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Clustering and vibrations in the time-dependent DFT approach

Time-dependent nuclear density functional theory (TDDFT) is a well-suited tool to describe heavy ion collisions and nuclear vibrations. Here we present a study of nuclear vibrations and reactions focusing on the aspect of nucleonic clustering in the intermediate states.

Nuclear vibrations are studied in 3D computational box without any symmetry assumptions on an equidistant grid. Usually periodic boundary conditions are considered in those calculations. However those are prone to introduce finite volume effects due to standing waves. A standard way to remedy this finite volume effect is to introduce absorbing boundary conditions altering the dynamics of the system. We demonstrate that by using twist-averaged boundary conditions (TABC), averaging over multiple calculations with different Bloch boundary conditions, one can reduce finite-volume effects drastically without adding any additional parameters associated with absorption at large distances. Moreover, TABC are an obvious choice for time-dependent calculations for infinite systems. Since TABC calculations for different twists can be performed independently, the method is trivially adapted to parallel computing.

To visualize emergent clusters, we use the nucleonic localization function, which is based on the probability of finding two nucleons with same spin and isospin in the vicinity of each other. This measure was originally introduced for electronic structure calculations and was proven to be an excellent indicator for clustering in time-independent nuclear DFT calculations.
We demonstrate that the localization function for the TDDFT solutions of collisions of light and intermediate nuclei reveals a variety of time-dependent modes involving nuclear cluster structures. For instance, the 16O + 16O collision results in a vibrational mode of a quasi-molecular 4He - 12C - 12C - 4He state. For heavier ions, a variety of cluster configurations are predicted.
We conclude that the nucleonic localization is also an excellent measure of clustering in time-dependent simulations and gives important insights into the reaction mechanism. It reveals the presence of collective vibrations involving cluster structures, which dominate the initial dynamics of the fusing system.

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