Nuclear kinetic density from \textit{ab initio} theory

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In collaboration with
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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 $N_{\text{max}}$ truncation

\[
\langle \tilde{r}_1 \cdots \tilde{r}_A \tilde{\sigma}_1 \cdots \tilde{\sigma}_A \tilde{\tau}_1 \cdots \tilde{\tau}_A | A\lambda J M \rangle_{SD} = \langle \tilde{\xi}_1 \cdots \tilde{\xi}_{A-1} \tilde{\sigma}_1 \cdots \tilde{\sigma}_A \tilde{\tau}_1 \cdots \tilde{\tau}_A | A\lambda J M \rangle \phi_{000}(\tilde{\xi}_0)
\]
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$$
Chiral effective field theory

- 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 – N⁴LO(500)+3Nlnl

- Two-nucleon (NN) interaction systematic from LO to N⁴LO

- Three-nucleon (3N) interaction at N²LO
  - Navrátil, 650 MeV local cut-off and 500 MeV non-local cut-off
Nuclear density

\[
\langle A \lambda_f J_f M_f | \rho_{\text{op}}(\vec{r} - \vec{R}, \vec{r}' - \vec{R}) | A \lambda_i J_i M_i \rangle \\
= \left( \frac{A}{A-1} \right)^{3/2} \sum \frac{1}{I_f} (I_i M_i K k | J_f M_f) \left( Y_i^* (\vec{r} - \vec{R}) Y_i^* (\vec{r}' - \vec{R}) \right)^{(K)}_k \\
\times R_{n,i} \left( \frac{A}{A-1} |\vec{r} - \vec{R}| \right) R_{n',i'} \left( \frac{A}{A-1} |\vec{r}' - \vec{R}| \right) \\
\times (M^K)^{-1}_{n,i,n',i',n_1,l_1,n_2,l_2} (-1)^{l_1+ l_2 + K + j_2} \hat{f}_1 \hat{f}_2 \hat{R} \left\{ \begin{array}{ccc} j_1 & j_2 & K \\ l_2 & l_1 & 1/2 \end{array} \right\} \\
\times \frac{(-1)^{SD}}{R} \langle A \lambda_f J_f \| (a_{n_1 l_1 j_1}^* \tilde{a}_{n_2 l_2 j_2})^{(K)} \| A \lambda_i J_i \rangle_{SD}
\]

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

Microscopic optical potentials derived from \textit{ab initio} translationally invariant nonlocal one-body densities

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Normalization

\[
\int d\vec{x} \langle A \lambda J M | \rho_{\text{op}}^{\text{phys}} (\vec{x}) | A \lambda J M \rangle = A
\]
Ground state density of $^4$He, $^{16}$O

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

Local density
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 \textit{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.

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

\[
\tau_N(\vec{r}) = \left[ \vec{\nabla} \cdot \vec{\nabla}' \rho_N(\vec{r}, \vec{r}') \right]_{\vec{r} = \vec{r}'}
\]

\[
\nabla_u \nabla'_{-u} \rho(\vec{r}, \vec{r}') = \sum_{n,l,n',l',K,k,m_l,m_{l'}} \alpha_{n,l,n',l'}^{K,i,f} (l m_l l' m_{l'} | LM) \\
\times \left[ \nabla_u R_{n,l}(r) Y^*_{l,m_l}(\hat{r}) \right] \left[ \nabla'_{-u} R_{n',l'}(r') Y^*_{l',m_{l'}}(\hat{r}') \right]
\]
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\textbf{Interaction}: \textit{NN-N^4LO(500)+3Nlnl}
COM treatment in DFT

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

\[
H_{kinetic}(\vec{r}) = \frac{\hbar^2}{2m} \left(1 - \frac{1}{A}\right) \tau_0(\vec{r})
\]

- 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 \textit{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.

\[ N_{\text{max}} = 10 \quad ^{8}\text{He} \]
\[ N_{\text{max}} = 14 \quad ^{4}\text{He} \]
\[ N_{\text{max}} = 8 \quad ^{12}\text{C} \]
\[ N_{\text{max}} = 8 \quad ^{16}\text{O} \]
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 $^{16}\text{O}$.
  - 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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