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

$$\langle \mathbf{r}_1 \cdots \mathbf{r}_A \sigma_1 \cdots \sigma_A \mathbf{\tau}_1 \cdots \mathbf{\tau}_A | A\lambda J M \rangle_{SD} = \langle \mathbf{\tilde{\xi}}_1 \cdots \mathbf{\tilde{\xi}}_{A-1} \tilde{\sigma}_1 \cdots \tilde{\sigma}_A \mathbf{\tilde{\tau}}_1 \cdots \mathbf{\tilde{\tau}}_A | A\lambda J M \rangle_{000} (\mathbf{\tilde{\xi}}_0)$$
No-core shell model (NCSM)

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\[
\langle \mathbf{r}_1 \ldots \mathbf{r}_A \mathbf{\sigma}_1 \ldots \mathbf{\sigma}_A \mathbf{\tau}_1 \ldots \mathbf{\tau}_A | \mathbf{A} \lambda J M \rangle_{SD} = \langle \tilde{\xi}_1 \ldots \tilde{\xi}_{A-1} \tilde{\sigma}_1 \ldots \tilde{\sigma}_A \tilde{\tau}_1 \ldots \tilde{\tau}_A | \mathbf{A} \lambda J M \rangle \varphi_{000}(\tilde{\xi}_0)
\]
Nuclear density

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

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

\[
\int d\tilde{x} \langle A\lambda JM | \rho_{op}^{\text{phys}} (\tilde{x}) | A\lambda JM \rangle = A
\]
NN and 3N interactions – N⁴LO(500)+3Nlnl

NN systematic from LO to N⁴LO

3N at N²LO
- Navrátil, 650 MeV local cut-off and 500 MeV non-local cut-off
Ground state density of $^4\text{He}$, $^{16}\text{O}$

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

Local density

$^4\text{He}$

$^{16}\text{O}$
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

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

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

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

Kinetic density

**Nuclear kinetic density from *ab initio* theory**

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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 a true two-parameter extrapolation scheme for nuclear observables using Gaussian processes
Thank you
Merci

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