Localization in light nuclei

P.-G. Reinhard,1 J. A. Maruhn,2 A. S. Umar,3 and V. E. Oberacker3

1Institut für Theoretische Physik, Universität Erlangen, D-91054 Erlangen, Germany
2Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt am Main, Germany
3Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235, USA

(Dated: February 28, 2011)

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.

PACS numbers: 21.60.-n,21.60.Jz,21.30.Fe,21.60.Cs,27.20.+n,27.30.+t

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, 6]. 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.
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

$$D_{q\sigma}(\mathbf{r}) = \left( \pi_{q\sigma} - \frac{1}{2} \left[ \nabla \rho_{q\sigma} \right]^{2} - \int_{\mathbb{R}^{3}} \rho_{q\sigma} \right) ,$$

which is also valid for time-dependent Slater determinants [11]. It is important to remember that $\pi_{q\sigma}$ is the short-range limit of the conditional like-spin partner 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. (4) is a reverse of the Thomas-Fermi kinetic energy 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 is calculated with boundary conditions at infinity as described in Ref. [14].

### 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 for even-even $N = Z$ nuclei from $A = 4$ to $A = 20$. The left panel shows the proton localization criterion $C_{p\uparrow}$ 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 $C = 1$ in all relevant regions where $\rho > 10^{-4}$ fm$^{-3}$. Smaller densities lead to erroneous results for $C$ 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.

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 $\alpha$ 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 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. 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. 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 $\alpha$-$^{12}$C-$\alpha$ configuration. The $\alpha$ 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 $^{12}\text{C}$ and $^{16}\text{O}$ shown here.

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

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 very elongated and resemble chains of alpha particles [20]. For somewhat heavier $N = Z$ nuclei, 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 $\alpha$ 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 isomeric state. Chain configurations were found immediately for $^{12}\text{C}$ and $^{16}\text{O}$ while the heavier systems preferred to maintain a compact core between the $\alpha$ 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 $^{12}\text{C}$ and $^{16}\text{O}$ nuclei. For both the density suggests an $\alpha$-chain structure which is, indeed, corroborated by the localization that also shows three or four clearly separated maxima, $C \approx 1$. 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 $^{12}\text{C}$ 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-$\alpha$ 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.

![Figure 3](https://example.com/fig3.png)

**FIG. 3:** (Color online) As figure[1] but for chain-like isomers of $^{12}\text{C}$ and $^{16}\text{O}$.

![Figure 4](https://example.com/fig4.png)

**FIG. 4:** (Color online) As figure[1] but for stretched isomers of $^{24}\text{Mg}$ and $^{28}\text{Si}$.

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

C. An example for $N > Z$: The $^{20}\text{C}$ Chain

Recently, much interest has been devoted to the study of cluster configurations for neutron-rich isotopes of light nuclei [1, 6, 15]. 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 $\alpha$ sub-structure requires a simultaneous analysis of proton and neutron localization. To that end we consider also as $\alpha$ localization the combination $\sqrt{\rho \bar{T} C_{\pi\uparrow}}$. The spin-up and spin-down wavefunctions are still degenerate such that it suffices to consider one of the
cloud from the excess neutrons, there appears still some average of the two left panels. In spite of the neutron linear-chain configuration of $^{20}\text{C}$. Lower left: proton localization. Upper left: neutron localization. Lower right: $\alpha$ localization ($\equiv \sqrt{C_{\uparrow\uparrow}C_{\downarrow\downarrow}}$). 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 $\alpha$ localization plots for the linear-chain isomer of the $^{20}\text{C}$ nucleus. As expected, due to the neutron excess of $^{20}\text{C}$ 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 $\alpha$ 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 $\alpha$ 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 [10]. 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 $^{46}\text{Ca}$ show that pronounced localization, associated with $\alpha$-particle substructures, appear only for the strongly prolate ground states of $^{8}\text{Be}$, $^{20}\text{Ne}$, and of course trivially for $^{4}\text{He}$. All other nuclei are more compact and show metallic binding. However, stretched isomers of light nuclei often show convincing $\alpha$ structures, particularly well developed for the $\alpha$ chains of $^{12}\text{C}$ and $^{16}\text{O}$, but also for the prolate $^{24}\text{Mg}$ and $^{28}\text{Si}$ 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.

This work has been supported by the U.S. Department of Energy under grant No. DE-FG02-96ER40963 with Vanderbilt University, and by the German BMBF under contract Nos. 06FY9086 and 06ER142D.

[1] L. R. Hafstad and E. Teller, Phys. Rev. 54, 681 (1938).
[2] H. Morinaga, Phys. Rev. 101, 254 (1956).
[3] K. Ikeda, N. Tagikawa, and H. Horiuchi, Prog. Theo. Phys. Suppl., extra number, 464 (1968).
[4] D. M. Brink and A. Weiguny, Nucl. Phys. A 120, 59 (1968).
[5] N. Itagaki and S. Okabe, K. Ikeda, and I. Tanihata, Phys. Rev. C 64, 041301 (2001).
[6] N. Itagaki, W. von Oertzen, and S. Okabe, Phys. Rev. C 74, 067304 (2006).
[7] W. von Oertzen, Martin Freer, and Yoshiko Kanada-En’yo, Phys. Rep. 432, 43 (2006).
[8] M. Ito, N. Itagaki, H. Sakurai and K. Ikeda, Phys. Rev. Lett. 100, 182502 (2008).
[9] J. A. Maruhn, N. Loebl, N. Itagaki and M. Kimura, Nucl. Phys. A 833, 1 (2010).
[10] A. D. Becke and K. E. Edgecombe, J. Chem. Phys. 92, 5397 (1990).
[11] T. Burnus, M. A. L. Marques, and E. K. U. Gross, Phys. Rev. A 71, 010501(R) (2005).
[12] Andreas Savin, Journal of Molecular Structure: THEOCHEM, 727, 127 (2005).
[13] P.-G. Reinhard and H. Flocard, Nucl. Phys. A584, 467 (1995).
[14] J. W. Eastwood and D. R. K. Brownrigg, J. Comp. Phys. 32, 24 (1979).
[15] J. Friedrich and N. Vögler, Nucl. Phys. A 373, 192 (1982).
[16] E. Chabanat, P. Bonche, P. Haensel, J. Meyer and R. Schaeffer, Nucl. Phys. A635, 231 (1998); A643, 441(E) (1998).
[17] A. S. Umar, J. A. Maruhn, N. Itagaki, and V. E. Oberacker, Phys. Rev. Lett. 104, 212503 (2010).
[18] J. A. Maruhn, N. Loebl, A. S. Umar, N. Itagaki, M. Kimura, H. Horiuchi, and A. Tohsaki, Mod. Phys. Lett. A 25, 1866 (2010).
[19] J.F. Dobson, J. Chem. Phys. 94, 4328 (1991).
[20] P.E. Hodgson, Z. Phys. A 349, 197 (1994).
[21] P.–G. Reinhard, D.J. Dean, W. Nazarewicz, J. Dobaczewski, J.A. Maruhn, and M.R. Strayer, Phys. Rev. C 60, 14316 (1999).