Nonlocal translationally invariant density

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Abstract

Nonlocal nuclear density is derived from the no-core shell model (NCSM) [1] one-body densities by generalizing the local density operator to a nonlocal form. The translational invariance (trinv) is generated by exactly removing the spurious center of mass (COM) component from the NCSM eigenstates expanded in the harmonic oscillator (HO) basis [2]. This enables the *ab initio* NCSM nuclear structure to be used in intermediate energy nuclear reactions and density functional theory (DFT). The ground state local and nonlocal density of ^4He, ^6He, ^{12}C and ^{16}O are calculated to display the effects of COM removal on predicted nuclear structure. We include nonlocal density in calculations of optical potentials [3] and show more accurate theoretical predictions for the differential cross sections for proton scattering on ^4He.The results of this work have been published in Ref. [4]. Additionally, we show amplified effects of COM removal in related DFT quantities like kinetic density [5].

Nuclear density

The general nonlocal nuclear density operator is shown below, where r is a coordinate for the final state and r' is a separate coordinate for the initial state.

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

In the NCSM basis, translational invariance of the internal wave function is preserved when the single-particle Slater Determinant (SD) basis is used with N_{max} truncation [1]. The factorization of the Jacobi and SD eigenstates allows us to decouple and remove the ground state COM component from the intrinsic part of the wavefunction [2].

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

We construct the local density [2] by taking the diagonal portion of the nonlocal density ($\vec{r}=\vec{r}'$). The local density provides additional confirmation of the effects of COM removal and is useful for studying convergence patterns of the density.

Microscopic optical potentials

Nonlocal nuclear density is an important input for constructing microscopic optical potentials of nuclear reactions at intermediate energy. These are computed by folding the density with the t-matrix computed using modern high precision two and three nucleon interactions [3].

$$U(\vec{q},\vec{K}) = \sum_{N=n,p}\int d\vec{P}\;\eta(\vec{q},\vec{K},\vec{P})\,t_{pN}(\vec{q},\vec{K},\vec{P})\,\rho_N(\vec{q},\vec{P})$$

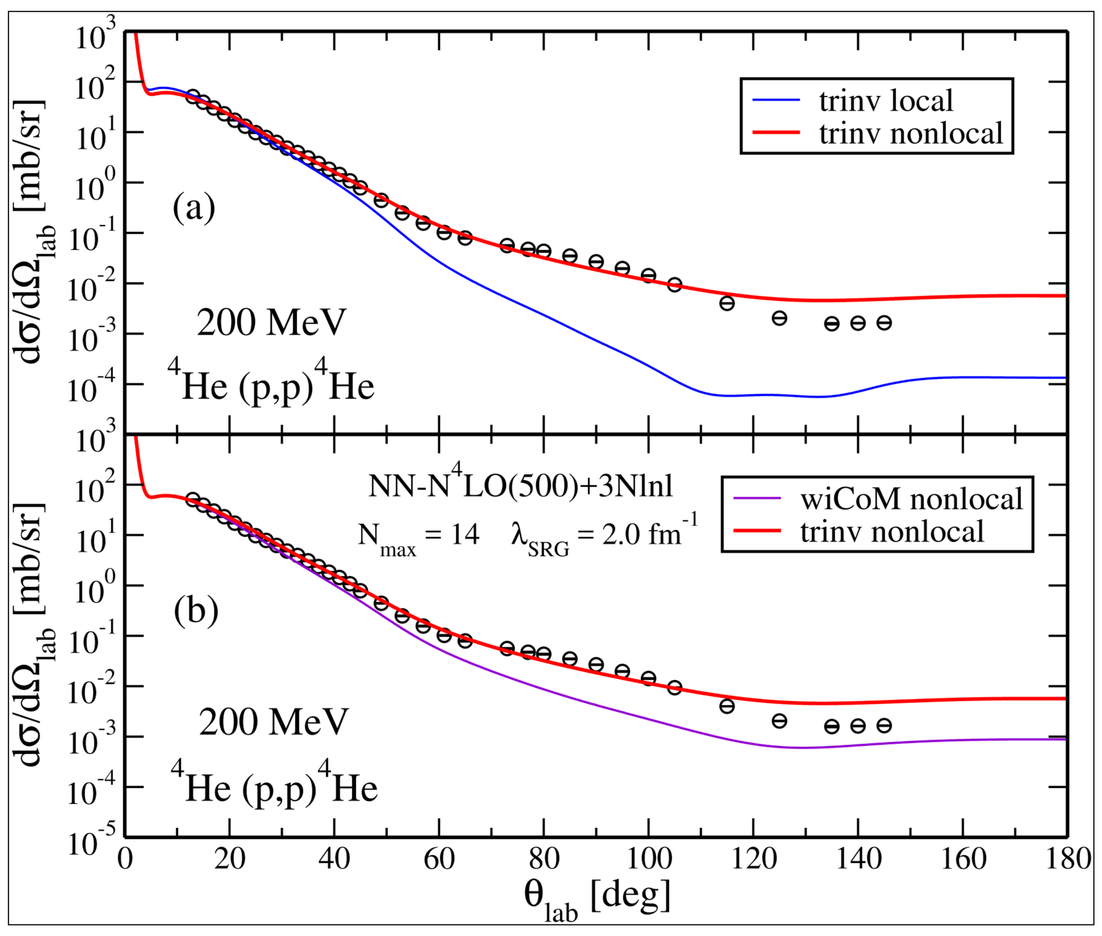

Figure 3: Comparisons between the wiCOM and trinv local density and nonlocal density calculations for the differential cross section of ^4He

See the talk titled "Microscopic optical potential for proton elastic scattering off light exotic nuclei" by Matteo Vorabbi for explicit discussion of the microscopic optical potentials.

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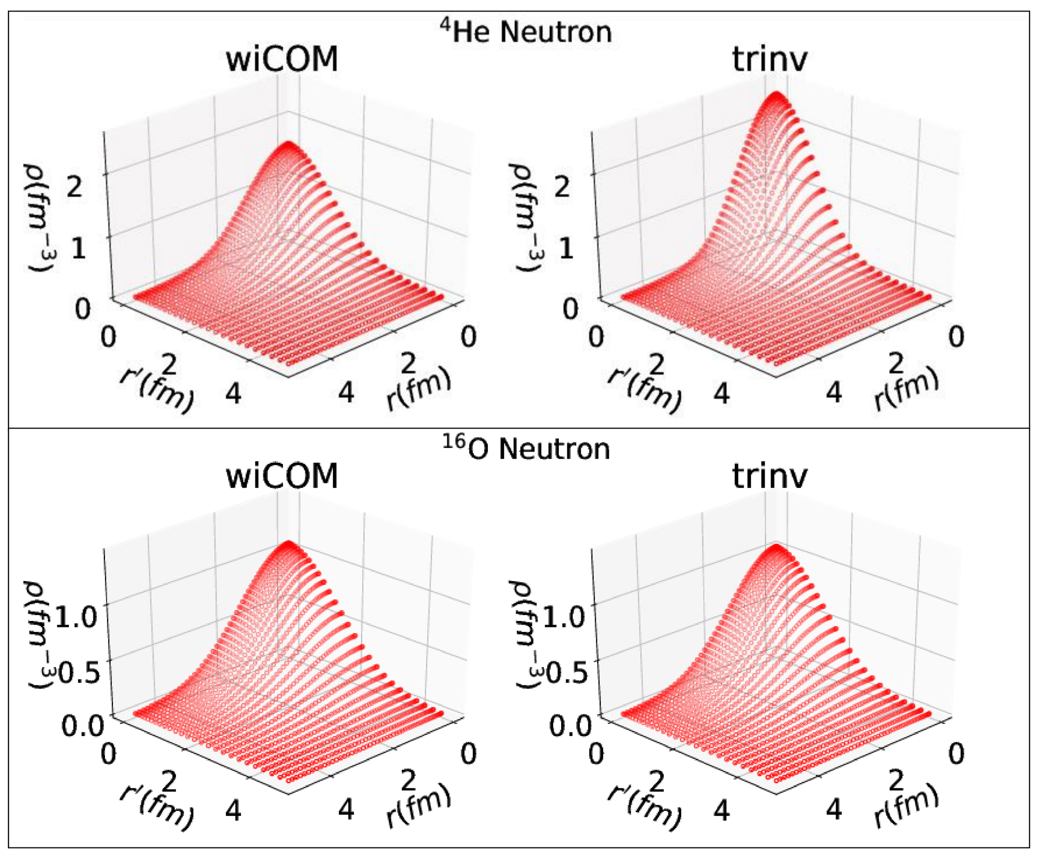

Figure 1: Comparisons between wiCOM and trinv nuclear density for ^4He and ^{16}O

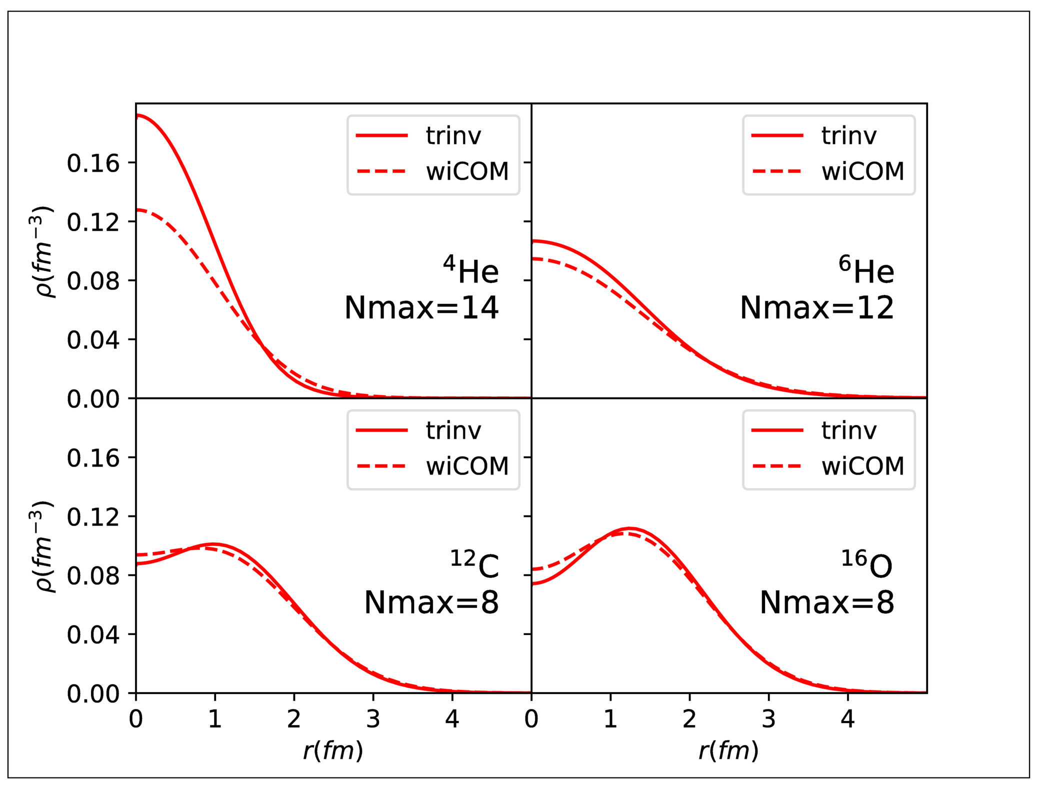

Figure 2: Comparisons of local wiCOM and trinv densities of ^4He, ^6He, ^{12}C and ^{16}O.

Kinetic density

The kinetic density is an example of one object in DFT [5] we can compute using ab initio wavefunctions. The kinetic density is given by the following relation,

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

The Laplacian-like operator is applied on the nonlocal density and should amplify effects of COM removal, the results of which are shown for $^{4,6}He$, ^{12}C, and ^{16}O.

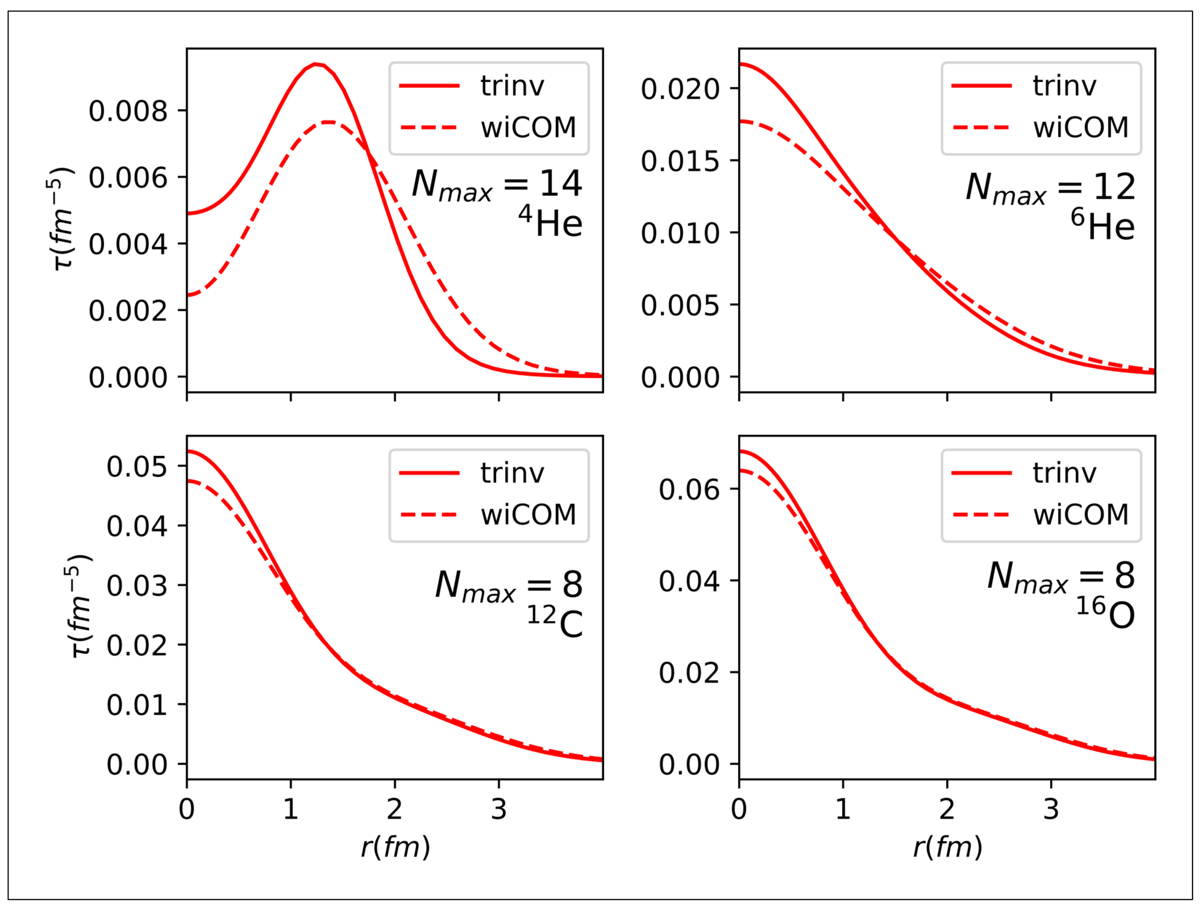

Figure 4: Comparison between the neutron wiCOM and trinv kinetic densities

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