat{l}_2(l_10l_20|K0)} \langle l_1, \tfrac{1}{2}, j_1 \| Y_K \| l_2, \tfrac{1}{2}, j_2 \rangle$$
$$\times \frac{-1}{\hat{K}}\, {}_{SD}\langle A\lambda_f J_f \left\| \left(a^\dagger_{n_1 l_1 j_1} \tilde{a}_{n_2 l_2 j_2}\right)^{(K)} \right\| A\lambda_i J_i \rangle_{SD}\; Y^*_{Kk}(\theta,\phi)$$

Non-Local TRINV Nuclear Density

$$\langle A\lambda_f J_f M_f | \rho_{op}(\vec{r}-\vec{R}, \vec{r}\,'-\vec{R}) | A\lambda_i J_i M_i \rangle$$
$$= \left(\frac{A}{A-1}\right)^{3} \frac{1}{\hat{J}_f} \sum (J_i M_i K k | J_f M_f)\, R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}\,'-\vec{R}|\right)$$
$$\times (M^K)^{-1}_{n,l,n',l',n_1,l_1,n_2,l_2} \frac{\sqrt{4\pi} \cdot (-1)^{l_1+l_2+K}\hat{K}}{\hat{l}_1\hat{l}_2(l_10l_20|K0)} \langle l_1, \tfrac{1}{2}, j_1 \| Y_K \| l_2, \tfrac{1}{2}, j_2 \rangle$$
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- Normalization is as previously shown: $\int d\vec{x}\, \langle A\lambda JM | \rho^{phys}_{op}(\vec{x}) | A\lambda JM \rangle = A$

Translationally Invariant (TRINV) Nuclear Density

Local TRINV Nuclear Density
- Navrátil, PRC 70, 014317 (2004)

$$\langle A\lambda_f J_f M_f|\rho_{op}(\vec{r}-\vec{R})|A\lambda_i J_i M_i\rangle$$
$$= \left(\frac{A}{A-1}\right)^{\frac{3}{2}} \frac{1}{\hat{J}_f} \sum (J_i M_i K k|J_f M_f)\, R_{n,l}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right) R_{n',l'}\left(\sqrt{\frac{A}{A-1}}|\vec{r}-\vec{R}|\right)$$
$$\times (M^K)^{-1}_{n,l,n',l',n_1,l_1,n_2,l_2} \frac{(-1)^K \cdot \hat{l}\hat{l}'(l0l'0|K0)}{\hat{l}_1\hat{l}_2(l_1 0 l_2 0|K0)} \langle l_1,\tfrac{1}{2},j_1\|Y_K\|l_2,\tfrac{1}{2},j_2\rangle$$
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Angular dependence factorized out for plotting

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

- Normalization is as previously shown: $\int d\vec{x}\, \langle A\lambda JM|\rho^{phys}_{op}(\vec{x})|A\lambda JM\rangle = A$

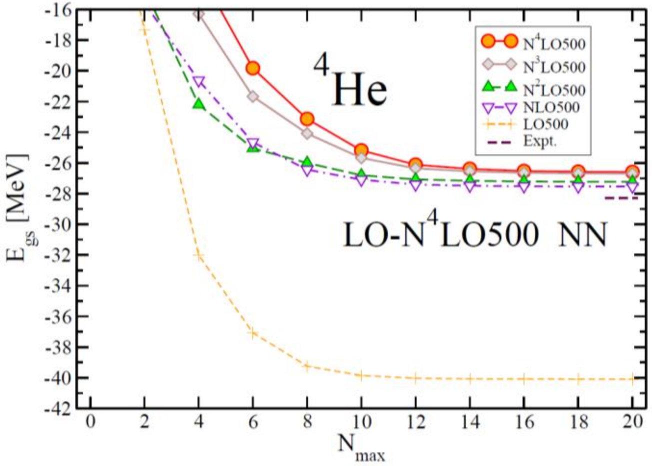
Chiral EFT Interactions

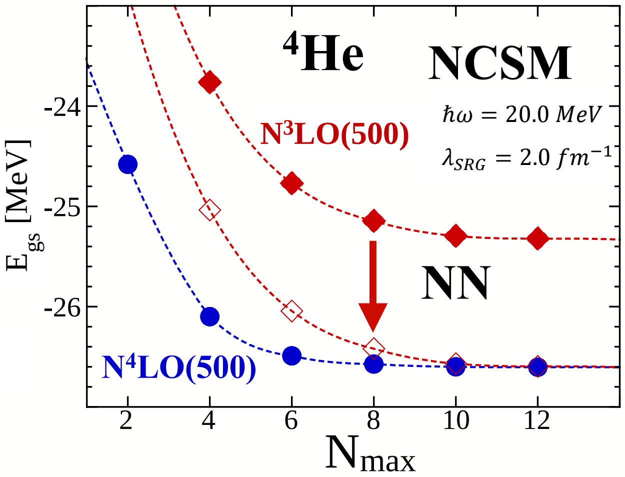
NN+3N(400)

- NN at N³LO: Entem & Machleidt from 2003, 500 MeV cut-off
- 3N at N²LO: Navrátil, local 400 MeV cut-off

N⁴LO(500)+3N

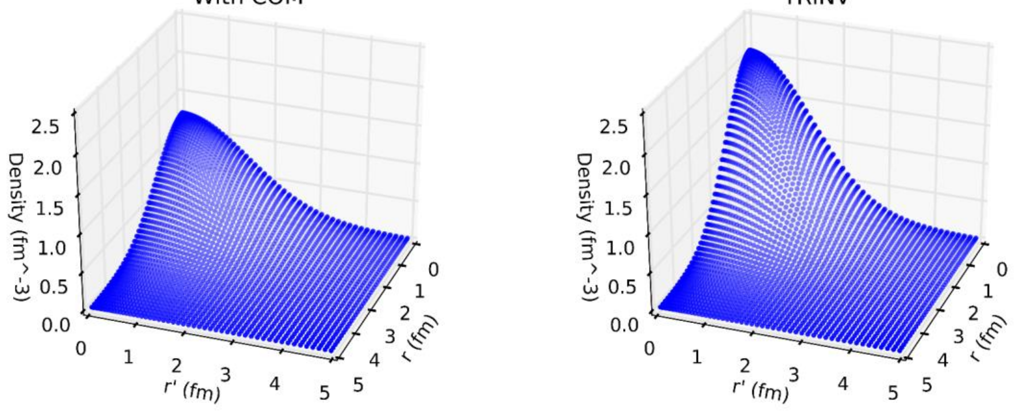
- NN systematic from LO to N⁴LO
  - D. R. Entem, N. Kaiser, R. Machleidt, and Y. Nosyk, Phys. Rev. C 91, 014002 (2015).
  - D. R. Entem, R. Machleidt, and Y. Nosyk, arXiv:1703.05454.
- 3N at N²LO: Navrátil, local 650 MeV cut-off and non-local 500 MeV cut-off



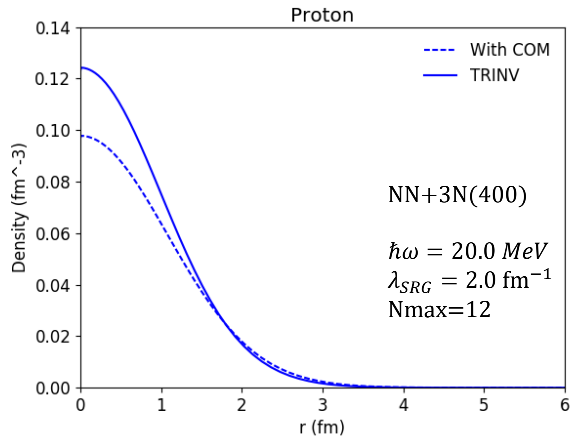


Density for Ground State ^{6}He with NN+3N(400)

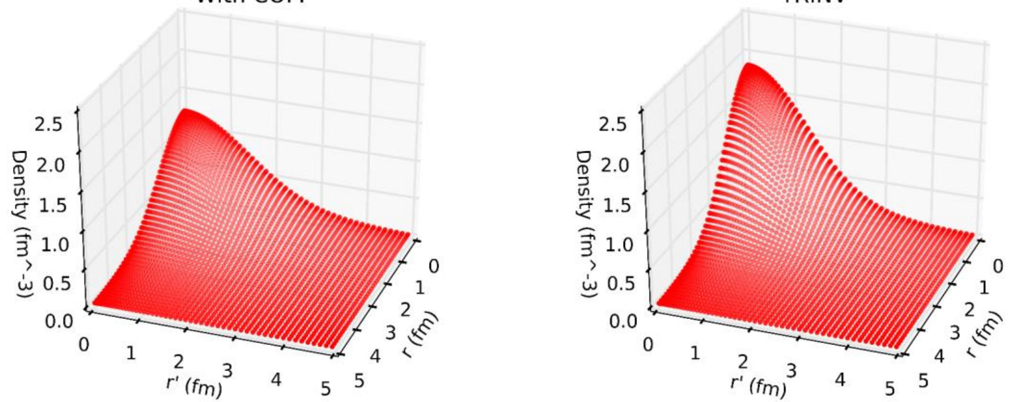
Non-Local Proton Density

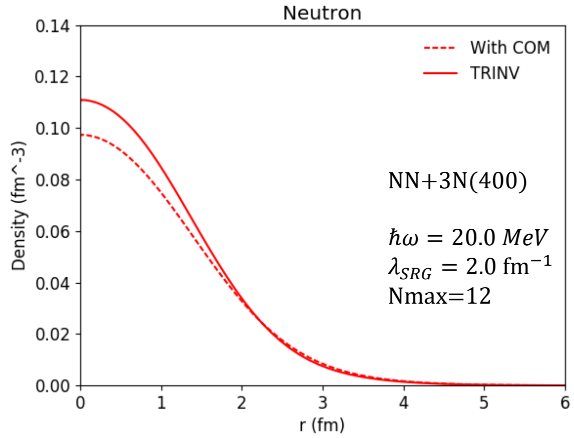


Local Density

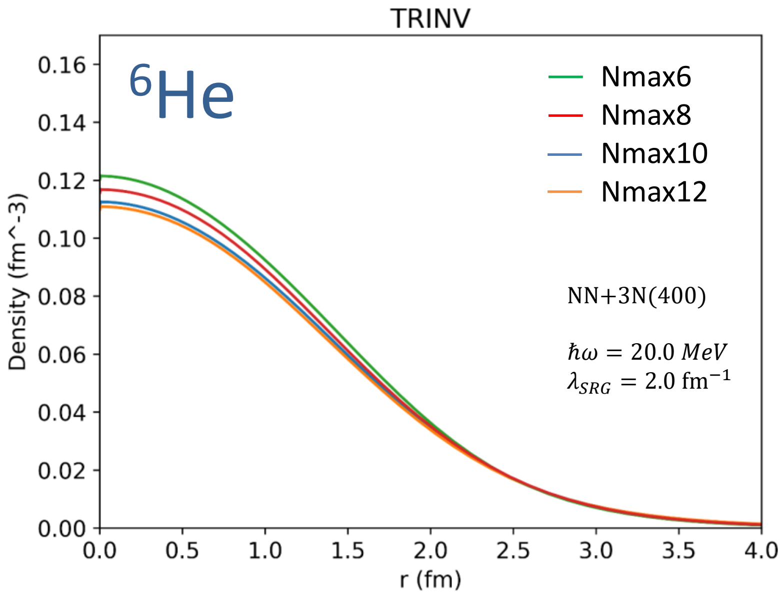


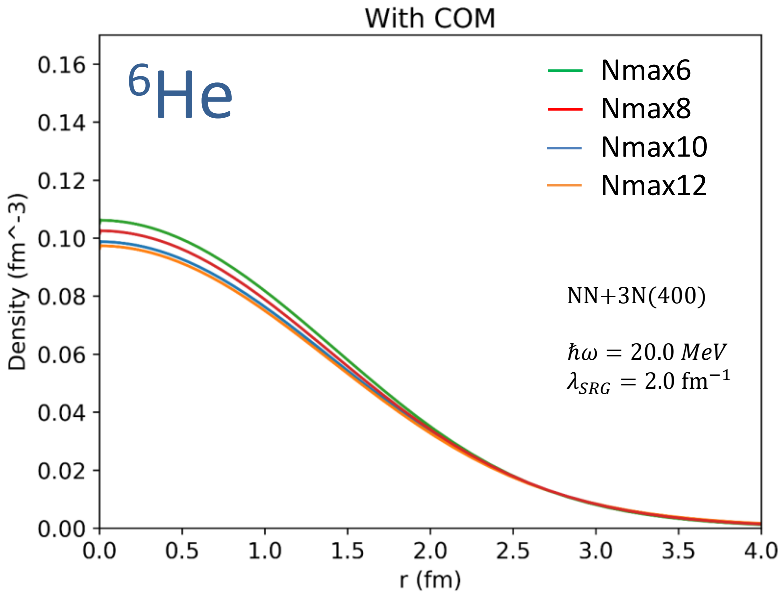
Non-Local Neutron Density





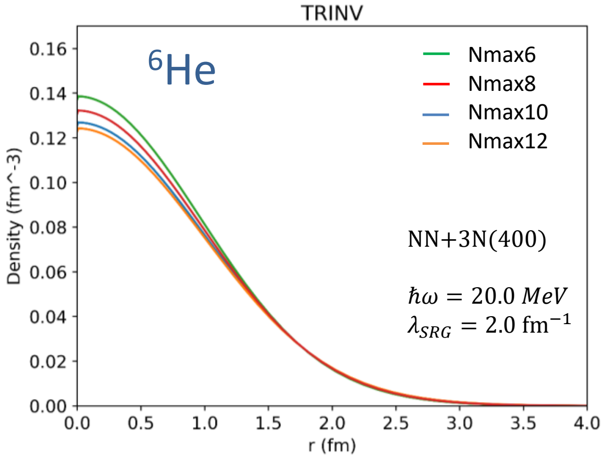
Neutron Density

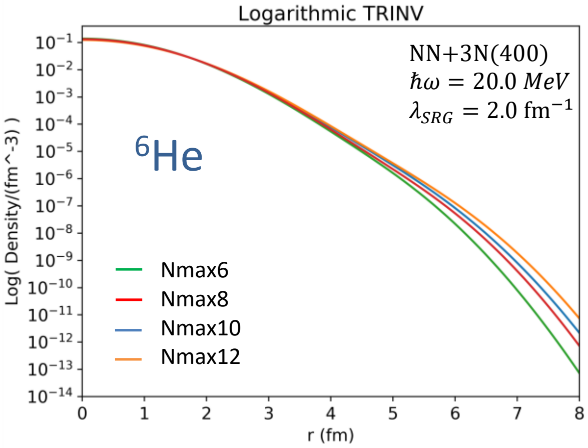


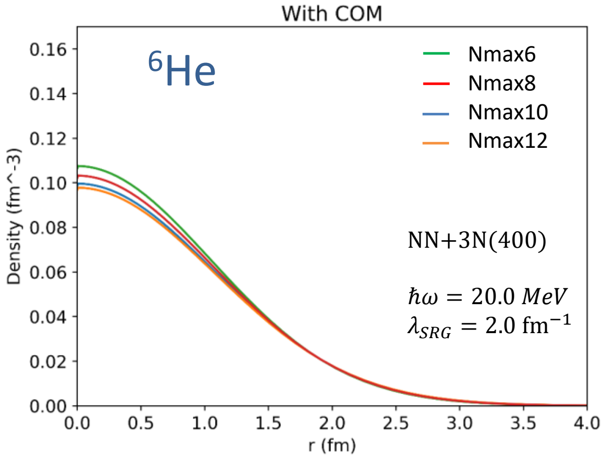


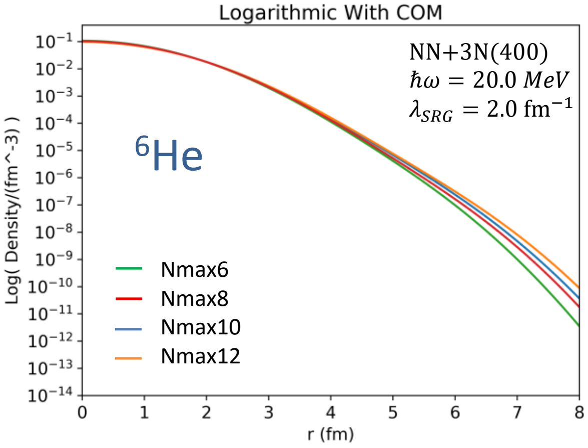
- We achieve good convergence in feasible model spaces

Convergence of Proton Density





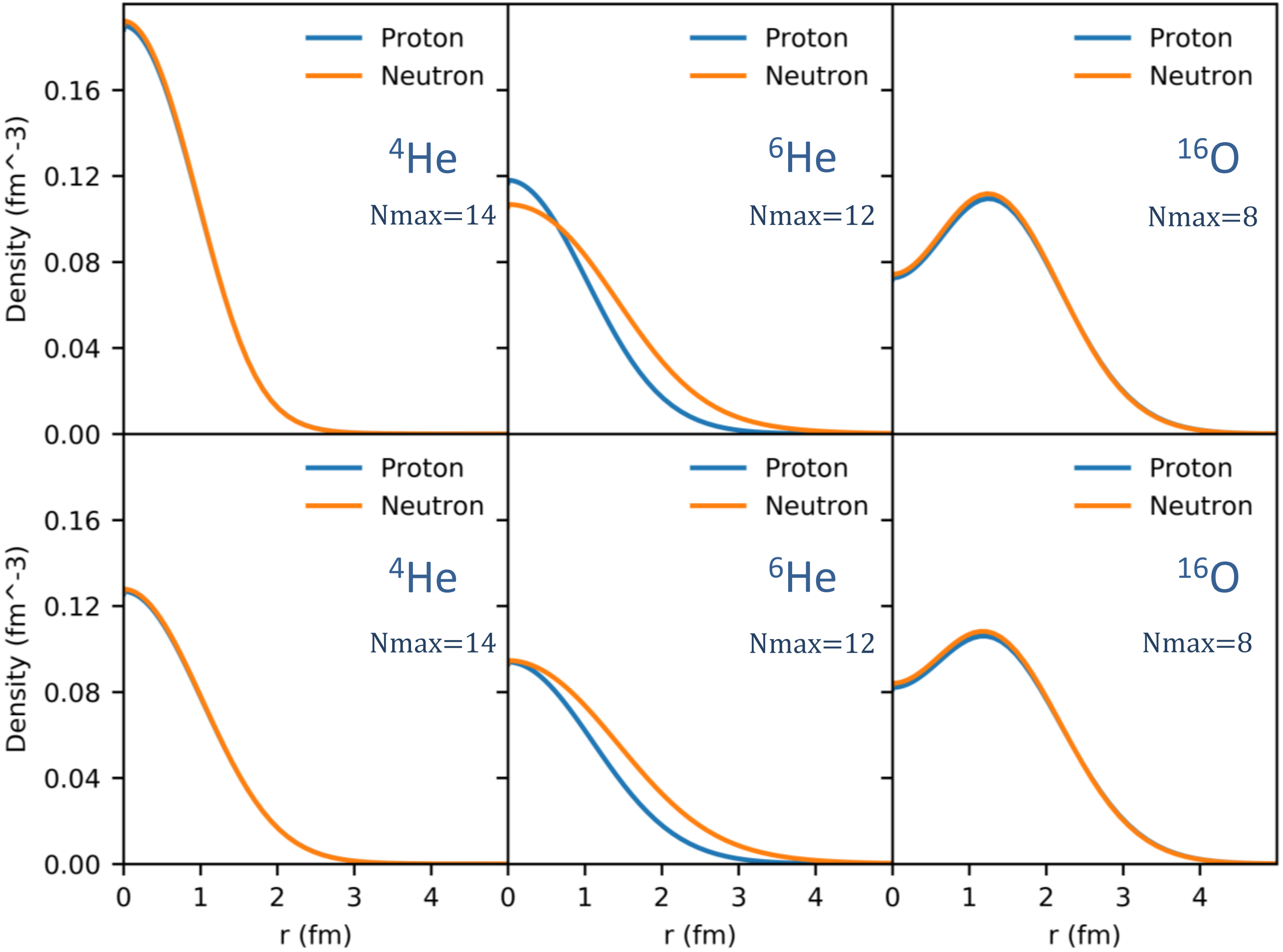




Ground State of ^4He, ^6He, ^{16}O with $N^4LO(500)$+3N

TRINV

With COM

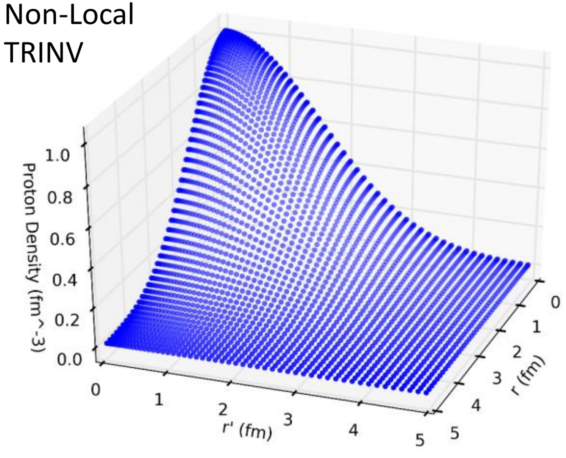


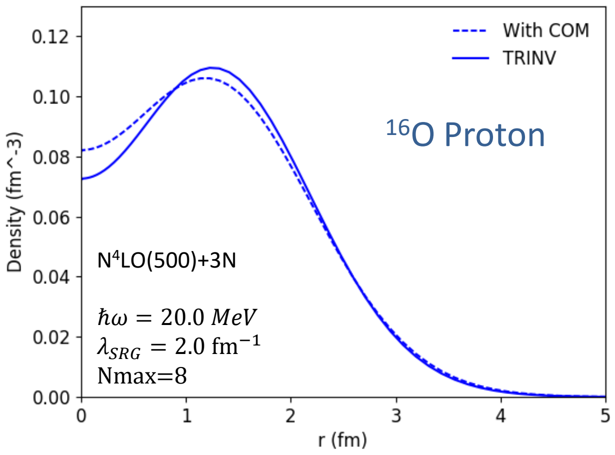
$N^4LO(500)$+3N

$\hbar\omega = 20.0\ MeV$
$\lambda_{SRG} = 2.0\ \mathrm{fm}^{-1}$

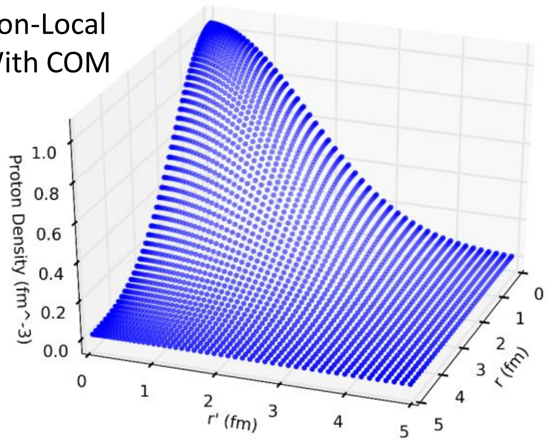
Density for Ground State ^{16}O with $N^4LO(500)+3N$

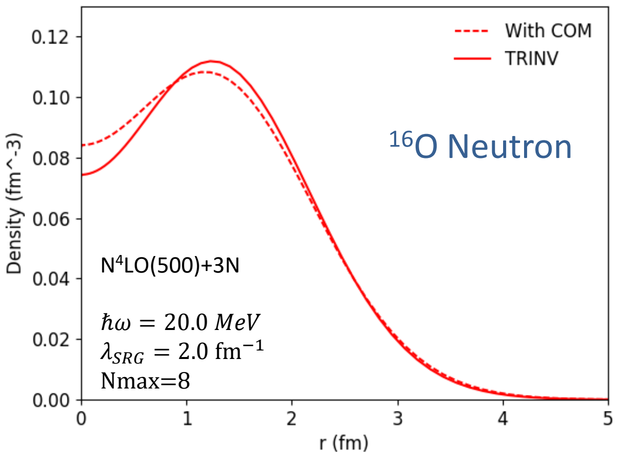
Non-Local
TRINV





Non-Local
With COM





- Removal of COM has less drastic effect on density compared to lighter nuclei

Motivation - Kinetic Density

- Kinetic density is essential object in density functional theory

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

- Effect of COM removal in nuclear densities should be amplified in kinetic density results due to application of gradients

$$\tau_T(\vec{r}) = \sum \beta^{i,f}_{n,l,n',l',K} \vec{\nabla} \left[R_{n,l} \left(\sqrt{\frac{A}{A-1}} |\vec{r} - \vec{R}| \right) Y^*_l(\theta, \phi) \right] \cdot \vec{\nabla}' \left[R_{n',l'} \left(\sqrt{\frac{A}{A-1}} |\vec{r} - \vec{R}| \right) Y^*_{l'}(\theta, \phi) \right]$$

- Gradients performed using spherical components of nabla operator

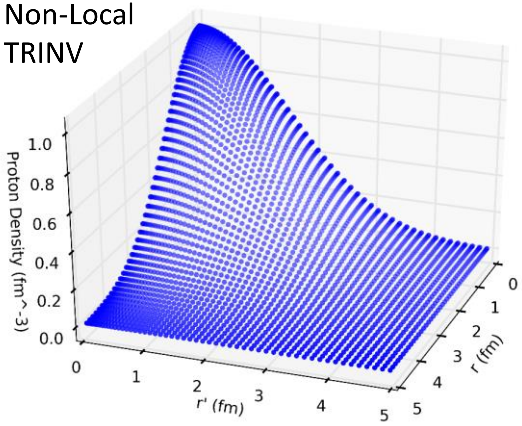
$$\nabla_{\pm 1}\left[R_{n,l}(r) Y_{l,m_l}(\theta,\phi)\right] = \alpha_{\pm 1} \left(\frac{dR_{n,l}(r)}{dr} - \frac{l}{r} R_{n,l}(r) \right) Y_{l+1,m_l \pm 1}(\theta,\phi) - \alpha_{\pm 2} \left(\frac{dR_{n,l}(r)}{dr} + \frac{l+1}{r} R_{n,l}(r) \right) Y_{l-1,m_l \pm 1}(\theta,\phi)$$

$$\nabla_0\left[R_{n,l}(r) Y_{l,m_l}(\theta,\phi)\right] = \alpha_3 \left(\frac{dR_{n,l}(r)}{dr} - \frac{l}{r} R_{n,l}(r) \right) Y_{l+1,m_l}(\theta,\phi) + \alpha_4 \left(\frac{dR_{n,l}(r)}{dr} + \frac{l+1}{r} R_{n,l}(r) \right) Y_{l-1,m_l}(\theta,\phi)$$

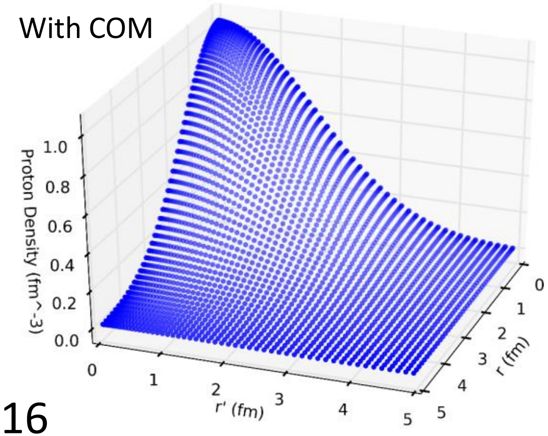
$$\frac{d}{dr} R_{n,l}(r) = \frac{l}{r} R_{n,l}(r) - \frac{1}{b} \left[\sqrt{n + l + \tfrac{3}{2}} \cdot R_{n,l+1}(r) + \sqrt{n} \cdot R_{n-1,l+1}(r) \right]$$

(Kinetic) Density for Ground State ^{16}O with $N^4LO(500)+3N$

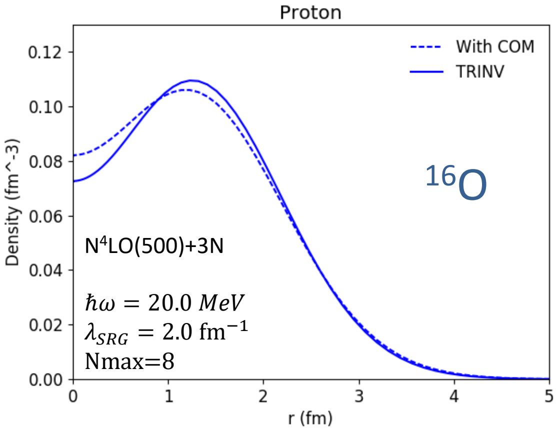
Non-Local
TRINV

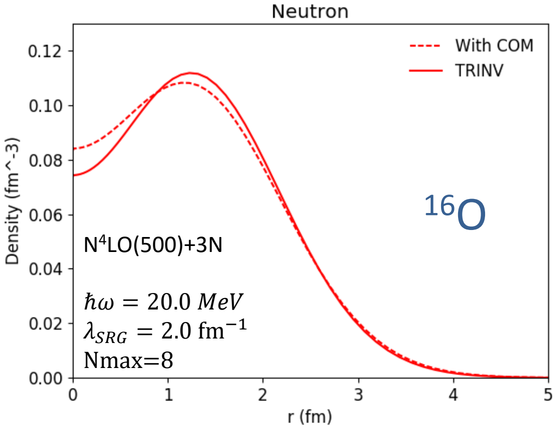


Non-Local
With COM

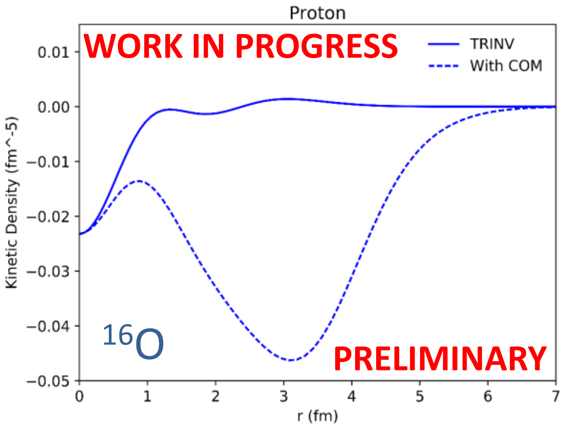


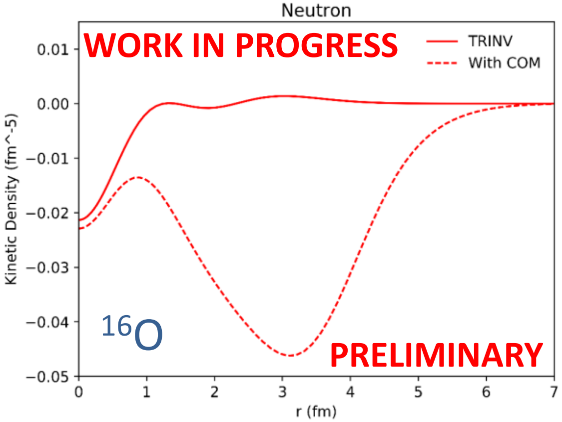
Local Density





Kinetic Density





Conclusions and Outlook

- Conclusions:
  - We observed significant difference for the nuclear density in light systems when the COM was removed
  - We can use the more general, non-local density for optical potentials and density functional theory

- Work to be done:
  - Continue benchmarking kinetic density term
  - Explore connection between the integral of kinetic density and the expectation value of kinetic energy operator

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