Nucleon localization function in rotating nuclei

T. Li (李通) 1,2, M. Z. Chen (陈孟之) 1,2, C. L. Zhang (张春莉) 1,2, W. Nazarewicz 2,3 and M. Kortelainen 4,5

1 National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824, USA
2 Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA
3 Facility for Rare Isotope Beams, Michigan State University, East Lansing, Michigan 48824, USA
4 Department of Physics, PO Box 35 (YFL), FI-40014 University of Jyväskylä, Finland
5 Helsinki Institute of Physics, P.O. Box 64, FI-00014 University of Helsinki, Finland

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Background: An electron localization function was originally introduced to visualize in positional space bond structures in molecules. It became a useful tool to describe electron configurations in atoms, molecules, and solids. In nuclear physics, a nucleon localization function (NLF) has been used to characterize cluster structures in light nuclei, formation of fragments in fission, and pasta phases appearing in the inner crust of neutron stars.

Purpose: We use the NLF to study the nuclear response to fast rotation.

Methods: We generalize the NLF to the case of nuclear rotation. The extended expressions involve both time-even and time-odd local particle and spin densities and currents. Since the current density and density gradient contribute to the NLF primarily at the surface, we propose a simpler spatial measure given by the kinetic-energy density. Illustrative calculations for the superdeformed yrast band of 152Dy were carried out by using the cranked Skyrme-Hartree-Fock method. We also employed the cranked harmonic-oscillator model to gain insights into spatial patterns revealed by the NLF at high angular momentum.

Results: In the case of a deformed rotating nucleus, several NLFs can be introduced, depending on the definition of the spin-quantization axis, direction of the total angular momentum, and self-consistent symmetries of the system. Contributions to the NLF from the current density, spin-current tensor density, and density gradient terms are negligible in the nuclear interior. The oscillating pattern of the simplified NLF can be explained in terms of a constructive interference between kinetic-energy and particle densities. The characteristic nodal pattern seen in the NLF in the direction of major axis of a rotating nucleus comes from single-particle orbits carrying large aligned angular momentum. The variation of the NLF along the minor axis of the nucleus can be traced back to deformation-aligned orbits.

Conclusions: The NLF allows a simple interpretation of the shell structure evolution in the rotating nucleus in terms of the angular-momentum alignment of individual nucleons. We expect that the NLF will be very useful for the characterization and visualization of other collective modes in nuclei and time-dependent processes.

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1. INTRODUCTION

Nuclear collective motion, such as rotations and vibrations, provides rich information about nuclear structure and nuclear response to external fields. When discussing nuclear collective motion, one is often making analogies to molecules and their collective modes. One has to bear in mind, however, that the A-body nuclear wave function cannot, in general, be expressed in terms of slow and fast components because the time separation between single-particle (s.p.) and collective nuclear motion is poor. Consequently, deviations from the perfect rotational and vibrational patterns are abundant. Such deviations indicate that the nuclear collective modes result from coherent superpositions of individual nucleonic excitations.

The observation of rotational bands in atomic nuclei has provided us with many insights into nuclear deformations and the underlying shell structure [1–4]. Theoretically, high-spin states can be described in a fully self-consistent way by the nuclear energy density functional (EDF) method [5], which is closely related to density-functional theory [6,7]. Although rotation is essentially a time-dependent problem, the introduction of a rotating intrinsic frame through the cranking approximation transforms the time-dependent problem into a time-independent one [8]. The cranking term added to the nuclear Hamiltonian can be interpreted as a constraint on the angular momentum, with the rotational frequency playing the role of the Lagrange multiplier.

The spatial electron localization function (ELF) was originally introduced in the context of electronic Hartree-Fock (HF) studies to characterize shell structure in atoms and chemical bonds in molecules [9–14]. In nuclear structure research, the nucleon localization function (NLF) turned out to be a useful tool for the identification of clusters in light nuclei [15–17] and nuclear reactions [18]; formation of fragments in fission [19–23]; and nuclear pasta phases in the inner crust of neutron stars [16]. Compared with nucleonic distributions
that are fairly constant in the nuclear interior, the NLF more effectively quantifies nuclear configurations through its characteristic oscillating pattern due to shell effects. Consequently, it is expected to be a good indicator of the competition between s.p. motion and collective nuclear modes.

In this work, we use the NLF to study the nuclear response to rotation. We consider the case of superdeformed (SD) $^{152}$Dy, a quintessential nuclear rotor that has been investigated in a number of self-consistent works [24–26].

This paper is organized as follows: Our theoretical framework is described in Sec. II, which contains a comprehensive discussion of the NFL and its extension to the case of rotation. Section III contains the results of HF calculations for $^{152}$Dy that are supplemented by cranked harmonic-oscillator model results that illuminate essential points. Finally, Sec. IV presents conclusions and perspectives for future studies.

II. THEORETICAL FRAMEWORK

A. Density matrices

The starting point in the derivation of the spatial localization function is the one-body HF density matrix in the coordinate representation:

$$\rho(q', q', s) = \langle \Psi | a_{r'q'}^\dagger a_{rq}|\Psi \rangle,$$

where $a_{r'q'}$ and $a_{rq}$ create and annihilate, respectively, a nucleon $(q = n$ or $p)$ at point $r$ with spin $s = \pm \frac{1}{2}$, and $|\Psi\rangle$ is the HF independent-particle state. In what follows, we consider pure proton and neutron HF states, i.e., $q' = q$, and we define $\rho_p(q, r', s') = \rho(r q, r' s')$.

Expressed in terms of spin components, the nonlocal HF density matrices can be written as [5,27,28]

$$\rho_p(q, r', s') = \frac{1}{2}\left[\rho_p(q, r')\delta_{ss'} + (s|\sigma|^s')s_q(r, r')\right],$$

where

$$\rho_p(q, r') = \sum_s \rho_p(q, r', s),$$

$$s_q(r, r') = \sum_{ss'} \rho_p(q, r', s') (s' | \sigma | s).$$

In the EDF method with the zero-range Skyrme interaction, the energy functional depends only on local densities and currents. Following the standard definitions [5,27], in the present study we employ the following densities:

$$\rho_p(q, r),$$

$$s_q(r),$$

$$\tau_p(q) = [\nabla \cdot \nabla']\rho_p(q, r'),$$

$$j^q_p(r) = \frac{1}{2}\nabla_{q'}\rho_p(q, r'),$$

$$j_{q_p}(r) = \frac{1}{2}[(\nabla - \nabla')\otimes s_q(r, r')]_{r'},$$

$$T_q(r) = [(\nabla - \nabla')s_q(r, r')]_{r'},$$

where $\otimes$ stands for the tensor product of vectors in the physical space.

B. Nucleon localization function

Let us first consider the probability of finding two nucleons of a given isospin $q$ and spin $s$ at spatial locations $r$ and $r'$:

$$P_{qs}(r, r') = \langle \Psi | a_{rq}^\dagger a_{r'q} a_{r'q} a_{rq} | \Psi \rangle.$$  (5)

For the HF product state $|\Psi\rangle$ this probability can be written as

$$P_{qs}(r, r') = \rho_p(q, r) \rho_p(q, r') - |\rho_p(q, r')|^2.$$  (6)

Because of the Pauli exclusion principle, $P_{qs}(r, r) = 0$. If a nucleon with spin $s$ and isospin $q$ is located with certainty at position $r$, the conditional probability of finding a second nucleon with the same spin and isospin at position $r'$ is

$$R_{qs}(q, r') = \frac{P_{qs}(r, r')}{\rho_p(q, r)}.$$  (7)

To study the local (short-range) behavior of $R_{qs}$, one assumes that the second nucleon is located within a shell of small radius $\delta$ around $r$. The corresponding conditional probability (7) can be written as

$$R_{qs}(r, r + \delta) = e^{\delta \nabla^2} R_{qs}(r, r')_{r' = r}.$$  (8)

After performing an angular averaging over the $\delta$ shell and carrying out a Taylor expansion in $\delta$, one obtains

$$e^{\delta \nabla^2} = 1 + \frac{1}{3!} \delta^2 \nabla^2 \delta^4 \nabla^4 \cdots.$$  (9)

The resulting local probability becomes

$$R_{qs}(r, \delta) = \frac{1}{6} \delta^2 \nabla^2 R_{qs}(r, r')_{r' = r} + O(\delta^4).$$  (10)

By introducing a localization measure $D_{qs}(r)$ through the relationship

$$R_{qs}(r, \delta) = \frac{1}{2} D_{qs}(r) \delta^2 + O(\delta^4),$$  (11)

one can capture the short-range limit of the conditional like-spin pair probability.

For a rotationally invariant and spin-unpolarized system, $D_{qs}(r)$ is independent of the choice of the spin-quantization axis. However, for the deformed and rotating nuclei considered in this study, one has to consider three different measures $D_{qs}^\mu(r)$ with $\mu = x, y, z$.

If one chooses $\mu$-axis as the spin-quantization axis, one can define three spin-dependent local densities:

$$\rho_{qs}^\mu(r) = \frac{1}{2} \rho_p(q, r) + \frac{1}{2} \sigma_\mu s_q(r),$$  (12a)

$$\tau_{qs}^\mu(r) = \frac{1}{2} \tau_p(q, r) + \frac{1}{2} \sigma_\mu T_{qs}(r),$$  (12b)

$$j_{qs}^\mu(r) = \frac{1}{2} j^q_p(r) + \frac{1}{2} \sigma_\mu j_{qs}^\mu(r),$$  (12c)

where $\sigma_\mu = 2 \delta_\mu = \pm 1$ and $e_\mu$ is the unit vector in the direction of the $\mu$ axis. After straightforward algebraic manipulations based on the density-matrix expansion technique [29,30], the measure $D_{qs}^\mu(r)$ can be expressed through the local densities (12)

$$D_{qs}^\mu = \tau_{qs}^\mu - \frac{1}{4} \frac{\nabla \rho_{qs}^\mu}{\rho_{qs}} - \frac{\left| j_{qs}^\mu \right|^2}{\rho_{qs}}.$$  (13)
Following Ref. [9], a dimensionless and normalized NLF can now be defined as

$$ C_{qs}(r) = \left[ 1 + \left( \frac{D_{qs}(r)}{\tau_{qs}(r)} \right) \right]^{-1}, \quad (14) $$

where the normalization $\tau_{qs}(r) = \frac{3}{2} (6\pi^2)^{2/3} \rho_0^{1/3}(r)$ is the Thomas-Fermi kinetic-energy density.

It should be noted that the densities (12) constituting the NLF contain both time-even and time-odd components. Indeed, the particle density $\rho_0(r)$, kinetic-energy density $\tau_p(r)$, and spin-current tensor density $\mathcal{J}_{qs}(r)$ are all time-even, while the spin vector density $s_{qs}(r)$, spin-kinetic vector density $T_{qs}(r)$, and current vector density $j_{qs}(r)$ are time-odd. If time-reversal symmetry is conserved, $s_{qs}(r) = 0$, $T_{qs}(r) = 0$, and $j_{qs}(r) = 0$. Consequently, for a system that conserves time-reversal symmetry and is governed by spin-independent interactions, one obtains

$$ D_{qs} = D_q = \frac{1}{2} \tau_q - \frac{1}{8} \left[ \nabla \rho_q \right]^2 || \rho_q $$

which is the familiar atomic physics expression [9].

In general, the tensor density $\mathcal{J}_{qs}(r)$ does not vanish even if the time-reversal symmetry is conserved [31]. It can be decomposed into trace, antisymmetric, and symmetric parts [28]. In many practical applications, the spin-current tensor is approximated by its antisymmetric (spin-orbit current) part [32]. However, all components of $\mathcal{J}_{qs}$ are important to characterize nuclear spin-orbit and tensor interactions [33–36] and the resulting spin polarization, which is sensitive to spin saturation of nucleonic shells. Consequently, the current $j_{qs}(r)$ does not vanish even in ground-state configurations of even-even nuclei. While its contribution to the NLF was ignored in even nuclei, it does not vanish even in ground-state configurations of even-even nuclei. Therefore, $D_{qs}$ can be interpreted as a measure of the excess of kinetic-energy density due to the Pauli exclusion principle:

$$ D_{qs} = \tau_{qs} - \tau_{qs,p} $$

This interpretation of the NLF is more flexible as it does not involve the notion of the conditional probability (7), which is not straightforwardly generalized to the case of point-group symmetries of the nuclear mean field.

### C. Cranked Hartree-Fock calculations

Superdeformed nuclei around $^{152}$Dy can be viewed as unique laboratories of extreme single-particle behavior [25,38]. The nucleus $^{152}$Dy plays a role of superdeformed double-magic core due to large shell closures at $Z = 66$ and $N = 86$. Because of this, $^{152}$Dy has been a subject of many studies of self-consistent nuclear response to collective rotation; see, e.g., Refs. [24,26,39,40]. Because of large deformed gaps and rapid rotation, pairing correlations are weak in SD $^{152}$Dy [41,42]. Indeed, with a reasonable pairing strength, adjusted to experimental odd-even mass difference in $^{128}$Sn, as done in Ref. [43], the static pairing vanishes in the SD yrast band of $^{152}$Dy in Hartree-Fock-Bogoliubov (HFB) calculations.

The intrinsic configurations of SD bands in the $A = 150$ mass region are well characterized by nucleons in the intruder orbitals carrying large principal harmonic-oscillator (HO) numbers $N$, namely, the proton $N = 6$ and neutron $N = 7$ states [44,45]. Because of their large intrinsic angular momenta, these orbitals strongly respond to nuclear rotation; hence, their occupations and alignment patterns well characterize SD bands.

To study the impact of rotation on shell structure through the nucleon localizations, we carry out unpaired cranked HF (CHF) calculations for superdeformed $^{152}$Dy using the HF solver HFODD [46]. Following Ref. [24], s.p. wave functions have been expanded in a stretched deformed HO basis with frequencies $h\omega_0 = 6.246$ MeV and $h\omega_1 = 11.200$ MeV along the directions parallel and perpendicular to the symmetry axis, respectively. The total number of basis states is 1013 with HO numbers $\hat{N} = 7$ states. Because of their large intrinsic angular momenta, these orbitals strongly respond to nuclear rotation; hence, their occupations and alignment patterns well characterize SD bands.

The corresponding s.p. kinetic-energy density is the sum of last two terms in $D_{qs}$ (13):

$$ \tau_{qs,p} = \left| \nabla \psi_{qs} \right|^2 = \frac{1}{4} \left[ \nabla \rho_{qs} \right]^2 + \frac{1}{\rho_{qs}} \left| \mathcal{J}_{qs} \right|^2, \quad (18) $$

where the first term is the von Weizsacker kinetic-energy density [37]. Therefore, $D_{qs}$ can be interpreted as a measure of the excess of kinetic-energy density due to the Pauli exclusion principle:

$$ D_{qs} = \tau_{qs} - \tau_{qs,p} $$

As discussed in Refs. [10,13], the localization function can also be interpreted in terms of the Pauli exclusion principle. Let us consider a situation in which an isolated fermion of given spin $s$ and isospin $q_s$ is located in some region of space. The wave function of this particle can be written as

$$ \psi_{qs}(r) = \sqrt{\rho_{qs}} e^{i\chi(r)}, \quad (16) $$

where $\chi(r)$ is a position-dependent phase factor related to the current density via

$$ j_{qs} = \rho_{qs} \nabla \chi. \quad (17) $$

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The angular momentum has been generated by means of a cranking term $-\hat{J} \omega$, where $\hat{J}$ is the $y$ component of the total angular-momentum operator and $\omega$ represents the angular velocity of rotation. In the presence of the cranking term, parity $\hat{P}$, y signature $\hat{R}_y \exp(-i\hat{J}y)$, and y simplex $\hat{R}_y = \hat{P} \hat{R}_y$ symmetries are preserved while time-reversal and axial symmetries are broken; see Refs. [49–51] for more discussion. Since the time-reversal operator commutes with the signature and simplex operators, the time-reversed s.p. CHF...
states (Routhians) belong to opposite signature and simplex eigenvalues.

Every CHF configuration can be labeled by using the standard notation in terms of parity-signature blocks \([N_{\pi,+},N_{\pi,-},N_{\eta,+},N_{\eta,-}]\), where \(N_{\pi,r}\) are the numbers of occupied s.p. orbitals having parity \(\pi\) and \(y\) signature \(r\). As discussed in Ref. [24], the yrast configuration of SD \(^{152}\text{Dy}\) is \([22,22,21,21]\)\(_n\) \(\otimes\) \([16,16,17,17]\)\(_p\). The relative variation of the quadrupole moment \(Q_{20}\) within this state is much less than 1\% in the frequency range \(\hbar\omega \approx 0.2 - 0.5\text{ MeV}\) [25], so we constrain it at the value \(Q_{20} = 42\) b to eliminate its possible impact on the computed localizations.

Single-particle Routhians obtained in the CHF + SkM* calculations for the SD yrast band of \(^{152}\text{Dy}\) are shown in Fig. 1. The large deformed shell closures at \(Z = 66\) and \(N = 86\) are clearly seen. The lowest \(N = 7\) neutron and \(N = 6\) proton Routhians indicated in the figure are rotation aligned, i.e., they are strongly impacted by the Coriolis coupling and their s.p. aligned angular momenta are large at high rotational frequencies. Many other states around the Fermi level are weakly impacted by rotation. Such states are usually referred to as deformation-aligned (strongly coupled) [1,52,53].

\textbf{D. Cranked harmonic-oscillator calculations}

In the previous study of the NLF, the harmonic-oscillator model was used to provide an illustrative guidance [16]. In this work, we study the NLF patterns of the SD cranked harmonic-oscillator (CHO) model with frequencies \(\omega_1 = \omega_\pi = \omega_y = 2\omega_z\). Since the HO potential is spin-independent, every s.p. HO level is doubly degenerate. As in the CHF calculations, we assume that the rotation takes place around the \(y\) axis. The s.p. Routhians and wave functions of the CHO can be obtained analytically [2,54,55]. We wish to emphasize that our CHO results were obtained without imposing the consistency relation between mean-field ellipsoidal deformation and the average density distribution [1,55].

To relate the CHO analysis to the CHF results for SD \(^{152}\text{Dy}\), we study a SD HO potential filled with 60 particles, which corresponds to a closed SD supershell \(N_{\text{shell}} \equiv 2(n_1 + n_2) + n_3 = 6\) [1,53,56,57]. The corresponding s.p. Routhians are shown in Fig. 2 as functions of \(\omega\). A supershell of a SD HO consists of degenerate positive- and negative-parity states. This degeneracy is lifted by rotation: the orbits with no CHO odd parts, they can be expressed in a form similar to Eq. (12):

\begin{equation}
\rho_q(r) = \rho_{q\eta,=+1}(r) + \rho_{q\eta,=-1}(r),
\end{equation}

where \(\delta_y \equiv r_y / i = \pm 1\). A similar decomposition holds for \(\tau_q(r)\) and \(f_q(r)\).

By decomposing these densities into time-even and time-odd parts, they can be expressed in a form similar to Eq. (12):

\begin{equation}
\rho_{q\eta}(r) = \frac{1}{2} \rho_q(r) + \frac{1}{2} \delta_y s_q(r),
\end{equation}

\begin{equation}
\tau_{q\eta}(r) = \frac{1}{2} \tau_q(r) + \frac{1}{2} \delta_y T_q(r),
\end{equation}

\begin{equation}
f_{q\eta}(r) = \frac{1}{2} f_q(r) + \frac{1}{2} \delta_y J_q(r),
\end{equation}

where

\(s_q(r) = \rho_{q\eta,=+1}(r) - \rho_{q\eta,=-1}(r)\),

\(T_q(r) = \tau_{q\eta,=+1}(r) - \tau_{q\eta,=-1}(r)\),

\(J_q(r) = f_{q\eta,=+1}(r) - f_{q\eta,=-1}(r)\).

The fields \(s'\) and \(T'\) are time-odd and \(J'\) is time-even.
FIG. 2. Single-particle Routhians of the SD CHO model belonging to the supershells $N_{\text{shell}} = 6$ and $7$. The CHO quantum numbers $[n_1, n_2, n_3]$ are given in brackets. Positive-parity and negative-parity states are indicated by solid and dashed lines, respectively. The rotational frequency $\omega$ is expressed in units of $\omega_0 = (\omega_z \omega_\perp)^{1/3}$ while the Routhians $E$ is in units of $\hbar \omega_z$. Each level is doubly degenerate due to the two possible spin orientations. The crossing between the lowest $N = 7$ Routhian $[0,0,7]$ and the $[3,0,0]$ level at $\omega/\omega_0 \approx 0.2$ is marked by the arrow.

III. RESULTS AND DISCUSSION

A. General considerations

In a rotating system, the current density $j$ characterizes the collective rotational behavior [26,58–65]. Figure 3 shows how the current density builds up in the CHO model. As rotational frequency increases, a pattern of the vector field $j$ resembling a rigid-body rotation gradually develops. At $\omega = 0.2\omega_0$, the lowest $N = 7$ Routhian $[0,0,7]$ becomes occupied and the $[3,0,0]$ level becomes empty, see Fig. 2. As the orbital $[0,0,7]$ is strongly prolate-driving and carries large s.p. angular momentum, and the Routhian $[3,0,0]$ has large negative quadrupole moment (oblate), the associated configuration change (band crossing) results in a large increase in the angular-momentum alignment and intrinsic deformation, see Fig. 3. This effect is also present in CHO calculations which consider the potential-density consistency relation [57].

When it comes to the realistic description, Fig. 4 shows the neutron and proton current densities of $^{152}$Dy calculated in the CHF method at four rotational frequencies up to $\hbar \omega = 0.8$ MeV (angular momentum $I_\omega \approx 90\hbar$). The leftmost column in Fig. 4 shows the result of the benchmark quasiparticle random-phase approximation calculation using the finite amplitude method (FAM-QRPA) [66], which corresponds to the $\omega \to 0$ limit. Both FAM-QRPA and full cranking calculations produce flow patterns close to the rigid-body rotation. As irrotational flow originates from pairing correlations [61,66] the result shown in Fig. 4 is consistent with our assumption of no static paring in the SD yrast band of $^{152}$Dy.

In addition to the current $j$, two other time-odd vector densities enter the expression for the NLF: spin density $s$ and spin-kinetic density $T$. They are displayed in Fig. 5 for several values of $\omega$. Both spin fields are polarized along the direction of the total angular momentum (here, $y$ axis). It is interesting to see that the distribution themselves hardly change with rotational frequency; what is changing is the magnitudes $|s|$ and $|T|$ that gradually increase with rotation. This is also seen in the FAM-QRPA calculation that produces flow patterns close to those obtained in the CHF calculations.

FIG. 3. Current density $j$ in the $x$-$z$ ($y = 0$) plane, calculated in the CHO model with 60 particles in a SD HO well for four values of rotational frequency $\omega$ (in units of $\omega_0$). The magnitude $|j|$ (in fm$^{-4}$) is shown by color and line thickness.

FIG. 4. Current density $j$ in the $x$-$z$ ($y = 0$) plane for neutrons (top) and protons (bottom) in the SD yrast band of $^{152}$Dy obtained in the CHF calculations, as a function of $\omega$ (in units of MeV/$\hbar$). The magnitude $|j|$ (in fm$^{-4}$) is shown by color and line thickness. The FAM-QRPA result is presented in the first column with a different color range.
from the density-gradient term

The same argument is also valid for the contribution to the NLF

The first column with a different color range.

by color and line thickness. The FAM-QRPA results are presented in

MeV
obtained in the CHF calculations, as functions of \( \omega \) (in units of MeV/\( \hbar \)). The magnitudes, \(|s|\) (in \( \text{fm}^{-1} \)) and \( |T| \) (in \( \text{fm}^{-3} \)), are shown by color and line thickness. The FAM-QRPA results are presented in the first column with a different color range.

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An irrotational flow exists (see examples in Refs. [61,66]). The

tensor density

\( j \) shown in Fig. 4, \( J \cdot e_y \), changes very weakly with \( \omega \). This field has a surface character, i.e., it practically

vanishes within the nuclear volume. Since \( \tilde{J}_y \cdot e_y \) is time-even, its contribution to \( C_{qs} \) does not vanish at \( \omega = 0 \).

B. Simplified nucleon localization function

An important consequence of the rigid-body flow is that the

current density only contributes significantly to the NLF at the

surface. This observation should be valid in most cases even if an

irrotational flow exists (see examples in Refs. [61,66]). The

same argument is also valid for the contribution to the NLF from the density-gradient term \(|\nabla \rho_s|^2\), which has a surface character. Consequently, we define a simplified localization measure as

\[
C^\tau_{qs} (\mathbf{r}) = \left[ 1 + \left( \frac{\tau_{qs, \mathbf{r}}}{\tau_{TF, qs} (\mathbf{r})} \right)^2 \right]^{-1},
\]

which does not include contributions from the current density and density gradient. Figure 7 shows \( C \), \( C^\tau \), and their difference obtained in the CHO model; we indeed see that \( C^\tau \) exhibits the same pattern as \( C \) inside the nuclear volume. A similar behavior is present in the CHF calculation for the SD yrast band of \(^{152}\text{Dy}\). Figure 8 shows \( C \) and \( C^\tau \) for neutrons with \( \tilde{\sigma}_y = -1 \) (y simplex \( \tau_y = -i \)) at \( \hbar \omega = 0.9 \text{ MeV} \); the two

localization functions differ only in the surface region. At lower frequencies, this difference is even less pronounced.

In previous work [19] the NLF was normalized as \( C_{qs} \rightarrow C_{qs} \rho_{qs} / [\max \rho_{qs}] \) (with \( \sigma \) being either spin, signature, or simplex) to avoid large values in the regions of small particle density. However, as shown in Figs. 7 and 8, replacing \( C \) with \( C^\tau \) mitigates this unwanted behavior and leaves the internal pattern unaffected, thus eliminating the need for this additional normalization. Coming back to the interpretation of \( D_{qs} \) as a measure of the Pauli repulsion, it is not surprising to see that \(|\nabla \rho_s|^2\) and \(|J_{qs}|^2\) are significant only at the surface where only a limited number of s.p. orbits are available and thus become “localized.” Therefore, the simplified localization function \( C^\tau \) is a useful tool to characterize intrinsic configurations in most cases, except perhaps for dynamic pro-

FIG. 5. Spin density \( s \) (top) and spin-kinetic density \( T \) (bottom) in the \( x-y \) (\( z = 0 \)) plane for neutrons in the SD yrast band of \(^{152}\text{Dy}\) obtained in the CHF calculations, as functions of \( \omega \) (in units of MeV/\( \hbar \)). The magnitudes, \(|s|\) (in \( \text{fm}^{-1} \)) and \( |T| \) (in \( \text{fm}^{-3} \)), are shown by color and line thickness. The FAM-QRPA results are presented in the first column with a different color range.

FIG. 6. Spin-current tensor density \( \tilde{J} \cdot e_y \) in the \( x-z \) (\( y = 0 \)) plane for neutrons in the SD yrast band of \(^{152}\text{Dy}\), as a function of \( \omega \) (in units of MeV/\( \hbar \)). Its magnitude (in \( \text{fm}^{-1} \)) is shown by color and line thickness.

FIG. 7. \( C \) (top), \( C^\tau \) (middle), and their difference (bottom) in the \( x-z \) (\( y = 0 \)) plane, calculated in the CHO model with 60 particles in a SD HO well for five values of rotational frequency \( \omega \) (in units of \( \omega_0 \)).

FIG. 8. \( C \) (left), \( C^\tau \) (middle), and their difference (right) in the \( x-z \) (\( y = 0 \)) plane for neutrons with \( \tilde{\sigma}_y = -1 \) (y simplex \( \tau_y = -1 \)), obtained in the CHF calculations for the SD yrast configuration of \(^{152}\text{Dy}\) at \( \hbar \omega = 0.9 \text{ MeV} \).
cesses and high-energy modes where the current density and density gradient can become appreciable inside the nucleus.

C. Dependence of nucleon localizations on the choice of spin-quantization axis

As discussed in Sec. II B, in the general case of deformed nuclei, nucleon localization functions $C_{qs\mu}$ (14) and $C_{qs\mu}^{TF}$ (23) depend on the choice of the spin-quantization direction $\mu$. This directional dependence is illustrated in Figs. 9 and 10 for the SD $^{152}\text{Dy}$ at $\hbar\omega = 0.5$ MeV. It is seen that the NLF slightly depends on the choice of $\mu$, especially in the case of the $y$-$z$ cross section. More importantly, $C_{qs\mu}^{TF} \approx C_{qs\mu}$ in the nuclear interior, independently of $\mu$.

D. Angular-momentum alignment: Cranked harmonic-oscillator analysis

In this section, we use the CHO model to illustrate some general features of NLFs and densities, which will help us understand the CHF results. First, to show the usefulness of $C^r$ when it comes to the visualization of nucleonic shell structure and angular-momentum alignment, we come back to Fig. 7. A characteristic regular pattern seen at $\omega = 0$ gradually gets blurred with $\omega$. At $\omega = 0.2\omega_0$, where the band crossing occurs, $C^r$ rapidly changes. Namely, the number of maxima along the $z$ axis increases as the $[0,0,7]$ orbit becomes occupied, and the number of maxima along the $x$ axis decreases as the $[3,0,0]$ state gets emptied.

To clearly see the evolution of $C^r$ with $\omega$, we consider the indicator

$$\Delta C^r(r; \omega) \equiv C^r(r; \omega) - C^r(r; \omega = 0).$$

This quantity is shown in Fig. 11 together with the corresponding variations $\Delta \tau$ and $\Delta \tau^{TF}$ relative to the nonrotating case.

One can notice that there is a clear correspondence between the peaks of $\Delta C^r$ and valleys (peaks) of $\Delta \tau$ ($\Delta \tau^{TF}$), which is consistent with Eq. (23). This observation suggests that $\Delta \tau$ and $\Delta \tau^{TF}$ are in antiphase, which results in a constructive interference when considering their ratio.

To analyze this pattern in more detail, Fig. 12(a) displays $\tau$, $\tau^{TF}$, and $C^r$ for 60 particles in the nonrotating SD HO along the $z$ axis ($y = 0$), together with the density profile of the $[0,0,6]$ state. One can see that valleys (peaks) of $\tau$, $\tau^{TF}$, and $C^r$ roughly coincide with maxima of the $[0,0,6]$ density, while other states contribute to a smooth background.

FIG. 9. Nucleon localizations functions $C_{qs\mu}$ (14) and $C_{qs\mu}^{TF}$ (23) in the $x$-$z$ ($y = 0$) plane for three spin-quantization directions $\mu = x, y, z$, obtained in the CHF calculation for the SD yrast configuration of $^{152}\text{Dy}$ at $\hbar\omega = 0.5$ MeV.

FIG. 10. Similar to Fig. 9 but shown in the $y$-$z$ ($x = 0$) plane.

FIG. 11. $C^r$ (top), $\tau$ (in fm$^{-5}$, middle) and $\tau^{TF}$ (in fm$^{-5}$, bottom) in the $x$-$z$ ($y = 0$) plane, calculated in the CHO model with 60 particles in a SD HO well. The first column shows the reference plots at $\omega = 0$ while the other columns show the rotational dependence relative to the $\omega = 0$ reference as a function of $\omega$ (in units of $\omega_0$).
orbits with quantum number $\tau$ in the nonrotating HO model plotted along the symmetry axis ($z$ axis) for the nonrotating HO model. The advantage of $C^\tau$ is that it amplifies the characteristic nodal structure of aligned orbits. The related $\Delta \tau$ plot exhibits a nodal pattern along the symmetry axis. On the other extreme, the $[2,0,2] \to [3,0,1]$ excitation corresponds to a $[420]1/2 \to [411]3/2$ transition, which involves deformation-aligned orbits. The related $\Delta \tau$ plot exhibits a nodal pattern along the minor axis. By summing up all six contributions, one arrives at a pattern in the last panel of Fig. 13, which is indicative of a change in $\tau$ due to rotation. Interestingly, this pattern is quite similar to that of Fig. 11 at $\omega = 0.15a_0$. We can thus conclude that, for a system that is strongly elongated along $z$ axis, rotation-aligned s.p. states with large $n_3$ leave a strong imprint on $\Delta \tau$ and $\Delta C^\tau$.

**E. Angular-momentum alignment: Cranked Hartree-Fock analysis**

In this section, we study the localization patterns obtained in the CHF calculations for the SD yrast band in $^{152}$Dy. Figure 14 shows the simplified NLF $C^\tau_{\phi^-}$ in the $\gamma = 0$ plane for different values of $\omega$. The first column corresponds to the nonrotating case, where we see NLF patterns characteristic of a deformed nucleus, similar to those for $^{100}$Zr, $^{232}$Th, and $^{240}$Pu discussed in Ref. [19]. As $\omega$ increases, new patterns gradually emerge inside the nucleus, with $C^\tau_{\phi^-} \neq C_{\phi^-}$ due to the time-reversal symmetry-breaking terms in Eq. (21).

For a better visualization of rotational dependence, we will be using relative indicators, cf. Eq. (24). Figure 15 presents the relative indicator $\Delta C^\tau_{\phi^-}$ in the $\gamma = 0$ plane. As the local densities and currents can be decomposed into time-even and time-odd parts, see Eqs. (12) and (21), their relative indicators

![Diagram](image)

**FIG. 12.** $C^\tau$ (thick solid line), $\tau$ (solid line), and $\tau^{\text{TF}}$ (dashed line) for the nonrotating HO model plotted along the $z$ axis ($x = y = 0$). (a) Three-dimensional SD HO case with 60 particles. The density profile of the $[0,0,6]$ orbit is marked by a dotted line. (b) One-dimensional case. HO orbits with principal quantum number $N \leq 6$ are occupied. The density profile of the $N = 6$ orbit is marked by a dotted line; here $\tau^{\text{TF}} = \pi^2 \rho^2/3$. Some quantities are scaled for a better visualization.

This effect is even more pronounced in the one-dimensional HO model, as shown in Fig. 12(b) where HO orbits with quantum number $N \leq 6$ are occupied. The antiphase relationship between $\tau$ and $\tau^{\text{TF}}$ is expected since $\tau$ is related to the gradients of s.p. wave functions while $\tau^{\text{TF}}$ depends on s.p. wave functions alone. The advantage of $C^\tau$ is that it amplifies the characteristic nodal structure of aligned high-$N$ s.p. orbitals thanks to the constructive interference between $\tau$ and $\tau^{\text{TF}}$.

As discussed above, the kinetic-energy density $\tau$ is sensitive to the nodal structure of s.p. wave functions. This sensitivity can thus be utilized for the visualization of the alignment process seen in the pattern of $\Delta \tau$ in Fig. 11. (For discussion of quasimolecular states in light nuclei based on the nodal structure of the s.p. densities and currents, see Ref. [65].) The cranking operator $\omega \hat{L}_z$ induces the particle-hole (p-h) excitations across the Fermi level. The low-energy excitations correspond to $\Delta N = 0$ ($\Delta n_1 = \pm 1$, $\Delta n_2 = 0$, $\Delta m_3 = \mp 1$) transitions.

Figure 13 shows the variation of $\tau$ at $\omega = 0$ induced by six such p-h excitations across the $N = 60$ gap from the occupied supershell $N_{\text{shell}} = 6$ to the empty supershell $N_{\text{shell}} = 7$, see Fig. 2. The $[0,0,6] \to [1,0,5]$ excitation is associated with that between the $[660]1/2 \to [651]3/2$ Nilsson levels. Both are rotation-aligned, prolate-driving orbits, and the corresponding $\Delta \tau$ plot exhibits a nodal pattern along the symmetry axis. On the other extreme, the $[2,0,2] \to [3,0,1]$ excitation corresponds to a $[420]1/2 \to [411]3/2$ transition, which involves deformation-aligned orbits. The related $\Delta \tau$ plot exhibits a nodal pattern along the minor axis. By summing up all six contributions, one arrives at a pattern in the last panel of Fig. 13, which is indicative of a change in $\tau$ due to rotation. Interestingly, this pattern is quite similar to that of Fig. 11 at $\omega = 0.15a_0$. We can thus conclude that, for a system that is strongly elongated along $z$ axis, rotation-aligned s.p. states with large $n_3$ leave a strong imprint on $\Delta \tau$ and $\Delta C^\tau$.

![Diagram](image)

**FIG. 13.** Changes in the kinetic-energy density $\tau$ due to p-h excitations (at $\omega = 0$) from the SD shell $N_{\text{shell}} = 6$ to the next supershell $N_{\text{shell}} = 7$ in Fig. 2. These excitations are induced in the CHO description of a 60-particle system by the cranking term. The rightmost panel shows the uniform average of individual p-h contributions.
can also be decomposed into time-even and time-odd components. For instance,
\[
\Delta \tau_{q\tilde{\sigma}}(r; \omega) = \frac{1}{2} \Delta \tau_q(r; \omega) + \frac{1}{2} \tilde{\sigma}_j T'_q(r; \omega), \tag{25}
\]
where the quantity
\[
\Delta \tau_q(r; \omega) = \tau_q(r; \omega) - \tau_q(r; \omega = 0) \tag{26}
\]
does not depend on simplex and provides a background that is an even function of \(\omega\). The simplex-dependent term in Eq. (25) is \(\omega\)-odd; together with the time-odd component of \(\rho_{q\tilde{\sigma}}(r; \omega)\) is responsible for the difference between the values of \(C^\tau_{q\tilde{\sigma}}\) of different simplex (the same argument also holds for signature). This difference is clearly shown in Fig. 15.

Also, to illustrate the directional dependence of \(\Delta C^\tau_{q\tilde{\sigma}}\), we show it in the \(x = 0\) plane in Fig. 16. A different pattern along the \(y\) direction results from the breaking of axial symmetry by the cranking term.

Figures 17 and 18 show the variations of \(\Delta \tau\) and \(\Delta \tau^{TF}\) with \(\omega\). Similar to the CHO case discussed in Sec. III D, \(\Delta \tau\) and \(\Delta \tau^{TF}\) are in antiphase that results in a constructive interference when it comes to \(\Delta C^\tau\). Furthermore, \(\Delta \tau\), \(\Delta \tau^{TF}\), and \(\Delta C_{q\tilde{\sigma}}\) of opposite values of \(\tilde{\sigma}\) change in the opposite direction with \(\omega\). That is, a ridge in \(\Delta C^\tau_{q\tilde{\sigma}}\) corresponds to a valley in \(\Delta C^\tau_{\tilde{\sigma}q}\). According to Eqs. (21), this is due to the contributions from time-odd densities which change sign between different values of \(\tilde{\sigma}\).

By investigating the behavior of the NLF from the perspective of individual s.p. orbits, we can gain useful insights on the s.p. motion in the rotating nucleus. Following the CHO dis-
FIG. 17. Similar to Fig. 15, but for $\Delta \tau_{q\phi}$ (in fm$^{-5}$). The reference value of $\tau_{q\phi}$ at $\omega = 0$ is shown in the first column.

discussion in Sec. III D, we focus on $\Delta \tau$. In particular, we shall study the rotational dependence of kinetic-energy densities of s.p. orbits near the Fermi level as these orbits are expected to primarily affect the nuclear response to rotation.

In the example discussed below, for the sake of simplicity we consider small rotational frequency $\hbar \omega = 0.1$ MeV, at which individual levels shown in Fig. 1 can easily be identified structurally. At higher rotational frequencies, this discussion can be repeated by following the diabatic Routhians within each parity-signature block.

FIG. 18. Similar to Fig. 17, but for $\Delta \tau_{q\phi}$ (in fm$^{-5}$).

Figure 19 shows $\Delta \tau$ at $\hbar \omega = 0.1$ MeV for different parity-signature blocks. The patterns of $\Delta \tau$ can be understood by inspecting the contributions from several individual s.p. orbits close to the Fermi energy shown in Fig. 20. The main contribution to $\Delta \tau_n$ in the negative-parity blocks comes from the high-$N$ orbits $7_1$ and $7_2$. For the $\pi = +$ neutrons, four close-lying deformation-aligned states $[651]1/2$, $[642]5/2$, $[413]5/2$, and $[411]1/2$, are most important. For the protons, the main contributions to $\Delta \tau$ come from the $N' = 6$ states $6_1$, $6_2$, $6_3$, and $6_4$ (for $\pi = +$) and $[541]1/2$ (for $\pi = -$). It is seen that the s.p. contributions shown in Figs. 20(a)–20(h) explain the behavior of $\Delta \tau$ in Fig. 19. As discussed earlier in Sec. III D, characteristic nodal structures of $\Delta \tau$ along the $z$-axis primarily come from the evolution of rotation-aligned
s.p. orbits with large $N$ and $n_\alpha$, below the Fermi energy. The features in the direction of the minor axis can be attributed to deformation-aligned s.p. states.

### IV. CONCLUSIONS

In this study, we extended the concept of the fermion localization function to anisotropic, spin-unsaturated, and spin-polarized systems. In particular, we considered the case of broken time-reversal symmetry. We demonstrated that, in spin-polarized systems, the localization function to anisotropic, spin-unsaturated, and spin-polarized systems can be easily extended to the case of self-consistent symmetries associated with point groups, such as signature or simplex, and there are no conceptual problems when viewing the NLF as a measure of the excess of kinetic-energy density due to the Pauli principle.

The localization function involves various local densities, among which the current density $j$, density gradient $\nabla \rho$, and spin-current tensor density $\mathbf{J}$ are appreciable only in the surface region. If one neglects these surface terms, one can define a simplified localization measure $C'$, which involves only the kinetic-energy density $\tau$ and the Thomas-Fermi kinetic-energy density $\tau^{\text{TF}}$. We argue that $C'$ is amplified by the out-of-phase spatial oscillation of $\tau$ and $\tau^{\text{TF}}$ attributed to the specific nodal structure of high-$N$ s.p. states.

To show the usefulness of the extended NLF, we carried out the Skyrme-CHF analysis of the superdeformed yrast band of $^{152}$Dy. As the rotational frequency increases, rotationally aligned s.p. states with high-$N$ and high-$n_\alpha$ produce a characteristic oscillating pattern in the NLF along the major axis of the nucleus, while the pattern variations along the minor axis come from deformation-aligned s.p. states close to the Fermi energy.

Our CHF and CHO results demonstrate that $C'$ is an excellent indicator of the nuclear response to collective rotation. Many applications of the NLF to the visualization of nuclear rotational and vibrational modes and time-dependent processes [18,36,66–71] are envisioned, especially after incorporating pairing correlations via the HFB extension of the formalism. One can also consider applying the concept of the NLF beyond the mean-field approach. In particular, since the kinetic-energy density can be computed within realistic A-body frameworks [72], studies of many-body correlations with the help of $C'$ could offer new perspectives.

Finally, let us note that, while in the usual atomic applications the current term in Eq. (13) is ignored, the contribution to ELF from the spin-current tensor density $\mathbf{J}$ is expected to be nonzero in relativistic superheavy atoms. For instance, the spin-orbit splitting for the valence $7p$ orbital of the element Og ($Z = 118$) is predicted to be very large, around 10 eV [14,73]. While $\mathbf{Og}$ is believed to be a spin-saturated system (the whole $7p$ shell is filled), this is not the case for, e.g., $\mathbf{Fl}$ ($Z = 114$, $7p_{3/2}$ shell empty) for which $\mathbf{J}$ and the resulting spin-orbit current should be consider when analyzing the corresponding ELF.

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[13] P. Fuenteaiba, E. Chamorro, and J. C. Santos, Understanding and using the electron localization function, in *Theoretical


