Nuclear kinetic density from *ab initio* theory

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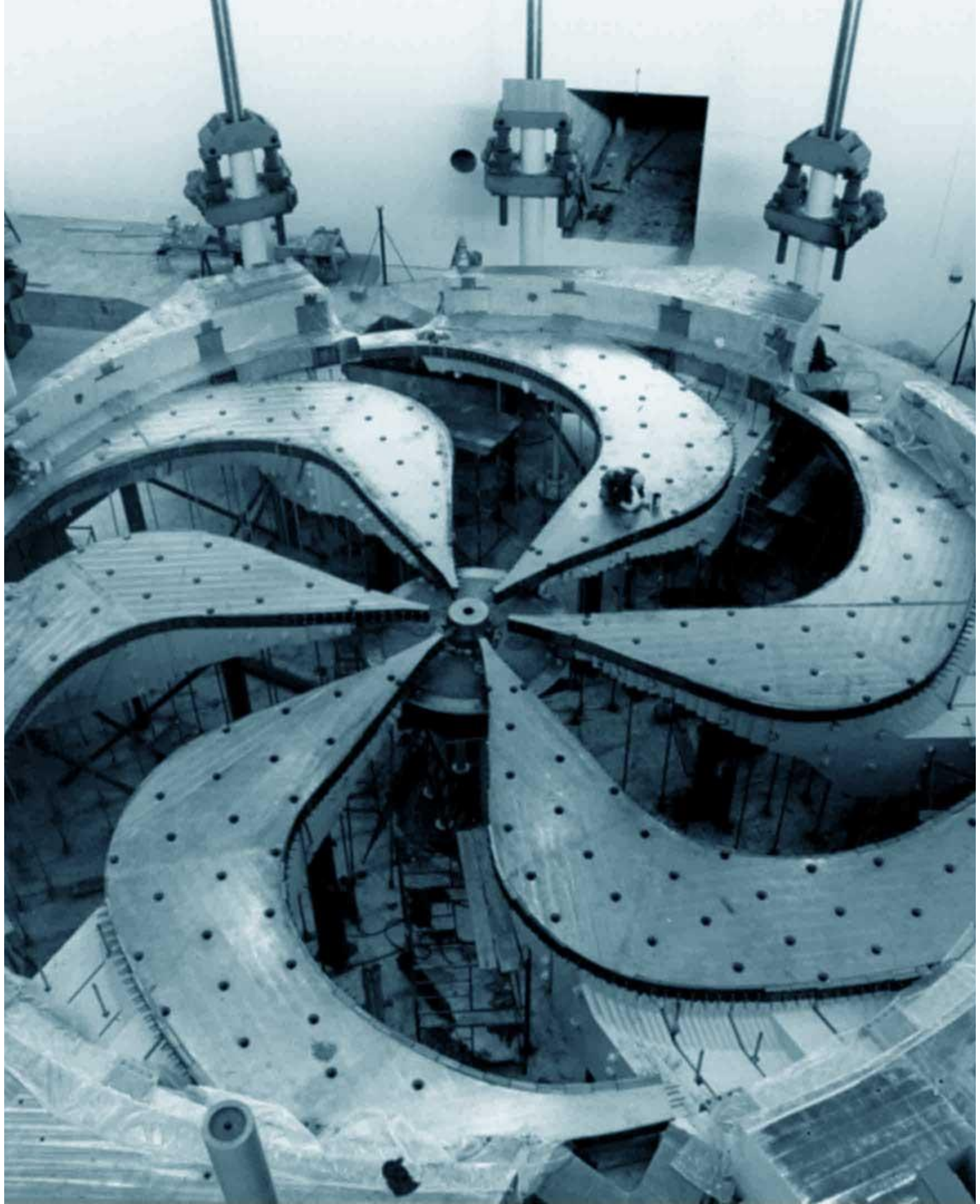
TRIUMF and University of Waterloo

In collaboration with

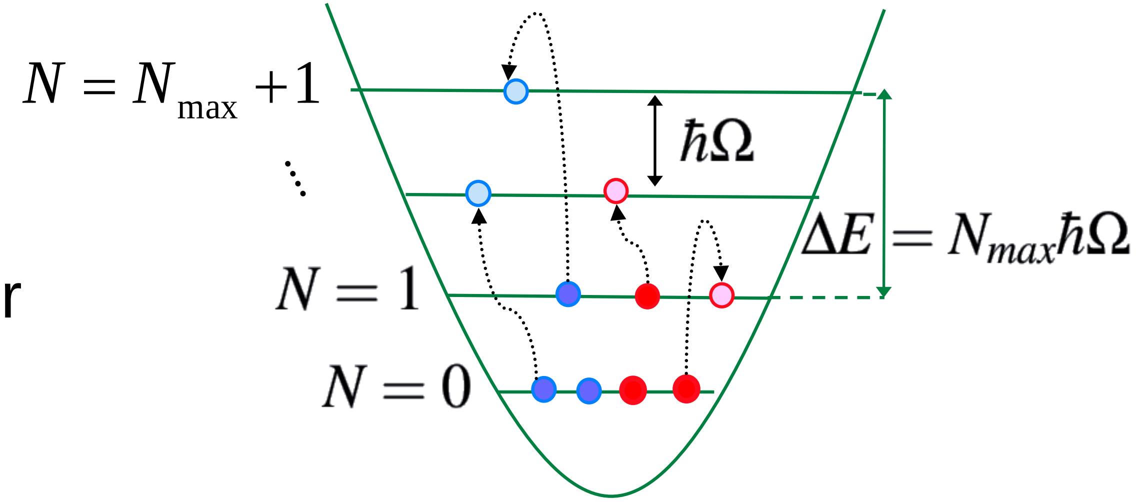
Petr Navrátil

2019-02-25

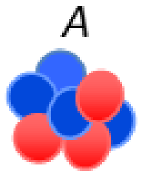


Discovery, accelerated

No-core shell model (NCSM)



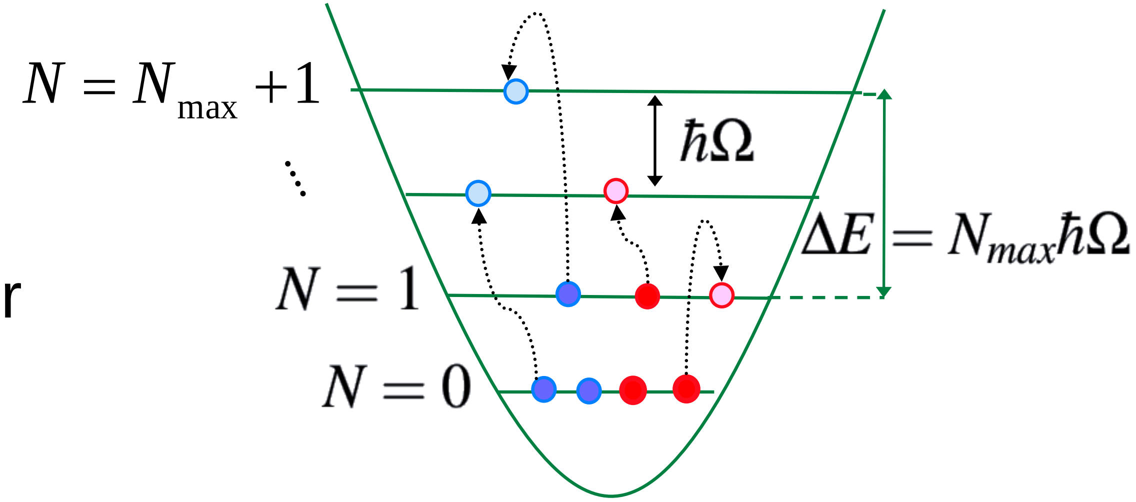
- NCSM is an *ab initio* approach to solve the many-body Schrödinger equation for bound states (narrow resonances) starting from *high-precision NN+NNN interactions*
- Uses large (but finite!) expansions in HO many-body basis states
- Translational invariance of the internal wave function is preserved when single-particle Slater Determinant (SD) basis is used with $N_{\max}$ truncation



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

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

No-core shell model (NCSM)



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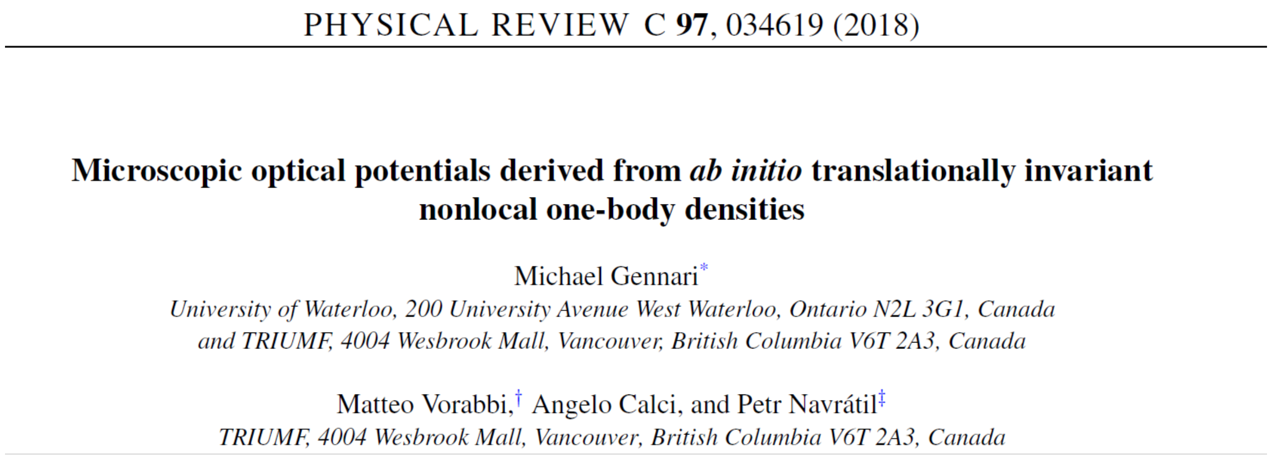
Nuclear density

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



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

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Nonlocal translationally invariant density (trinv)

- 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

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

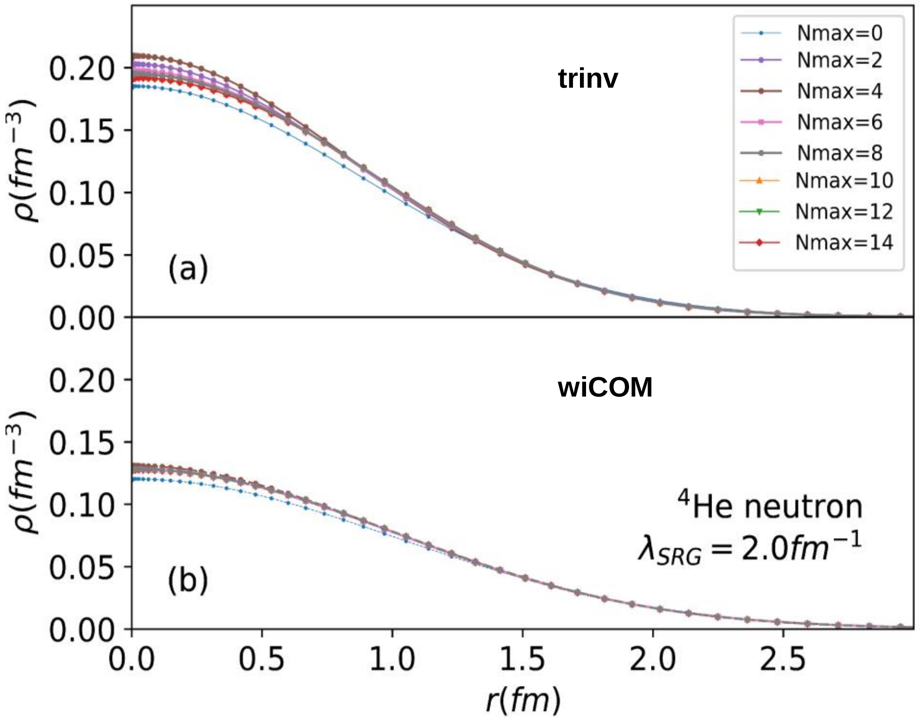
NN and 3N interactions – $N^4LO(500)$+3NlnI

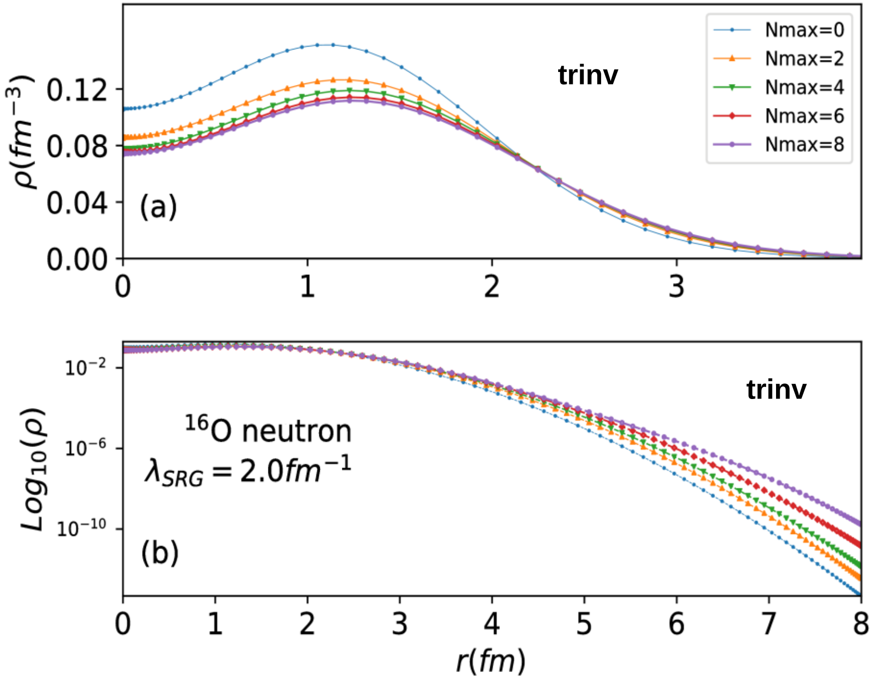
NN systematic from LO to N^4LO

- 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 96.2, 024004 (2017)

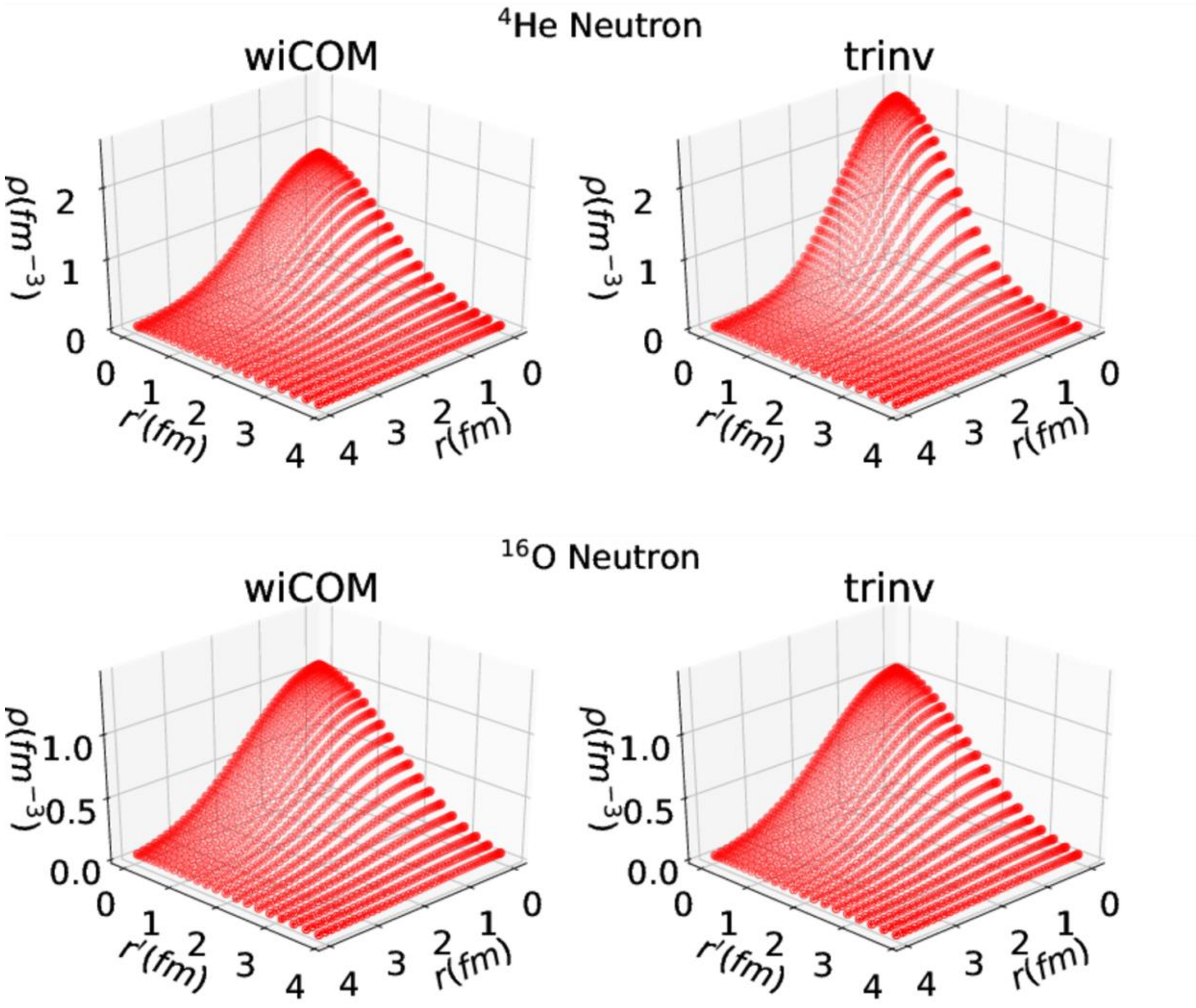
3N at N^2LO

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

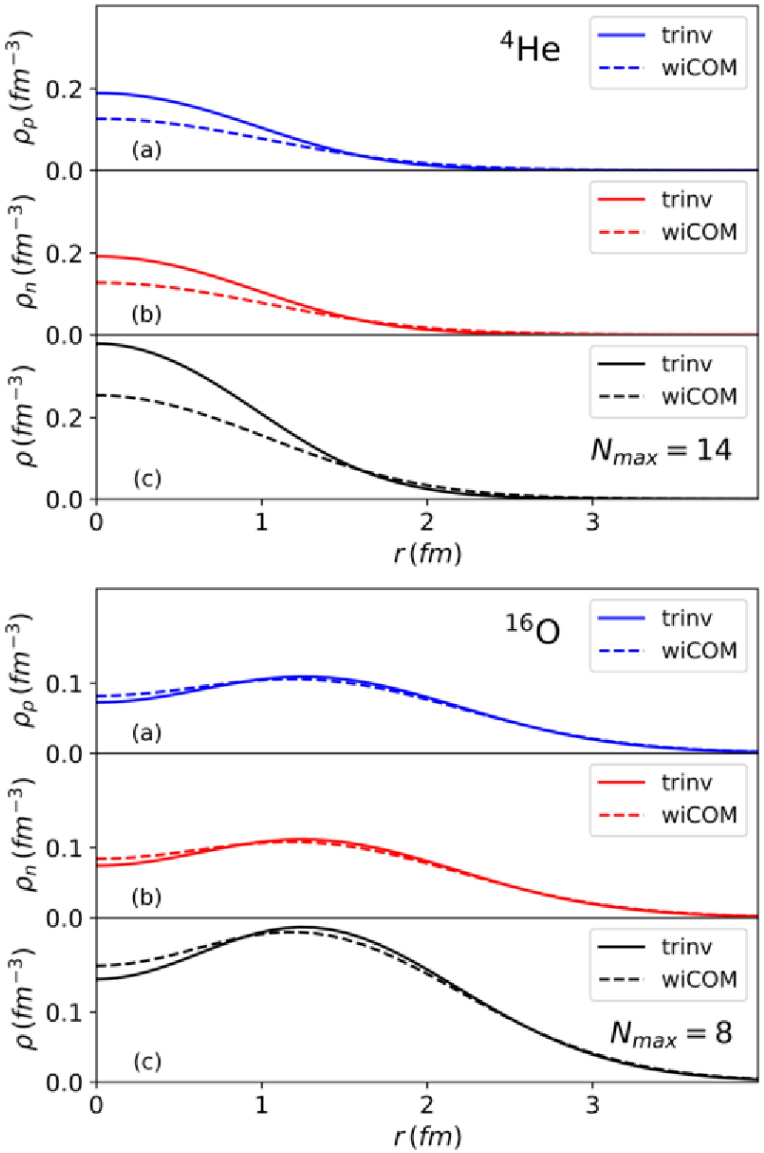




Ground state density of ^{4}He, ^{16}O



Local density



Interaction: NN-N^{4}LO(500)+3NlnI

Nuclear kinetic density

- Nuclear kinetic density is a fundamental, non-observable quantity of density functional theory (DFT)
- With the nonlocal density, we can compute the kinetic density from the *ab initio* NCSM
- Effects of COM removal in nuclear density should be amplified in DFT quantities like the kinetic density, due to the application of gradients on the nuclear density

$$\mathcal{H}_{kinetic}(\vec{r}) = \frac{\hbar^2}{2m}\tau_0(\vec{r})$$

$$\Big\downarrow$$

$$\tau_{\mathcal{N}}(\vec{r}) = \left[\vec{\nabla}\cdot\vec{\nabla}\,'\rho_{\mathcal{N}}(\vec{r},\vec{r}\,')\right]_{\vec{r}=\vec{r}\,'}$$

$$\Big\downarrow$$

$$\nabla_u\nabla'_{-u}\rho(\vec{r},\vec{r}\,') = \sum_{n,l,n',l',K,k,m_l,m_{l'}} \alpha^{K,i,f}_{n,l,n',l'}\,(l\,m_l\,l'\,m_{l'}|LM) \times \left[\nabla_u R_{n,l}(r)Y^*_{l,m_l}(\hat{r})\right]\left[\nabla'_{-u}R_{n',l'}(r')Y^*_{l',m_{l'}}(\hat{r}')\right]$$

Nuclear kinetic density

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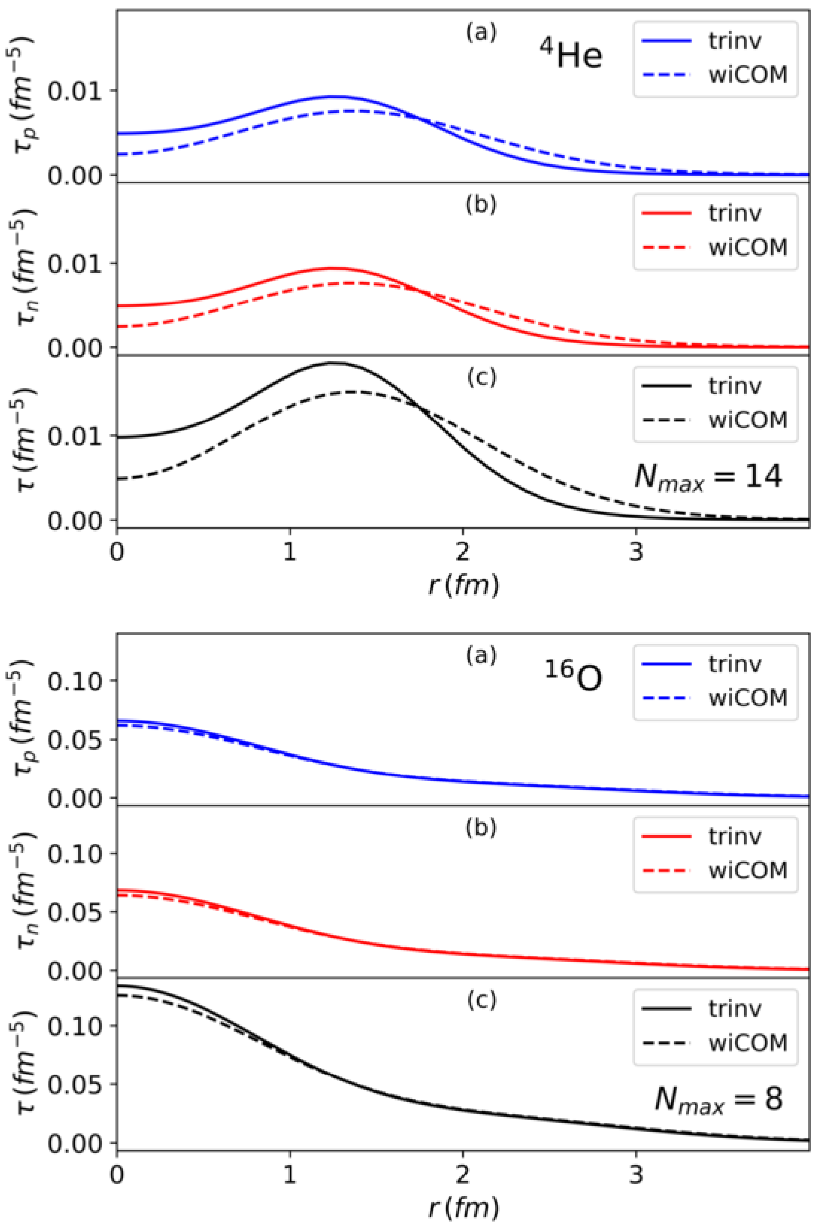
Interaction: NN-N^{4}LO(500)+3Nlnl

Kinetic density



COM treatment in DFT

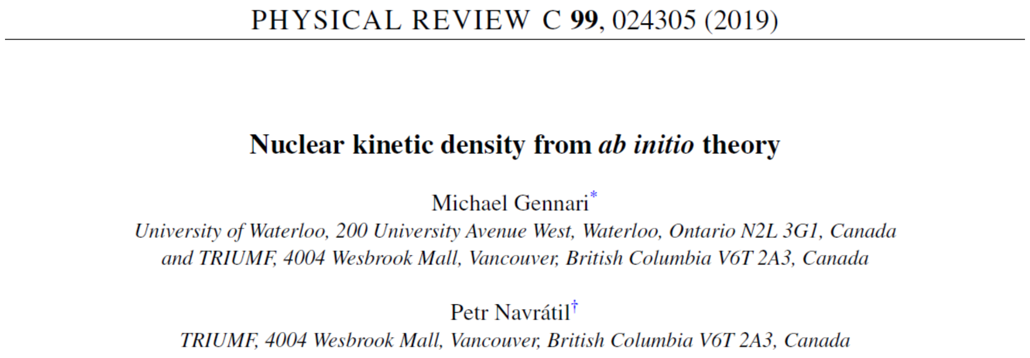
- Basic treatment for COM contamination can be introduced in the kinetic density term

$$\mathcal{H}_{kinetic}(\vec{r}) = \frac{\hbar^2}{2m}\left(1 - \frac{1}{A}\right)\tau_0(\vec{r})$$

- In the NCSM, $\tau_0(\vec{r})$ is the COM contaminated nuclear density (wiCOM)
- Can compare COM removal techniques by
  - computing translationally invariant kinetic density
  - computing COM contaminated kinetic density and applying removal procedure shown above

Comparison of COM removal techniques

- Inverse proportionality in A pushes DFT curve further from the *ab initio* kinetic density curve
- Still a notable difference in systems like ^{12}C and ^{16}O
- COM removal procedure likely important in deformed nuclei



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Nuclear kinetic density from *ab initio* theory

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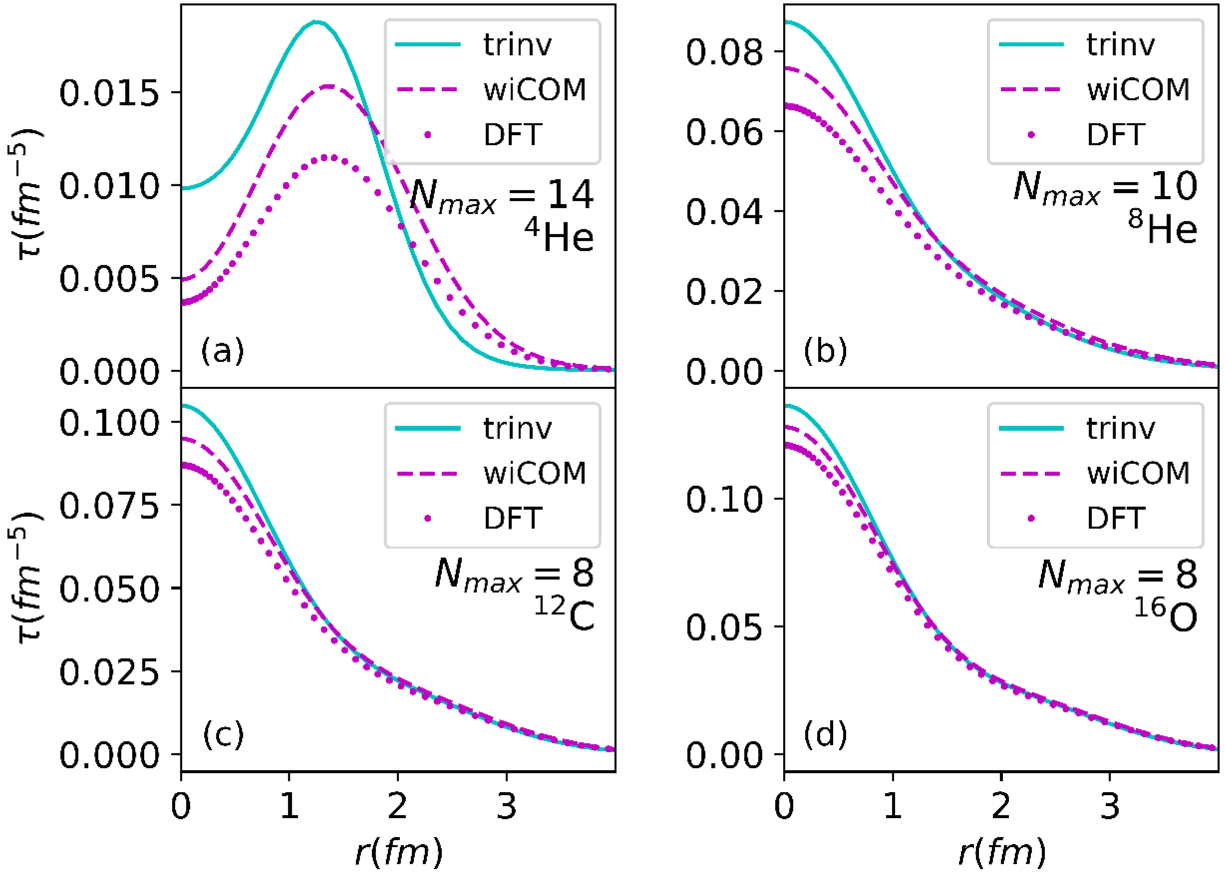
Kinetic density



Conclusions and outlook

- **Conclusions**
  - We observed significant differences in the kinetic density of light systems when the COM was removed
  - The effect of COM removal is significant in larger systems like ^{16}O
  - More details on some of these results can be found in Phys. Rev. C 99, 024305 (2019)

- **Outlook**
  - Pursuing implementation and extensions to natural orbitals framework in in the NCSM
  - Attempting a true two-parameter extrapolation scheme for nuclear observables using Gaussian processes

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Thank you
Merci

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