

# Nuclear kinetic density from *ab initio* theory

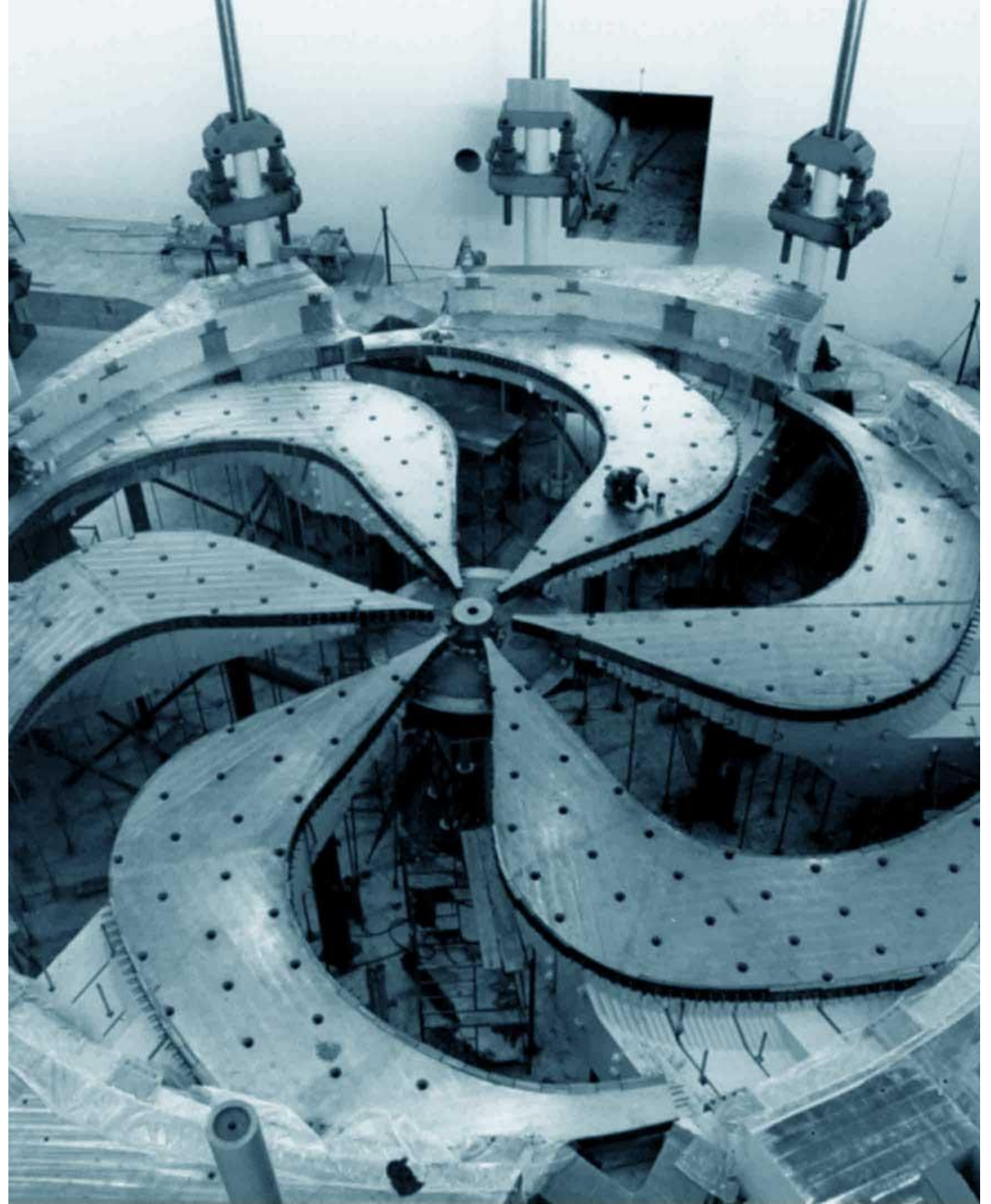
Michael Gennari

TRIUMF

In collaboration with

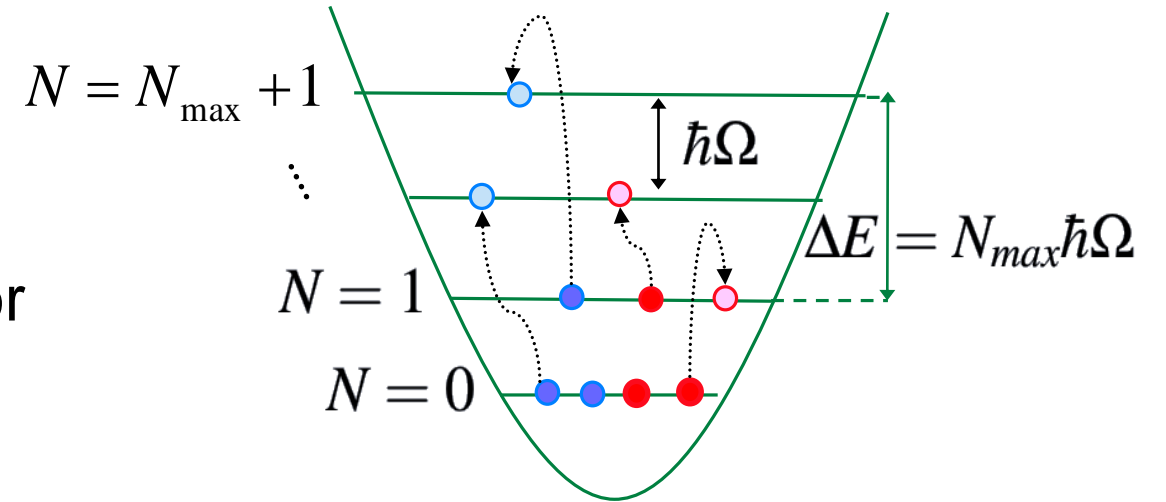
Petr Navrátil


2019-06-05



# 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



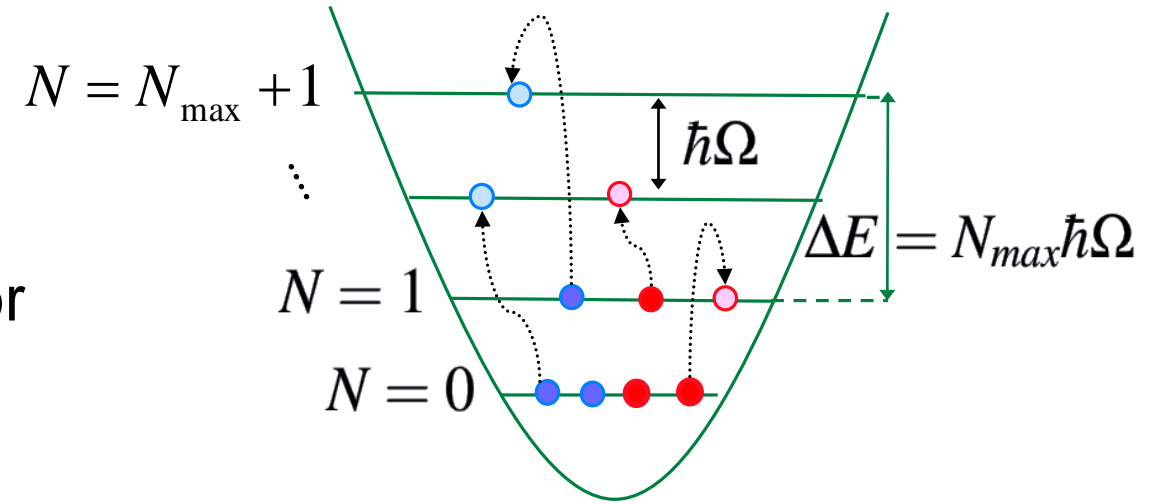


$$\Psi^A = \sum_{N=0}^{N_{\max}} \sum_i c_{Ni} \Phi_{Ni}^A$$

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

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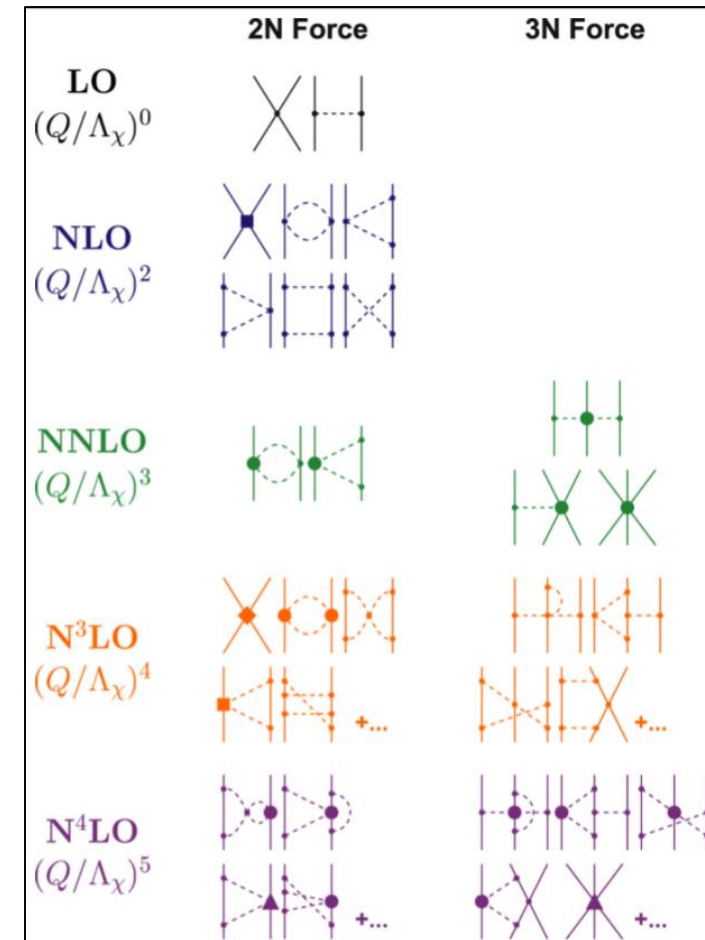
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$$\langle \vec{r}_1 \cdots \vec{r}_A \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots \vec{\tau}_A | A\lambda JM \rangle_{SD} = \underbrace{\langle \vec{\xi}_1 \cdots \vec{\xi}_{A-1} \vec{\sigma}_1 \cdots \vec{\sigma}_A \vec{\tau}_1 \cdots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

# Chiral effective field theory

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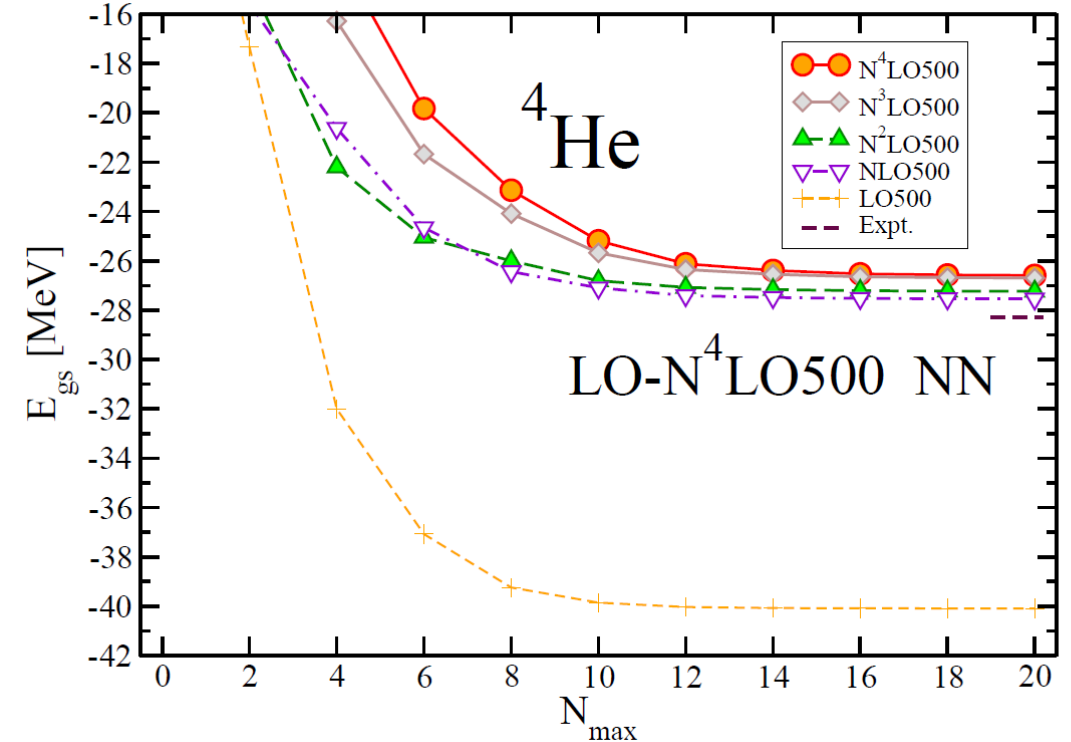
- NCSM requires diagonalization of Hamiltonian built from kinetic terms and realistic nuclear potentials rooted in QCD
- Interaction matrix elements are generated from chiral effective field theory approach (EFT) by
  - a) identifying relevant symmetries and degrees of freedom of low-energy QCD
  - b) identifying relevant separation scales of low-energy QCD ( $\Lambda_\chi \approx 1$  GeV hard scale)
- Allows for high quality control over truncation error at each chiral level



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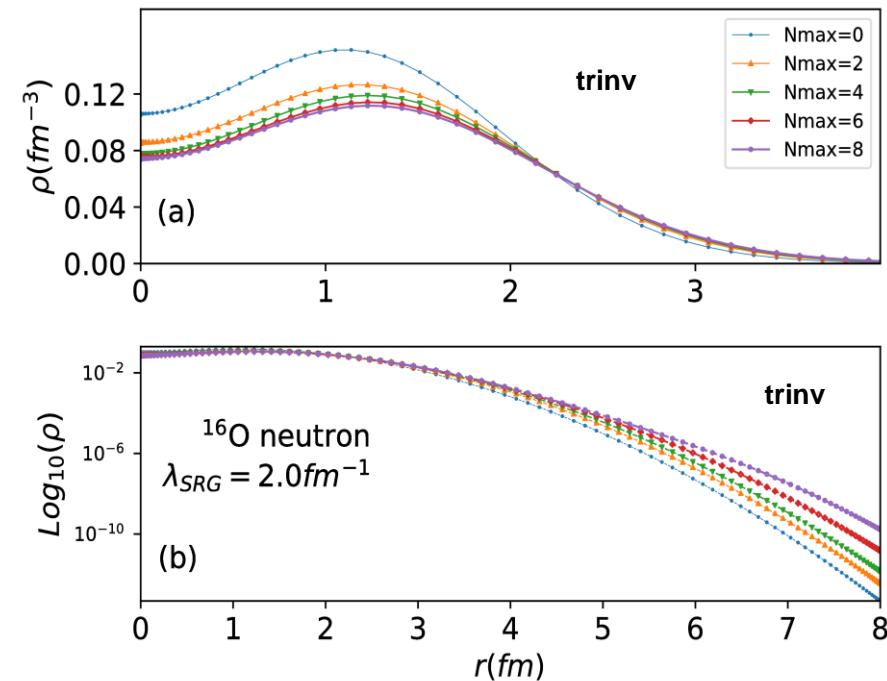
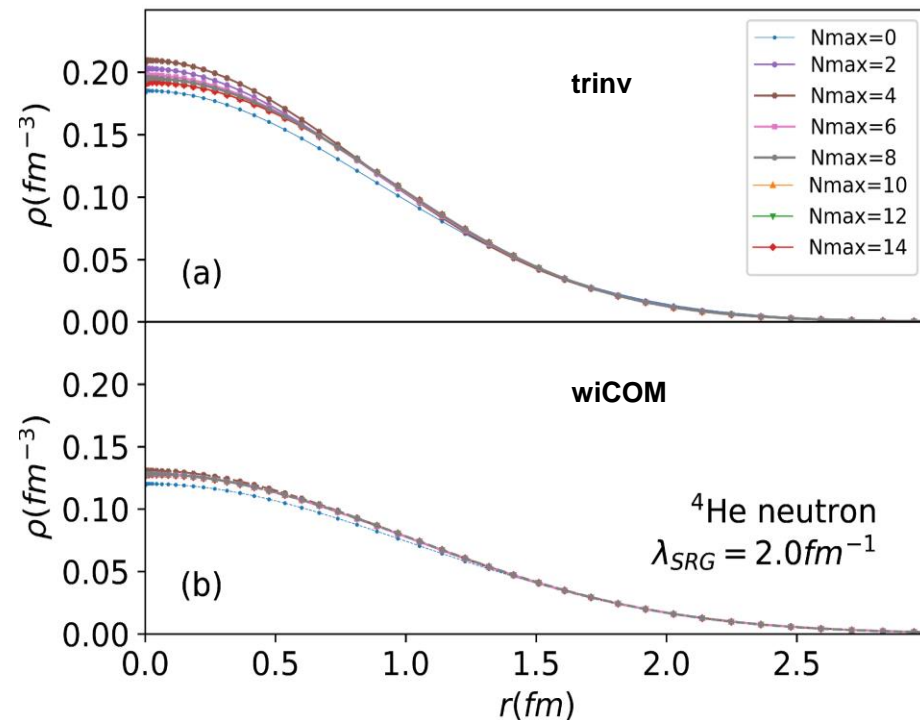




# NN and 3N interactions – $N^4\text{LO}(500)+3\text{N}^{\text{nl}}$

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- Two-nucleon (NN) interaction systematic from LO to  $N^4\text{LO}$ 
  - 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 96.2, 024004 (2017)
- Three-nucleon (3N) interaction at  $N^2\text{LO}$ 
  - Navrátil, 650 MeV local cut-off and 500 MeV non-local cut-off



# Nuclear density

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

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

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

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Matteo Vorabbi,<sup>†</sup> Angelo Calci, and Petr Navrátil<sup>‡</sup>

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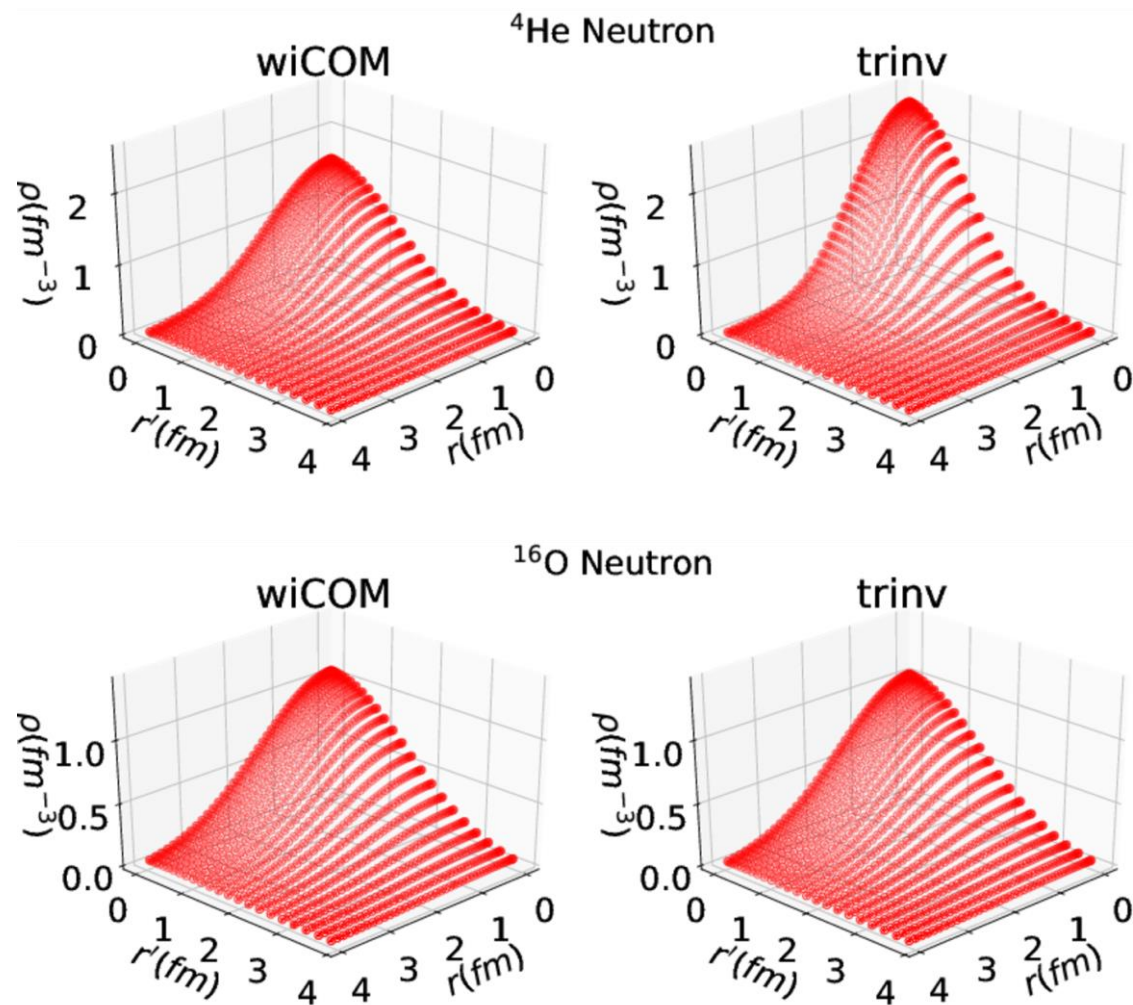
## Nonlocal translationally invariant density (trinv)

- 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

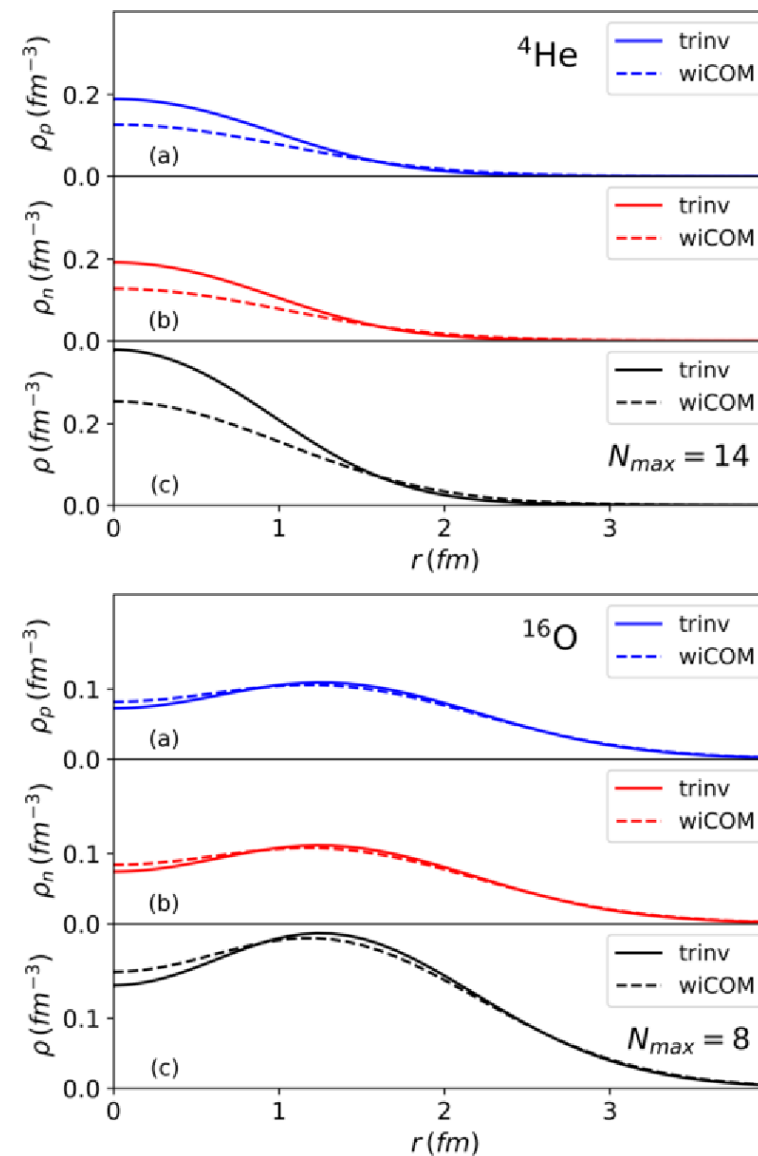
## Normalization

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

# Ground state density of $^4\text{He}$ , $^{16}\text{O}$



## Local density



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



# 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

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



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



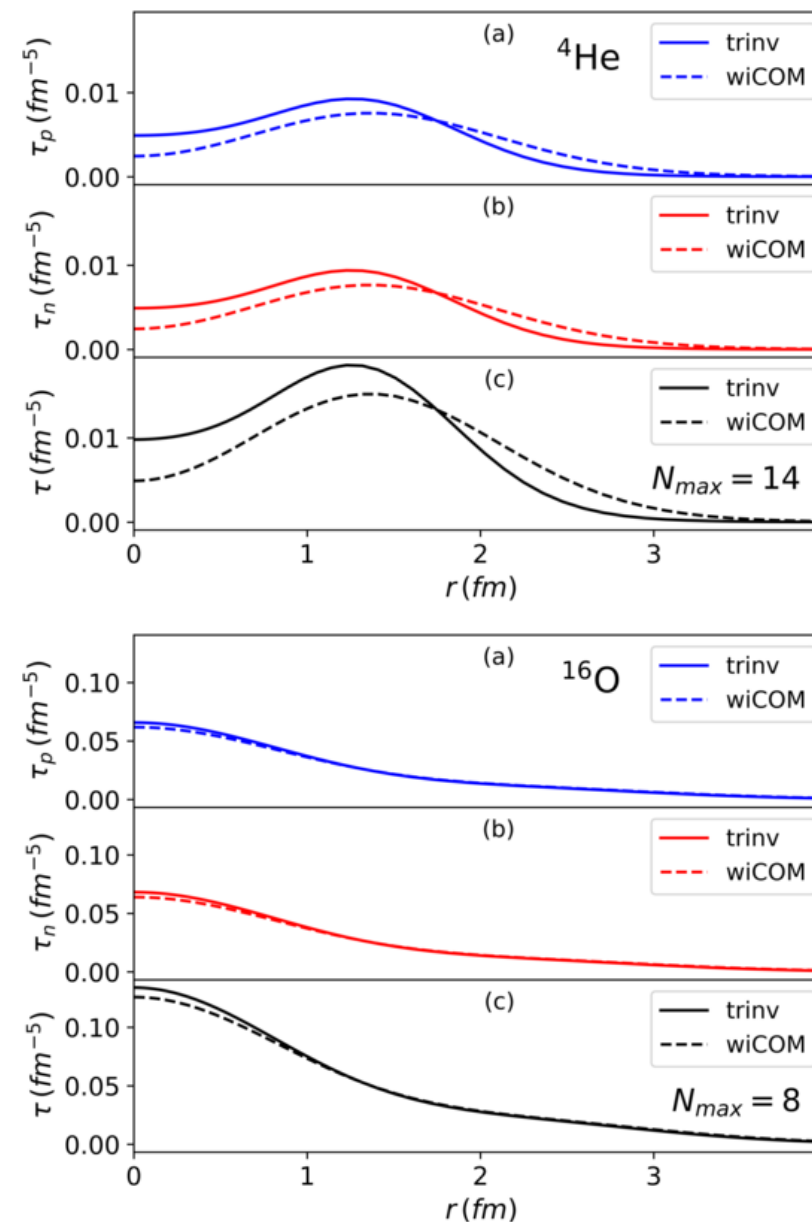
$$\begin{aligned} \nabla_u \nabla'_{-u} \rho(\vec{r}, \vec{r}') = & \sum_{n,l,n',l',K,k,m_l,m_{l'}} \alpha_{n,l,n',l'}^{K,i,f} (l m_l l' m_{l'} | LM) \\ & \times \left[ \nabla_u R_{n,l}(r) Y_{l,m_l}^*(\hat{r}) \right] \left[ \nabla'_{-u} R_{n',l'}(r') Y_{l',m_{l'}}^*(\hat{r}') \right] \end{aligned}$$

# Nuclear kinetic density

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Interaction: NN-N<sup>4</sup>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

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

PHYSICAL REVIEW C **99**, 024305 (2019)

Nuclear kinetic density from *ab initio* theory

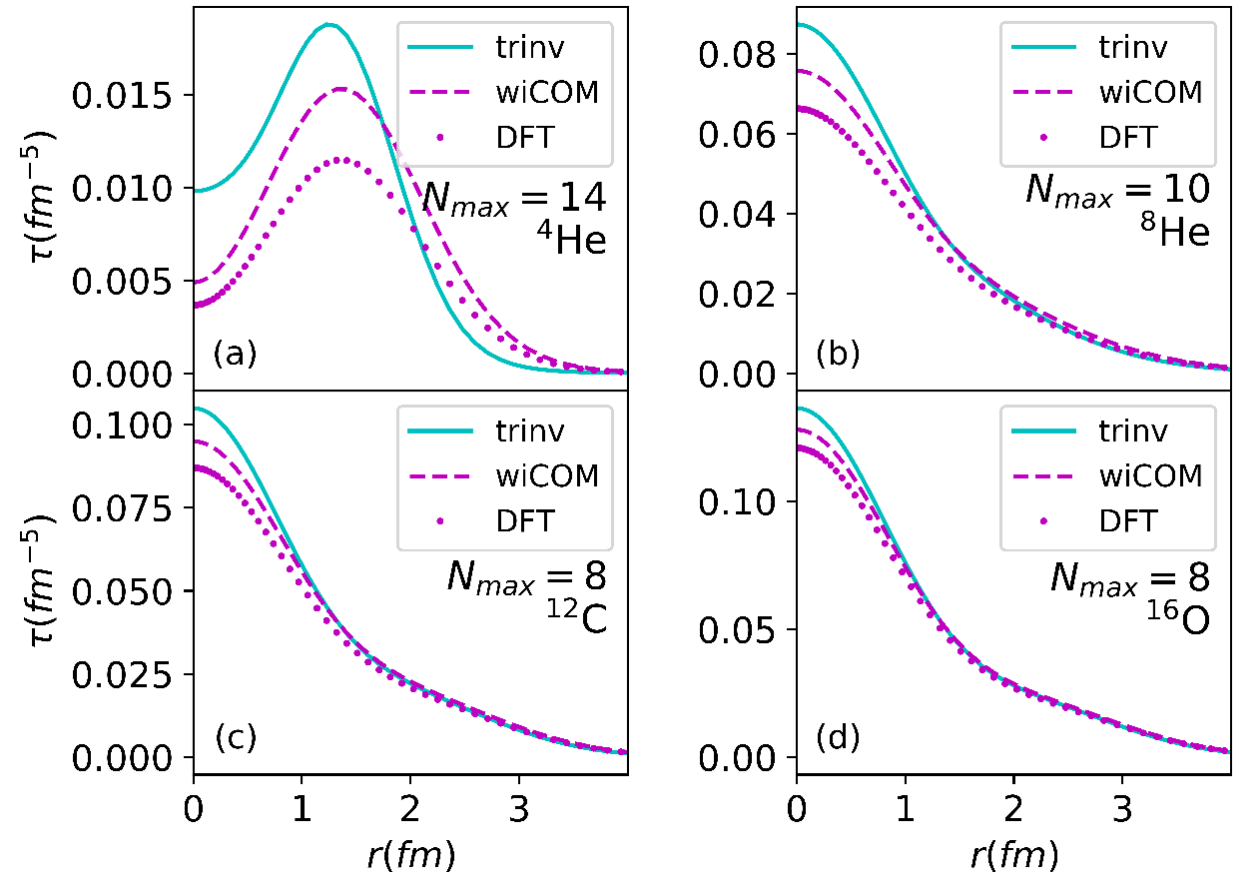
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Kinetic density



# Conclusions and outlook

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## ■ 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  $^{16}\text{O}$
- 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 the NCSM
- Attempting an extrapolation scheme for nuclear observables using Gaussian processes



Thank you  
Merci

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