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We investigate the presence of spatial localization in nuclei using a method that maps the nucleon same-spin pair probability and is based on the density-matrix. The method is used to study spatial localization of light nuclei within the Hartree-Fock approximation. We show that the method provides an alternative tool for studying spatial localization in comparison to the localization observed from maxima in the nuclear mass density.

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I. INTRODUCTION

Clustering phenomena in light nuclei have always been an intriguing aspect of nuclear structure physics. Theoretical understanding of why and how conglomeration of nucleons to subunits within a nucleus results in an increase in stability remains an actively investigated question. In particular, alpha clustering in light nuclei has a long history [1–4] and suggests the existence of configurations resembling the formation of *nuclear molecules* [5–7]. It has also been suggested that neutron rich isotopes of some light nuclei may give rise to new types of cluster structures [7, 8]. Most of the theoretical analyses for the cluster structures have been performed with the *a priori* initialization in terms of clusters and effective interactions, which are determined such as to reproduce the binding energies and scattering phase shifts of these configurations. On the other hand, nuclear structure calculations based on the independent-particle approximation or density functionals also manifest cluster-like substructures as marked concentration of density in the visualization of the total nuclear mass density. For example, Hartree-Fock (HF) calculations for light nuclei often show such formations [9], however since the HF single-particle states are generally spread across the whole nucleus they are delocalized, which makes the entanglement of these substructures in terms of the single-particle orbitals very difficult. Furthermore, the identification of cluster and shell structures based only on the mass density may be an oversimplification since it is missing other aspects of the many-body system, for example the kinetic energy density or density gradients, which may help to provide a more detailed understanding of the underlying structure. Finally, with the rising popularity of the density functional approach in nuclear physics it may be desirable to have a new localization measure that stems directly from the nuclear density-matrix, since all of the information is contained in this quantity.

II. THE LOCALIZATION MEASURE

A. Outline of formalism

An alternative measure of localization had been developed in the context of a mean-field description for electronic systems [10]. A fermionic mean-field state is fully characterized by the one-body density-matrix

$$\rho_{q\sigma\sigma'}(\mathbf{r},\mathbf{r}') = \sum_{\alpha\in q} \phi_\alpha(\mathbf{r}\sigma)\phi^*_\alpha(\mathbf{r}'\sigma') \; . \tag{1}$$

The probability of finding two nucleons with the same spin at spatial locations $\mathbf{r}$ and $\mathbf{r}'$ (same-spin pair probability) for isospin q is given by

$$P_{q\sigma}(\mathbf{r},\mathbf{r}') = \rho_{q\sigma}(\mathbf{r})\rho_{q\sigma}(\mathbf{r}') - \left|\rho_{q\sigma\sigma}(\mathbf{r},\mathbf{r}')\right|^2 \; , \tag{2}$$

where $\rho_{q\sigma}(\mathbf{r}) = \rho_{q\sigma\sigma}(\mathbf{r},\mathbf{r})$ is the local density. The conditional probability for finding a nucleon at $\mathbf{r}'$ when we know with certainty that another nucleon with the same spin and isospin is at $\mathbf{r}$ is

$$R_{q\sigma}(\mathbf{r},\mathbf{r}') = \rho_{q\sigma}(\mathbf{r}') - \frac{\left|\rho_{q\sigma\sigma}(\mathbf{r},\mathbf{r}')\right|^2}{\rho_{q\sigma}(\mathbf{r})} \; . \tag{3}$$

Since we are interested in the localization aspects of this probability it is sufficient to consider only the local short-range behavior of the conditional probability, which one can obtain by performing a spherical averaging over a shell of radius δ about the point $\mathbf{r}$ and then Taylor expanding the resulting expression to get [10]

$$R_{q\sigma}(\mathbf{r},\delta) \approx \frac{1}{3}\left(\tau_{q\sigma} - \frac{1}{4}\frac{[\nabla\rho_{q\sigma}]^2}{\rho_{q\sigma}} - \frac{\mathbf{j}^2_{q\sigma}}{\rho_{q\sigma}}\right)\delta^2 + \mathcal{O}(\delta^3) \; , \tag{4}$$

where $\tau_{q\sigma}$ and $\mathbf{j}_{q\sigma}$ are the kinetic energy density and current density given by

$$\tau_{q\sigma}(\mathbf{r}) = \sum_{\alpha\in q} \left|\nabla\phi_\alpha(\mathbf{r}\sigma)\right|^2$$

$$\mathbf{j}_{q\sigma}(\mathbf{r}) = \sum_{\alpha\in q} \mathrm{Im}\left[\phi^*_\alpha(\mathbf{r}\sigma)\nabla\phi_\alpha(\mathbf{r}\sigma)\right]$$

$$\nabla\rho_{q\sigma}(\mathbf{r}) = 2\sum_{\alpha\in q} \mathrm{Re}\left[\phi^*_\alpha(\mathbf{r}\sigma)\nabla\phi_\alpha(\mathbf{r}\sigma)\right] \; .$$

The reason for writing $\nabla\rho_{q\sigma}$ explicitly is to emphasize that to have a smooth behavior of the quantities calculated below it is essential to calculate all quantities directly from the wavefunctions. The expression shown in Eq. (4) suggests the definition of a localization measure

$$D_{q\sigma}(\mathbf{r}) = \left(\tau_{q\sigma} - \frac{1}{4}\frac{[\nabla\rho_{q\sigma}]^2}{\rho_{q\sigma}} - \frac{\mathbf{j}_{q\sigma}^2}{\rho_{q\sigma}}\right) , \qquad (5)$$

which is also valid for time-dependent Slater determinants [11]. It is important to remember that $D_{q\sigma}$ is the short-range limit of the conditional like-spin *pair* probability and may contain correlations that are not evident in simple one-body observables, such as the mass density. The localization measure defined by Eq. (5) is a reverse relation, e.g. the larger the probability of finding two like-spin particles in vicinity of each other the smaller the value of D. For this reason it is customary to define a reversed and normalized localization measure

$$\mathcal{C}_{q\sigma}(\mathbf{r}) = \left[1 + \left(\frac{\tau_{q\sigma}\rho_{q\sigma} - \frac{1}{4}[\nabla\rho_{q\sigma}]^2 - \mathbf{j}_{q\sigma}^2}{\rho_{q\sigma}\tau_{q\sigma}^{\mathrm{TF}}}\right)^2\right]^{-1} \qquad (6)$$

$$\tau_{q\sigma}^{\mathrm{TF}} = \frac{3}{5}\left(6\pi^2\right)^{2/3}\rho_{q\sigma}^{5/3} ,$$

where $\tau_{q\sigma}^{\mathrm{TF}}$ is the Thomas-Fermi kinetic energy density. The latter is used to provide a natural scale which then allows to define a dimensionless measure. The current density vanishes in the static case which we will consider in the following.

B. Limiting cases and interpretation

This criterion (6) is known in electronic systems as electron localization function (ELF) and it is used as one ingredient to analyze the bond structure of molecules in the static [10] and dynamic domain [11]. The information content of the localization function is understood from considering limiting cases.

The extreme case of ideal metallic bonding is realized for homogeneous matter where $\tau = \tau_{q\sigma}^{\mathrm{TF}}$. This yields $\mathcal{C} = \frac{1}{2}$, a value which thus signals a region with a nearly homogeneous Fermi gas as it is typical for metal electrons, nuclear matter, or neutron stars. The opposite regime are space regions where exactly one single-particle wavefunction of type $q\sigma$ contributes. This is called *localization* in molecular physics. Such a situation yields $D_{q\sigma}(\mathbf{r}) = 0$, since it is not possible to find another like-spin state in the vicinity, and consequently $\mathcal{C} = 1$, the value which signals *localization*. It should be noted that the localization function is invariant under unitary transformations amongst the single-particle wavefunctions in a Slater state [12]. In the nuclear case, it is the α particle which is perfectly localized in this sense, i.e. which has $\mathcal{C} = 1$ everywhere for all states. Well bound nuclei show usually metallic bonding and predominantly have $\mathcal{C} = \frac{1}{2}$. Light nuclei are often expected to contain pronounced α-particle sub-structures. Such a sub-structure means that in a certain region of space only an α particle is found which in turn is signaled by $\mathcal{C} = 1$ in this region. In fact, an α sub-structure is a correlation of four particles: $p\uparrow$, $p\downarrow$, $n\uparrow$, and $n\downarrow$. Thus it is signaled only if we find simultaneously for all four corresponding localization functions $\mathcal{C}_{q\sigma} \approx 1$. In the following, we will consider mainly $N = Z$ nuclei for which the four different particles have very similar wavefunctions. In this case, it suffices to consider, pars pro toto, only one localization function. Furthermore, it should be noted that a full identification of α-cluster sub-structures requires also to check the correlations between the four nucleons gathering in a "localized" region of the nucleus. The localization function is just the first step to identify those regions, namely the minimum necessary condition.

III. RESULTS AND DISCUSSION

In our calculations, the static HF equations are solved on a Cartesian three-dimensional mesh without any symmetry assumptions. The grid spacing was 1 fm with a box size of $(-15.5, +15.5)$ fm in each dimension. The Skyrme energy functional was employed with the parametrization SkI3 [13]. The spatial derivatives are calculated using the fast Fourier transform and periodic boundary conditions are employed, except for the Coulomb potential, which is calculated with boundary conditions at infinity as described in Ref. [14].

A. Ground states of $N = Z$ nuclei

Fig. 1 shows an x-z-cut of the localization function (6) for even-even $N = Z$ nuclei from $A = 4$ to $A = 20$. The left panel shows the proton localization criterion $\mathcal{C}_{p\uparrow}$ complemented in the right panel by the corresponding total density. As mentioned above, the states are spin symmetric which yields identical localization plots for spin-up and spin-down. Moreover, for light $N = Z$ nuclei proton and neutron localizations are very similar due to the small Coulomb interaction. (For neutron rich isotopes this is no longer true as we will show below.) The color (gray scale) coding is shown on top of each column and remains the same throughout the column. The position of the density contour at half nuclear matter density ($\rho = 0.08$ fm^{-3}) is indicated with color cyan in the maps of proton localization. One should keep in mind that the maxima and minima of the total nuclear density need not be correlated with that of the localization function, which is a topological quantity to describe localization (see also Fig. 2 and discussion thereof). The top panel of Fig. 1 shows the calculations for the ^{4}He nucleus. As we have described previously we see a perfect localization with $\mathcal{C} = 1$ in all relevant regions where $\rho > 10^{-4}$ fm^{-3}. Smaller densities lead to erroneous results for $\mathcal{C}$ due to the

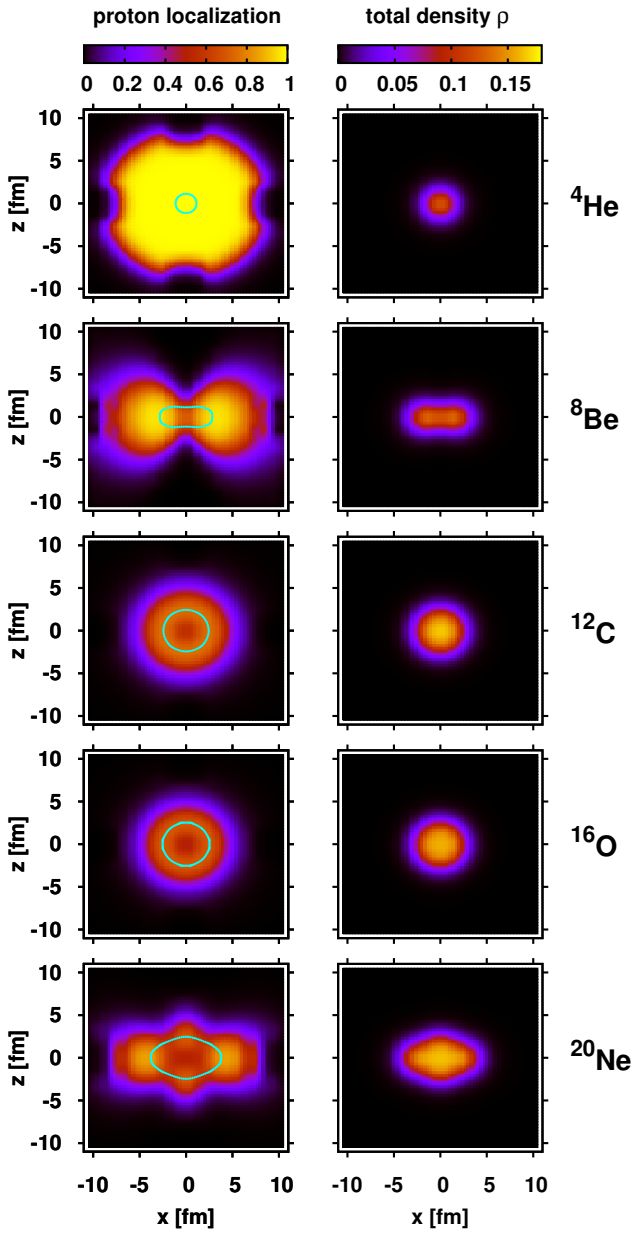

FIG. 1. (Color online) Color map (gray scale) plots of proton localization (left column) and total density in fm^{-3} (right column), for the $Z = N$ nuclei up to ^{20}Ne. The position of the density contour at half nuclear matter density ($\rho = 0.08$ fm^{-3}) is indicated with color cyan (light gray) in the maps of proton localization.

very subtle cancellations required. The strongly prolate ^{8}Be shows very distinct localization pattern with perfect localization in the left and right halves of the contour plane and much smaller localization in the contact region where the wavefunctions overlap. As can be seen this is much more pronounced in comparison to the total mass density plot. Here, it is probably reasonable to conclude that ^{8}Be can be considered as an α-α molecule.

With this version of the Skyrme force the ground state of ^{12}C is oblate deformed as shown in the right pane of Fig. 1. One may be tempted to consider this as a planar arrangement of three α particles. A slight indication of that may be spotted in the localization plot. But it is not well developed, the configuration is too compact, and shows preferably metallic binding as we can see from the localization (left column) which stays safely in a regime $\mathcal{C} \approx 1/2$. The strongly bound ^{16}O nucleus mostly shows

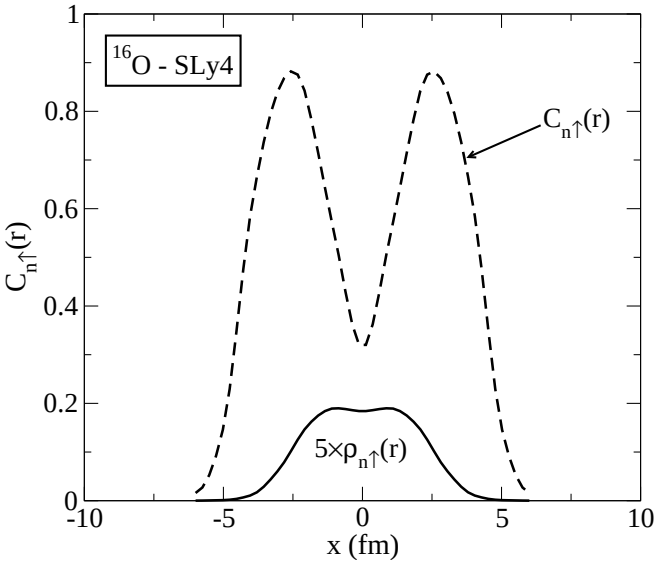

FIG. 2. (Color online) Density profile and localization function for the ^{16}O nucleus.

a localization value of $\mathcal{C} = \frac{1}{2}$ throughout as one would have expected. Its density is known to have a dip at the center [15]. This cannot be discriminated in the density plot here but can be observed as a region of lower localization in the localization map plot. To examine this further we have repeated the same calculation for ^{16}O using the SLy4 interaction [16]. In Fig. 2 we show a cut through the profile of the density and similarly through the localization function. We observe that the central dip in the total density is barely visible. The localization function, however, shows a very pronounced dip indicating a strong and irreducible overlap of all wavefunctions in this center region. Note, furthermore, that the maxima of mass density and localization do not coincide. The localization has a preference towards the surface where the lower density enhances the chance of finding one prevailing wavefunction.

Finally, the last panel of Fig. 1 shows results for the strongly prolate ^{20}Ne nucleus. The localization map shows two regions of high localization at the outer ends and a ring of somewhat enhanced localization at the center around the elongation axis. One can interpret this as a quasi-molecular α-^{12}C-α configuration. The α substructures on both sides are almost as well developed as in ^{8}Be. We have also computed the further series of $N = Z$ nuclei, ^{24}Mg, ^{28}Si, ^{32}S, ^{36}Ar, and ^{40}Ca. These nuclei

are increasingly compact and all show basically metallic binding similar to ^{12}C and ^{16}O shown here.

B. Strongly deformed configurations of light $N = Z$ nuclei

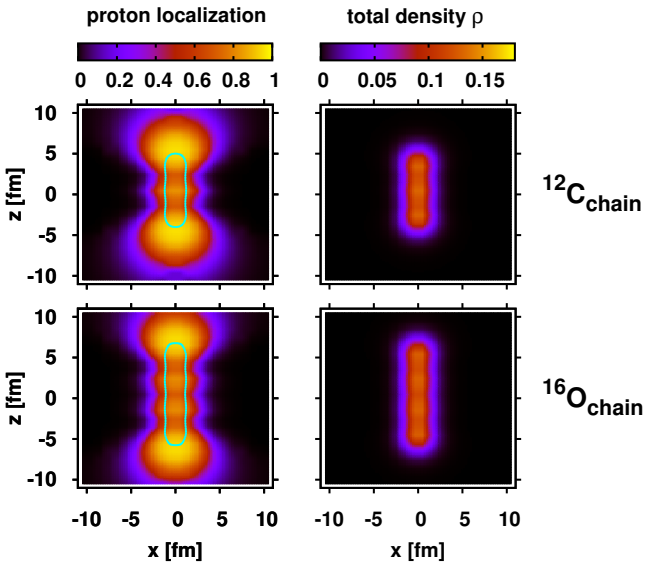

FIG. 3. (Color online) As figure 1, but for chain-like isomers of ^{12}C and ^{16}O.

Very light $N = Z$ nuclei are likely to display isomeric, or at least transiently stable, configurations which are very elongated and resemble chains of *alpha* particles [20]. For somewhat heavier $N = Z$ one finds often shape coexistence with strongly prolate deformed nuclear configurations [21]. Such less bound and spatially more extended configurations are more likely to allow for α sub-structures. We thus have also considered such isomeric configurations for a number of light $N = Z$ nuclei. These configurations were found numerically by starting the static iteration from a sufficiently prolate configuration such that the iteration converged to the elongated isomeric state. Chain configurations were found immediately for ^{12}C and ^{16}O while the heavier systems preferred to maintain a compact core between the α satellites. It is to be noted that these configurations are stable minima in a mean field calculation. They may hybridize with the ground state in correlated calculations. Still such configurations may show up as transient configurations in nuclear reactions [20].

Fig. 3 shows the total density and localization plots for the linear-chain states of ^{12}C and ^{16}O nuclei. For both the density suggests an α-chain structure which is, indeed, corroborated by the localization that also shows three or four clearly separated maxima, $\mathcal{C} \approx 1$. The region of high localization is very large at both ends, but much smaller for the maxima in the interior due to larger wavefunction overlap. One interesting point about the ^{12}C linear-chain configuration localization plot is that in studying the dynamical formation of this chain state, as it was done in Ref. [17], we have observed that the dynamical vibrations of the mass density resembled the localization plot with only the equilibrium shape having the triple-α structure. This is consistent with the kinetic interpretation of the localization function, suggesting that kinetic energies of the same-spin pairs peak mostly around the ends of the linear-chain.

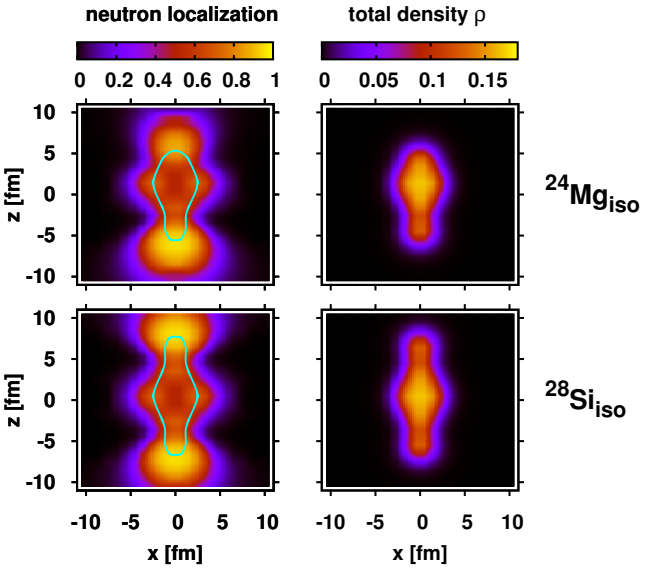

FIG. 4. (Color online) As figure 1, but for stretched isomers of ^{24}Mg and ^{28}Si.

Fig. 4 shows strongly prolate (not yet chain-like isomers which lie higher in energy) isomers of ^{24}Mg and ^{28}Si. Unlike the compact ground-state configurations these isomers indicate interesting molecular substructures. One may interpret ^{24}Mg as a α-^{12}C-α-α molecule and ^{28}Si as α-α-^{12}C-α-α. Again, the outermost α's are best developed with large regions of high localization. The inner α's have already degraded localization due to neighboring wavefunctions from both sides.

C. An example for $N > Z$: The ^{20}C chain

Recently, much interest has been devoted to the study of cluster configurations for neutron-rich isotopes of light nuclei [5, 6, 18]. In particular the linear-chain configurations of C isotopes and their stability against bending modes has been of interest. For nuclei with $N > Z$ where proton and neutron wavefunctions are naturally different the search for α sub-structure requires a simultaneous analysis of proton and neutron localization. To that end we consider also as α localization the combination $\sqrt{\mathcal{C}_{p\uparrow}\mathcal{C}_{n\uparrow}}$. The spin-up and spin-down wavefunctions are still degenerate such that it suffices to consider one of the

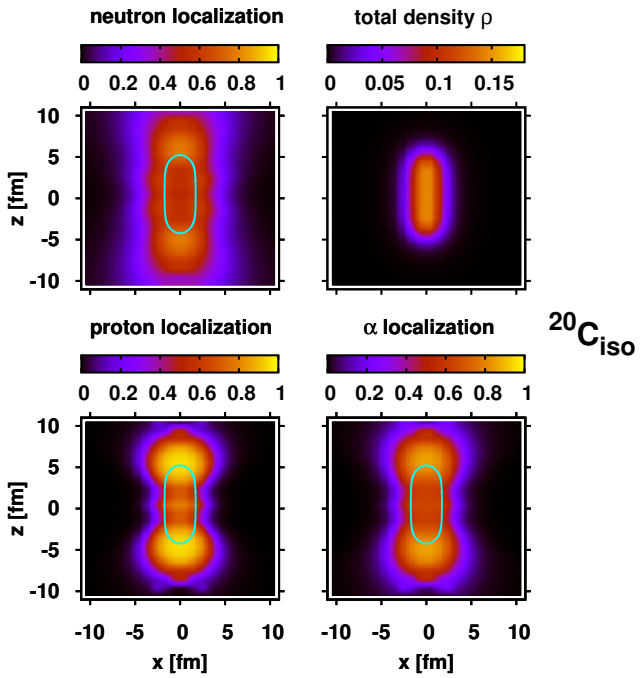

FIG. 5. Color map plots of localizations and density for the linear-chain configuration of ^{20}C. Lower left: proton localization. Upper left: neutron localization. Lower right: α localization ($\equiv \sqrt{\mathcal{C}_{p\uparrow}\mathcal{C}_{n\uparrow}}$). Upper right: total density (in fm^{-3}). The position of the density contour at half nuclear matter density ($\rho = 0.08$ fm^{-3}) is indicated with color cyan (light gray) in the maps of localization.

spins. In Fig. 5 we show proton, neutron, and α localization plots for the linear-chain isomer of the ^{20}C nucleus. As expected, due to the neutron excess of ^{20}C the localization plots for neutrons and protons look considerably different. The protons show more distinct regions with high localization value in comparison to the neutron case, where the wavefunctions have more overlap due to the large number of neutrons. The α localization is the obvious average of the two left panels. In spite of the neutron cloud from the excess neutrons, there appears still some faint α sub-structure at the edges of the chain. It is also interesting to observe that the total mass density does not show any pronounced features due to the smoothing effect of the surplus neutrons while the localization plots still reveal noteworthy structures.

IV. CONCLUSION

In summary, we have applied a localization measure which was developed originally for analyzing bonding structures in molecules to a study of *alpha* sub-structures in light nuclei. The localization function is obtained directly from the density-matrix, in the mean-field approximation. It depends on kinetic-energy density and current density, in addition to the mass density. It can be easily implemented for density functional theory calculations of nuclear structure. One of the fundamental reasons why the new localization measure is such an excellent predictor of correlation and localization is due to the fact that it incorporates the kinetic energy of the relative motion of spin-parallel nucleons at a particular point in space in addition to the mass density for the system [19]. In most cases this localization function shows more detailed localization or clustering features in comparison to the total mass density. Results for $N = Z$ nuclei up to ^{40}Ca show that pronounced localization, associated with α-particle substructures, appear only for the strongly prolate ground states of ^{8}Be, ^{20}Ne, and of course trivially for ^{4}He. All other nuclei are more compact and show metallic binding. However, stretched isomers of light nuclei often show convincing α structures, particularly well developed for the α chains of ^{12}C and ^{16}O, but also for the prolate ^{24}Mg and ^{28}Si isomers. In the future we also plan to study the new localization function in time-dependent HF calculations of systems related to nuclear molecular configurations.

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