

Nonlocal Translationally Invariant Nuclear 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, ¹²C and ¹⁶O 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. Additionally, we show amplified effects of COM removal in related DFT quantities like kinetic density [4].

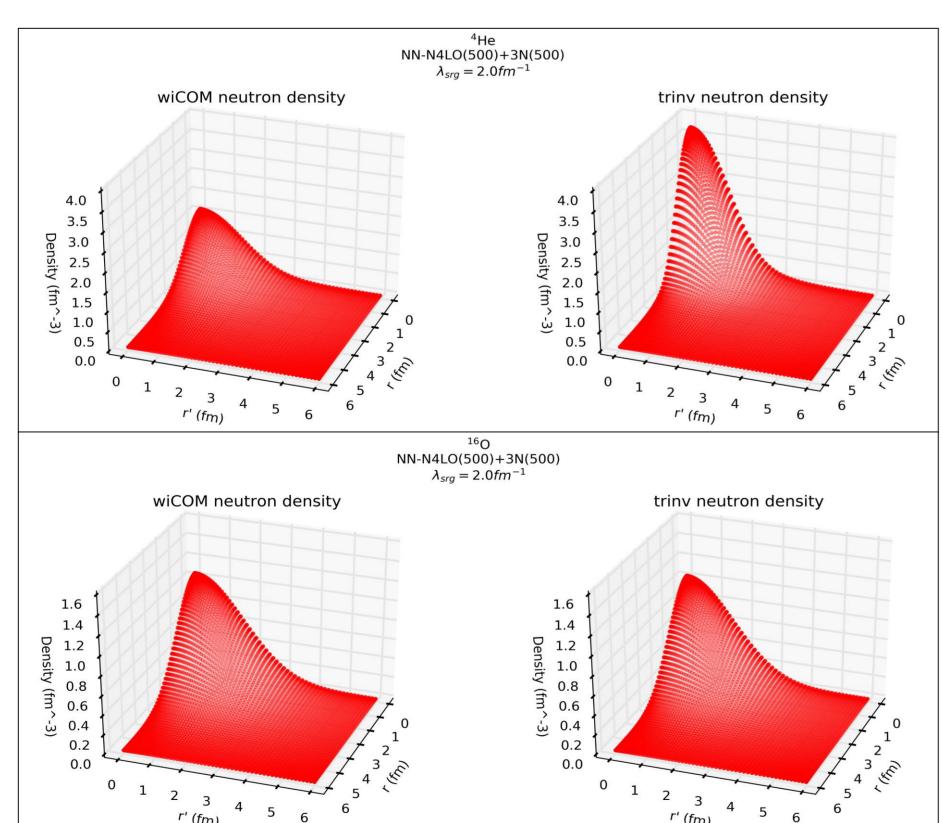
Nonlocal Trinv Nuclear Density

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.

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

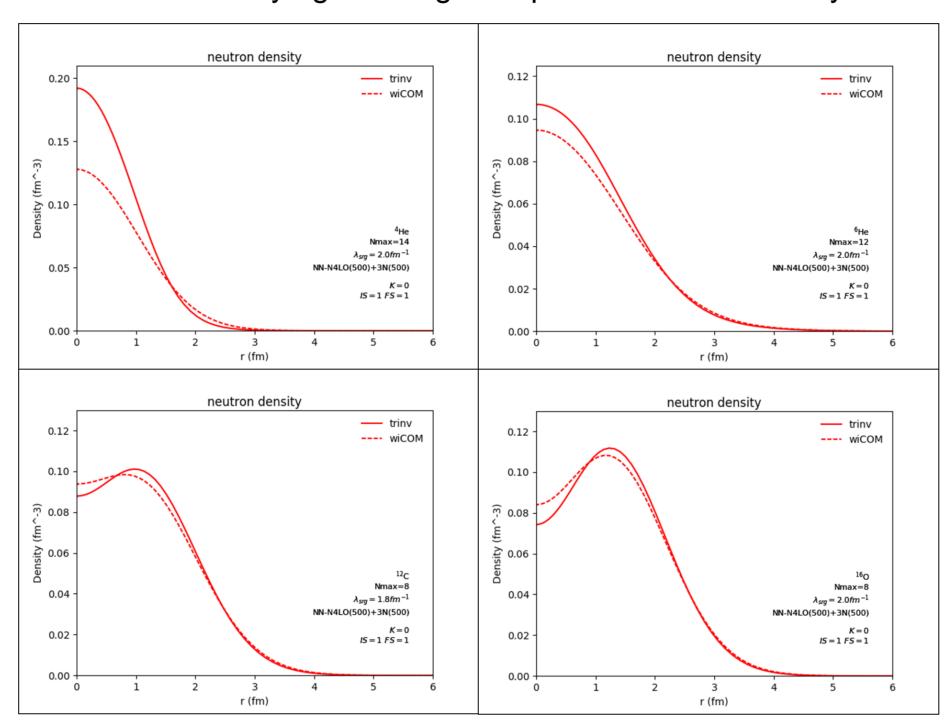
In the NCSM basis, translational invariance of the internal wave function is preserved when the single-particle Slater Determinant (SD) basis is used with N_{max} truncation [1]. The factorization of the Jacobi and SD eigenstates allows us to decouple and remove the ground state COM component from the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

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



Nonlocal Nuclear Density: This figure shows comparisons between COM contaminated and trinv nuclear density for ⁴He and ¹⁶O

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.

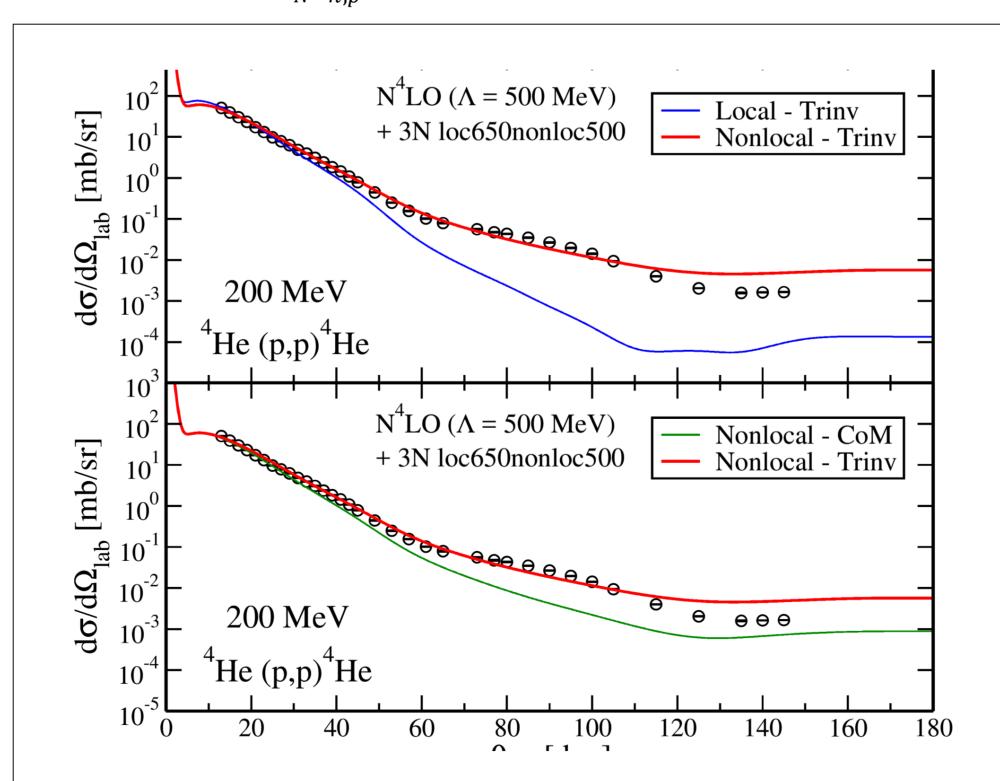


Density Comparison: This figure shows comparisons of local COM contaminated and trinv densities of ⁴He, ⁶He, ¹²C and ¹⁶O.

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].

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



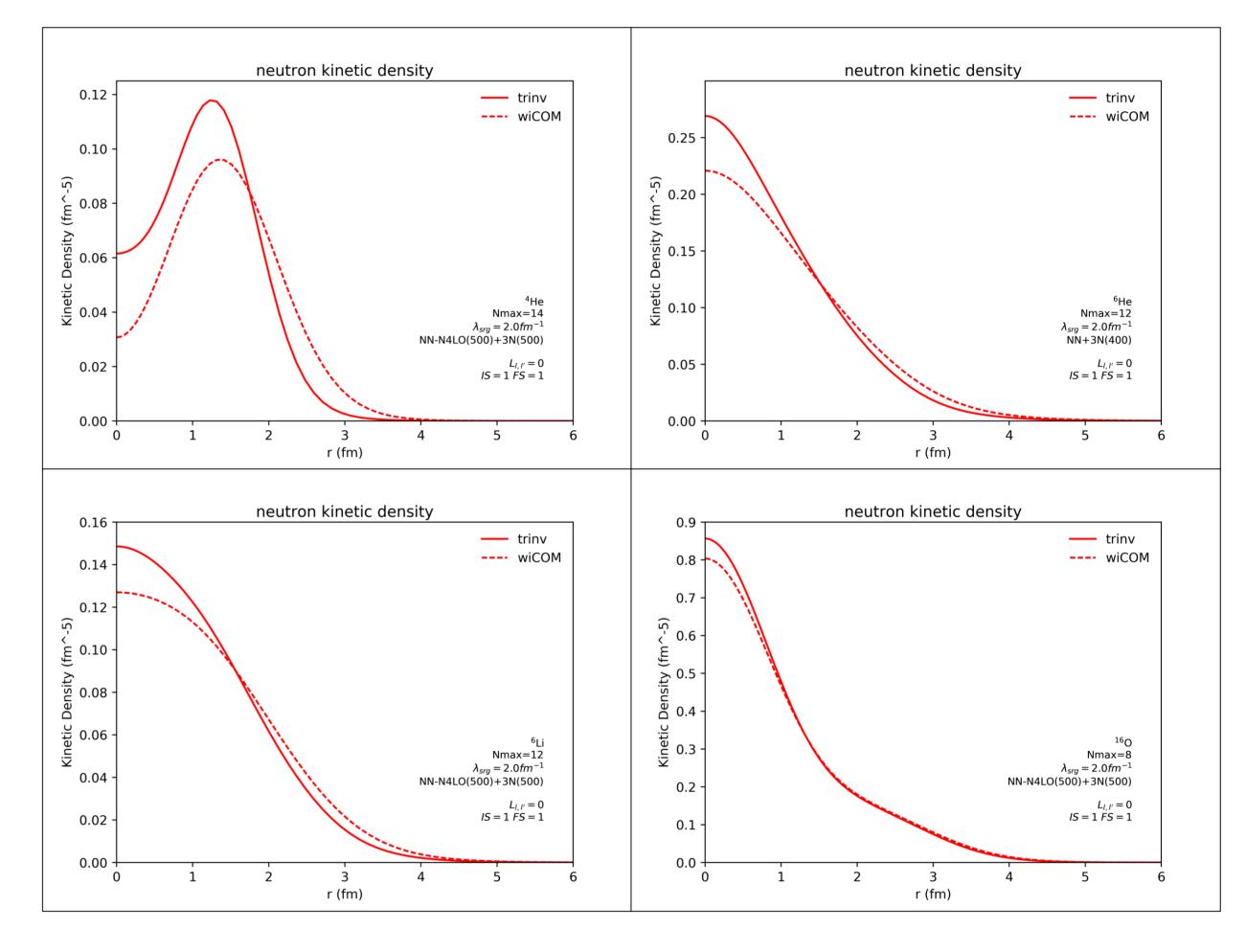
Cross Sections ⁴He: This figure shows comparisons between the local density approximation and nonlocal density calculations for the differential cross section of ⁴He, in addition to the effects observed by COM removal

Kinetic Density

The kinetic density is an example of one object in DFT [4] we can now calculate using *ab initio* wavefunctions. Kinetic density is given by the following relation,

$$\tau_T(\vec{r}) = \overrightarrow{\nabla} \cdot \overrightarrow{\nabla}' \, \rho_T(\vec{r}, \vec{r}')|_{\vec{r} = \vec{r}'}$$

The Laplacian-like operator being applied on the nonlocal density should amplify the effects of COM removal, the results of which are shown below.



Nuclei Comparison: This figure shows the comparison between the COM contaminated and trinv kinetic densities, in addition to the effects in higher A-nucleon systems

References

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