

This is a self-archived version of an original article. This version may differ from the original in pagination and typographic details.

Author(s): Li, T.; Chen, M. Z.; Zhang, C. L.; Nazarewicz, W.; Kortelainen, M.

Title: Nucleon localization function in rotating nuclei

Year: 2020

Version: Published version

Copyright: ©2020 American Physical Society

Rights: In Copyright

Rights url: http://rightsstatements.org/page/InC/1.0/?language=en

Please cite the original version:

Li, T., Chen, M. Z., Zhang, C. L., Nazarewicz, W., & Kortelainen, M. (2020). Nucleon localization function in rotating nuclei. Physical Review C, 102(4), Article 044305. https://doi.org/10.1103/physrevc.102.044305

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

(Received 13 July 2020; accepted 21 September 2020; published 7 October 2020)

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 timeeven 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.

DOI: 10.1103/PhysRevC.102.044305

I. 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) ¹⁵²Dy, 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 ¹⁵²Dy 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:

$$\rho(\mathbf{r}sq, \mathbf{r}'s'q') \equiv \langle \Psi | a_{\mathbf{r}'s'q'}^{\dagger} a_{\mathbf{r}sq} | \Psi \rangle, \tag{1}$$

where a_{rsq}^{\dagger} and a_{rsq} 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 $\rho_q(\mathbf{rs}, \mathbf{r's'}) = \rho(\mathbf{rsq}, \mathbf{r's'q})$.

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

$$\rho_q(\mathbf{r}s, \mathbf{r}'s') = \frac{1}{2} [\rho_q(\mathbf{r}, \mathbf{r}')\delta_{ss'} + (s|\boldsymbol{\sigma}|s')s_q(\mathbf{r}, \mathbf{r}')], \quad (2)$$

where

$$\rho_q(\boldsymbol{r}, \boldsymbol{r}') = \sum_{s} \rho_q(\boldsymbol{r}s, \boldsymbol{r}'s), \qquad (3a)$$

$$\mathbf{s}_q(\mathbf{r}, \mathbf{r}') = \sum_{ss'} \rho_q(\mathbf{r}s, \mathbf{r}'s') \langle s' | \boldsymbol{\sigma} | s \rangle.$$
(3b)

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:

$$\rho_q(\mathbf{r}) = \rho_q(\mathbf{r}, \mathbf{r}), \tag{4a}$$

$$\boldsymbol{s}_q(\boldsymbol{r}) = \boldsymbol{s}_q(\boldsymbol{r}, \boldsymbol{r}), \tag{4b}$$

$$\tau_q(\mathbf{r}) = \left[\nabla \cdot \nabla' \rho_q(\mathbf{r}, \mathbf{r}') \right]_{\mathbf{r} = \mathbf{r}'},\tag{4c}$$

$$\boldsymbol{j}_{q}(\boldsymbol{r}) = \frac{1}{2i} [(\boldsymbol{\nabla} - \boldsymbol{\nabla}')\rho_{q}(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}, \qquad (4d)$$

$$\mathbb{J}_{q}(\boldsymbol{r}) = \frac{1}{2i} [(\boldsymbol{\nabla} - \boldsymbol{\nabla}') \otimes \boldsymbol{s}_{q}(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}, \qquad (4e)$$

$$\boldsymbol{T}_{q}(\boldsymbol{r}) = [(\boldsymbol{\nabla} \cdot \boldsymbol{\nabla}')\boldsymbol{s}_{q}(\boldsymbol{r}, \boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}, \qquad (4f)$$

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':

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

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

$$P_{qs}(\boldsymbol{r},\boldsymbol{r}') = \rho_q(\boldsymbol{r}s,\boldsymbol{r}s)\rho_q(\boldsymbol{r}'s,\boldsymbol{r}'s) - |\rho_q(\boldsymbol{r}s,\boldsymbol{r}'s)|^2.$$
(6)

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

$$R_{qs}(\boldsymbol{r}, \boldsymbol{r}') = \frac{P_{qs}(\boldsymbol{r}, \boldsymbol{r}')}{\rho_q(\boldsymbol{rs}, \boldsymbol{rs})}.$$
(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 δ around r. The corresponding conditional probability (7) can be written as

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

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

$$\langle e^{\delta \cdot \nabla'} \rangle = \frac{1}{4\pi} \int e^{\delta \cdot \nabla'} d\Omega$$
$$= 1 + \frac{1}{3!} \delta^2 \nabla'^2 + \frac{1}{5!} \delta^4 \nabla'^4 + \cdots .$$
(9)

The resulting local probability becomes

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

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

$$R_{qs}(\boldsymbol{r},\delta) = \frac{1}{3}D_{qs}(\boldsymbol{r})\delta^2 + O(\delta^4), \qquad (11)$$

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

For a rotationally invariant and spin-unpolarized system, $D_{qs}(\mathbf{r})$ 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 $D_{as_u}(\mathbf{r})$ with $\mu = x, y, z$.

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

$$\rho_{qs_{\mu}}(\boldsymbol{r}) = \frac{1}{2}\rho_{q}(\boldsymbol{r}) + \frac{1}{2}\sigma_{\mu}s_{q\mu}(\boldsymbol{r}), \qquad (12a)$$

$$\tau_{qs_{\mu}}(\boldsymbol{r}) = \frac{1}{2}\tau_{q}(\boldsymbol{r}) + \frac{1}{2}\sigma_{\mu}T_{q\mu}(\boldsymbol{r}), \qquad (12b)$$

$$\boldsymbol{j}_{qs_{\mu}}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{j}_{q}(\boldsymbol{r}) + \frac{1}{2}\sigma_{\mu}\mathbb{J}_{q}(\boldsymbol{r}) \cdot \boldsymbol{e}_{\mu}, \qquad (12c)$$

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

$$D_{qs_{\mu}} = \tau_{qs_{\mu}} - \frac{1}{4} \frac{\left| \nabla \rho_{qs_{\mu}} \right|^2}{\rho_{qs_{\mu}}} - \frac{\left| \boldsymbol{j}_{qs_{\mu}} \right|^2}{\rho_{qs_{\mu}}}.$$
 (13)

Following Ref. [9], a dimensionless and normalized NLF can now be defined as

$$\mathcal{C}_{qs_{\mu}}(\boldsymbol{r}) = \left[1 + \left(\frac{D_{qs_{\mu}}(\boldsymbol{r})}{\tau_{qs_{\mu}}^{\mathrm{TF}}(\boldsymbol{r})}\right)^{2}\right]^{-1},$$
(14)

where the normalization $\tau_{qs_{\mu}}^{\text{TF}}(\mathbf{r}) = \frac{3}{5}(6\pi^2)^{2/3}\rho_{qs_{\mu}}^{5/3}(\mathbf{r})$ 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 $\rho_q(\mathbf{r})$, kinetic-energy density $\tau_q(\mathbf{r})$, and spin-current tensor density $\mathbb{J}_q(\mathbf{r})$ are all time-even, while the spin vector density $s_{q\mu}(\mathbf{r})$, spin-kinetic vector density $T_{q\mu}(\mathbf{r})$, and current vector density $\mathbf{j}_q(\mathbf{r})$ are time-odd. If time-reversal symmetry is conserved, $s_{q\mu}(\mathbf{r}) = 0$, $T_{q\mu}(\mathbf{r}) = 0$, and $\mathbf{j}_q(\mathbf{r}) = 0$. Consequently, for a system that conserves time-reversal symmetry and is governed by spin-independent interactions, one obtains

$$D_{q\pm\frac{1}{2}} = D_q = \frac{1}{2}\tau_q - \frac{1}{8}\frac{|\nabla\rho_q|^2}{\rho_q},$$
 (15)

which is the familiar atomic physics expression [9].

In general, the tensor density $\mathbb{J}_{a}(\mathbf{r})$ 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 \mathbb{J}_q 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 $j_{qs_u}(\mathbf{r})$ does not vanish even in ground-state configurations of eveneven nuclei. While its contribution to the NLF was ignored in several previous calculations [15,18,19], the current-density contribution to the NLF practically vanishes in the nuclear interior, see discussion in Sec. III A. Consequently, one can safely neglect this term when the goal is to use the NLF as a configuration-characterization tool.

The choice of the normalization function in Eq. (14) is somehow arbitrary. In atomic physics applications and for time-reversal-invariant nuclear configurations, the density $\rho_{qs_{\mu}}$ does not depend on spin. In the general case, however, nucleonic densities depend on the spin polarization. In this work, in order to emphasize the rotation-induced effects, we decided to stick to the normalization function $\tau_{qs_{\mu}}^{\text{TF}}$, which is different for spin-up and spin-down subsystems.

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*, is located in some region of space. The wave function of this particle can be written as

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

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

$$\boldsymbol{j}_{as} = \rho_{qs} \boldsymbol{\nabla} \boldsymbol{\chi}. \tag{17}$$

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

$$\tau_{qs}^{\text{s.p.}} = |\nabla \psi_{qs}|^2 = \frac{1}{4} \frac{|\nabla \rho_{qs}|^2}{\rho_{qs}} + \frac{|\mathbf{j}_{qs}|^2}{\rho_{qs}}, \quad (18)$$

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:

$$D_{qs} = \tau_{qs} - \tau_{qs}^{\text{s.p.}}.$$
(19)

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 ¹⁵²Dy can be viewed as unique laboratories of extreme single-particle behavior [25,38]. The nucleus ¹⁵²Dy plays a role of superdeformed double-magic core due to large shell closures at Z = 66 and N = 86. Because of this, ¹⁵²Dy 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 ¹⁵²Dy [41,42]. Indeed, with a reasonable pairing strength, adjusted to experimental odd-even mass difference in ¹²⁰Sn as done in Ref. [43], the static pairing vanishes in the SD yrast band of ¹⁵²Dy 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 \mathcal{N} , namely, the proton $\mathcal{N} = 6$ and neutron $\mathcal{N} = 7$ 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 ¹⁵²Dy using the HF solver HFODD [46]. Following Ref. [24], s.p. wave functions have been expanded in a stretched deformed HO basis with frequencies $\hbar\omega_z = 6.246$ MeV and $\hbar\omega_{\perp} = 11.200$ MeV along the directions parallel and perpendicular to the symmetry axis, respectively. The total number of basis states is 1013 with HO quanta not exceeding 15 in each direction. We employed the Skyrme energy density functional parametrization SkM* [47], with its generic time-odd terms [24,48].

The angular momentum has been generated by means of a cranking term $-\omega \hat{J}_y$, where \hat{J}_y is the *y* component of the total angular-momentum operator and ω represents the angular velocity of rotation. In the presence of the cranking term, parity \hat{P} , *y* signature $\hat{R}_y = \exp(-i\pi \hat{J}_y)$, and *y* simplex $\hat{\Re}_y = \hat{P}\hat{R}_y$ 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



FIG. 1. Single-particle (a) neutron and (b) proton Routhians as functions of ω , obtained in the CHF + SkM* calculations for the SD yrast band of ¹⁵²Dy. The (πr_y) combinations are indicated by solid lines (+, +i), dotted lines (+, -i), dot-dashed lines (-, +i), and dashed lines (-, -i). The Routhians originating from the lowest neutron $\mathcal{N} = 7$ and proton $\mathcal{N} = 6$ and [541]1/2 levels are marked by thicker lines.

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 $[N_{+,+i}, N_{+,-i}, N_{-,+i}, N_{-,-i}]$, where $N_{\pi r_y}$ are the numbers of occupied s.p. orbitals having parity π and y signature r_y . As discussed in Ref. [24], the yrast configuration of SD ¹⁵²Dy 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 $\hbar \omega = 0.2 \approx 0.5$ 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 ¹⁵²Dy are shown in Fig. 1. The large deformed shell closures at Z = 66 and N = 86 are clearly seen. The lowest $\mathcal{N} = 7$ neutron and $\mathcal{N} = 6$ 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].

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 harmonicoscillator (CHO) model with frequencies $\omega_{\perp} = \omega_x = \omega_y = 2\omega_z$. 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 ¹⁵²Dy, we study a SD HO potential filled with 60 particles, which corresponds to a closed SD supershell $\mathcal{N}_{\text{shell}} \equiv 2(n_1 + n_2) + n_3 = 6$ [1,53,56,57]. The corresponding s.p. Routhians are shown in Fig. 2 as functions of ω . 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 quanta along the rotation axis ($n_2 = 0$) and the largest possible value of the difference ($n_3 - n_1$) carry the largest s.p. angular momentum. In Fig. 2 those are the [0,0,7] ($\mathcal{N} = 7$) and [0,0,6] ($\mathcal{N} = 6$) Routhians.

E. Nucleon localization function at high spins

Since parity, y signature r_y , and y simplex r_y are selfconsistent symmetries in our cranking calculations, in order to see the angular-momentum alignment effects caused by different orbits, it is convenient to study the NLFs of a given r_y or r_y . This can be done by expressing local densities and currents in terms of their symmetry-conserving components. In practice, this can be done by summing up the contributions from HF s.p. wave functions belonging to a given symmetry block [49–51]. For instance, if the y simplex is conserved,

$$\rho_q(\mathbf{r}) = \rho_{q\check{\sigma}_v = +1}(\mathbf{r}) + \rho_{q\check{\sigma}_v = -1}(\mathbf{r}), \qquad (20)$$

where $\check{\sigma}_y \equiv \mathfrak{r}_y/i = \pm 1$. A similar decomposition holds for $\tau_q(\mathbf{r})$ and $\mathbf{j}_q(\mathbf{r})$.

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

$$\rho_{q\breve{\sigma}_y}(\mathbf{r}) = \frac{1}{2}\rho_q(\mathbf{r}) + \frac{1}{2}\breve{\sigma}_y s'_q(\mathbf{r}), \qquad (21a)$$

$$\tau_{q\breve{\sigma}_{y}}(\boldsymbol{r}) = \frac{1}{2}\tau_{q}(\boldsymbol{r}) + \frac{1}{2}\breve{\sigma}_{y}T_{q}'(\boldsymbol{r}), \qquad (21b)$$

$$\boldsymbol{j}_{\boldsymbol{q}\boldsymbol{\check{\sigma}}_{\boldsymbol{y}}}(\boldsymbol{r}) = \frac{1}{2}\boldsymbol{j}_{\boldsymbol{q}}(\boldsymbol{r}) + \frac{1}{2}\boldsymbol{\check{\sigma}}_{\boldsymbol{y}}\boldsymbol{J}_{\boldsymbol{q}}'(\boldsymbol{r}), \qquad (21c)$$

where

$$S'_{q}(\mathbf{r}) = \rho_{q\check{\sigma}_{y}=+1}(\mathbf{r}) - \rho_{q\check{\sigma}_{y}=-1}(\mathbf{r}), \qquad (22a)$$

$$T'_{q}(\boldsymbol{r}) = \tau_{q\breve{\sigma}_{y}=+1}(\boldsymbol{r}) - \tau_{q\breve{\sigma}_{y}=-1}(\boldsymbol{r}), \qquad (22b)$$

$$\mathbf{J}'_{q}(\mathbf{r}) = \mathbf{j}_{q\breve{\sigma}_{y}=+1}(\mathbf{r}) - \mathbf{j}_{q\breve{\sigma}_{y}=-1}(\mathbf{r}).$$
(22c)

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 ω is expressed in units of $\omega_0 = (\omega_z \omega_{\perp}^2)^{1/3}$ 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 $\mathcal{N} = 7$ Routhian [0,0,7] and the [3,0,0] Routhian 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 $\mathcal{N} = 7$ 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].



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 ω (in units of ω_0). The magnitude |j| (in fm⁻⁴) is shown by color and line thickness.

When it comes to the realistic description, Fig. 4 shows the neutron and proton current densities of ¹⁵²Dy calculated in the CHF method at four rotational frequencies up to $\hbar\omega =$ 0.8 MeV (angular momentum $I_y \approx 90\hbar$). 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 $\omega \rightarrow 0$ 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 ¹⁵²Dy.

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 ω . 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. 4. Current density j in the *x*-*z* (y = 0) plane for neutrons (top) and protons (bottom) in the SD yrast band of ¹⁵²Dy obtained in the CHF calculations, as a function of ω (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.



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 ¹⁵²Dy obtained in the CHF calculations, as functions of ω (in units of MeV/ \hbar). The magnitudes, |s| (in fm⁻³) and |T| (in fm⁻⁵), are shown by color and line thickness. The FAM-QRPA results are presented in the first column with a different color range.

To complete the discussion of spin fields, the spin-current tensor density $\mathbb{J} \cdot \boldsymbol{e}_y$ is shown in Fig. 6. As compared with the current density \boldsymbol{j} shown in Fig. 4, $\mathbb{J} \cdot \boldsymbol{e}_y$ changes very weakly with ω . This field has a surface character, i.e., it practically vanishes within the nuclear volume. Since $\mathbb{J}_q \cdot \boldsymbol{e}_y$ is time-even, its contribution to C_{qs_u} 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 $|\nabla \rho_{qs}|^2$, which has a surface character. Consequently, we define a simplified localization measure as

$$\mathcal{C}_{qs_{\mu}}^{\tau}(\boldsymbol{r}) = \left[1 + \left(\frac{\tau_{qs_{\mu}}(\boldsymbol{r})}{\tau_{qs_{\mu}}^{\mathrm{TF}}(\boldsymbol{r})}\right)^{2}\right]^{-1},$$
(23)

which does not include contributions from the current density and density gradient. Figure 7 shows C, C^{τ} , and their difference obtained in the CHO model; we indeed see that C^{τ} 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 ¹⁵²Dy. Figure 8 shows C and C^{τ} for neutrons with $\breve{\sigma}_y = -1$ (y simplex $\mathfrak{r}_y = -i$) at $\hbar\omega = 0.9$ MeV: the two



FIG. 6. Spin-current tensor density $\mathbb{J} \cdot \mathbf{e}_{y}$ in the *x*-*z* (*y* = 0) plane for neutrons in the SD yrast band of ¹⁵²Dy, as a function of ω (in units of MeV/ \hbar). Its magnitude (in fm⁻⁴) is shown by color and line thickness.



FIG. 7. C (top), C^{τ} (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 ω (in units of ω_0).

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 $C_{q\sigma} \rightarrow C_{q\sigma}\rho_{q\sigma}/[\max \rho_{q\sigma}]$ (with σ 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^{τ} 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 $|\nabla \rho_{qs}|^2$ 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^{τ} is a useful tool to characterize intrinsic configurations in most cases, except perhaps for dynamic pro-



FIG. 8. C (left), $C^{\mathfrak{r}}$ (middle), and their difference (right) in the *x*-*z* (*y* = 0) plane for neutrons with $\check{\sigma}_y = -1$ (*y* simplex $\mathfrak{r}_y = -1$), obtained in the CHF calculations for the SD yrast configuration of ¹⁵²Dy at $\hbar\omega = 0.9$ MeV.



FIG. 9. Nucleon localizations functions $C_{qs_{\mu}}$ (14) and $C_{qs_{\mu}}^{\tau}$ (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 ¹⁵²Dy at $\hbar\omega = 0.5$ 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 $C_{qs_{\mu}}^{\tau}$ (23) depend on the choice of the spin-quantization direction μ . This directional dependence is illustrated in Figs. 9 and 10 for the SD ¹⁵²Dy at $\hbar\omega = 0.5$ MeV. It is seen that the NLF



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



FIG. 11. C^{τ} (top), τ (in fm⁻⁵, middle) and τ^{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 ω (in units of ω_0).

slightly depends on the choice of μ , especially in the case of the *y*-*z* cross section. More importantly, $C_{qs_{\mu}}^{\tau} \approx C_{qs_{\mu}}$ in the nuclear interior, independently of μ .

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^{τ} 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 ω . At $\omega = 0.2\omega_0$, where the band crossing occurs, C^{τ} rapidly changes. Namely, the number of maxima along the *z* axis increases as the [0,0,7] orbit becomes occupies, and the number of maxima along the *x* axis decreases as the [3,0,0] state gets emptied.

To clearly see the evolution of \mathcal{C}^{τ} with ω , we consider the indicator

$$\Delta \mathcal{C}^{\tau}(\boldsymbol{r};\omega) \equiv \mathcal{C}^{\tau}(\boldsymbol{r};\omega) - \mathcal{C}^{\tau}(\boldsymbol{r};\omega=0).$$
(24)

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 ΔC^{τ} 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 τ , τ^{TF} , and C^{τ} for 60 particles in the nonrotating SD HO along the *z* axis (x = y = 0), together with the density profile of the [0,0,6] state. One can see that valleys (peaks) of τ , τ^{TF} , and C^{τ} roughly coincide with maxima of the [0,0,6] density, while other states contribute to a smooth background.



FIG. 12. C^{τ} (thick solid line), τ (solid line), and τ^{TF} (dashed line) for the nonrotating HO model plotted along *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 $\mathcal{N} \leq 6$ are occupied. The density profile of the $\mathcal{N} = 6$ orbit is marked by a dotted line; here $\tau^{\text{TF}} = \pi^2 \rho^3/3$. Some quantities are scaled for a better visualization.

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

As discussed above, the kinetic-energy density τ 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 $\omega \hat{L}_y$ induces the particle-hole (p-h) excitations across the Fermi level. The low-energy excitations correspond to $\Delta \mathcal{N} = 0$ ($\Delta n_1 = \pm 1$, $\Delta n_2 = 0$, $\Delta n_3 = \pm 1$) transitions.

Figure 13 shows the variation of τ 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 $[0, 0, 6] \rightarrow [1, 0, 5]$ excitation can be associated with that between the $[660]1/2(6_{1,2})$ and $[651]3/2(6_{3,4})$ 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 $[2, 0, 2] \rightarrow$ [3, 0, 1] excitation corresponds to a $[420]1/2([422]3/2) \rightarrow$ [411]3/2 ([413]5/2) transition, which involves deformationaligned 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 τ due to rotation. Interestingly, this pattern is quite similar to that of Fig. 11 at $\omega = 0.15\omega_0$. 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 ΔC^{τ} .

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 ¹⁵²Dy. Figure 14 shows the simplified NLF $C_{q\bar{d}y}^{\tau}$ in the y = 0 plane for different values of ω . The first column corresponds to the nonrotating case, where we see NLF patterns characteristic of a deformed nucleus, similar to those for ¹⁰⁰Zr, ²³²Th, and ²⁴⁰Pu discussed in Ref. [19]. As ω increases, new patterns gradually emerge inside the nucleus, with $C_{q\uparrow}^{\tau} \neq C_{q\downarrow}^{\tau}$ 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 $\Delta C_{q\bar{d}y}^{\tau}$ in the y = 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



FIG. 13. Changes in the kinetic-energy density τ due to p-h excitations (at $\omega = 0$) from the SD shell $N_{shell} = 6$ to the next supershell $N_{shell} = 7$ 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.



FIG. 14. $C_{q\check{\sigma}y}^{\tau}$ in the *x*-*z* (*y* = 0) plane as a function of ω (in units of MeV/ \hbar), obtained in the CHF calculation for the SD yrast band of ¹⁵²Dy. The symbols \uparrow and \downarrow represent $\check{\sigma}_y = +1$ and -1 (*y* simplex $\mathfrak{r}_y = +i$ and -i), respectively.



FIG. 15. Similar as in Fig. 14 but for $\Delta C^{\tau}_{q\bar{\sigma}y}$. The reference value of C^{τ} at $\omega = 0$ is shown in the first column of Fig. 14.



FIG. 16. Similar to Fig. 15 but for $\Delta C_{q\bar{q}y}^{\tau}$ in the *y*-*z* (*x* = 0) plane.

y (fm)

-5 0 5

can also be decomposed into time-even and time-odd components. For instance,

$$\Delta \tau_{q\breve{\sigma}_y}(\boldsymbol{r};\omega) = \frac{1}{2} \Delta \tau_q(\boldsymbol{r};\omega) + \frac{1}{2} \breve{\sigma}_y T'_q(\boldsymbol{r};\omega), \qquad (25)$$

where the quantity

z (fm)

-10

0

-10

 $10 \Delta C_{\rm pl}^{\tau}$

0 5

-5

-5 0 5

$$\Delta \tau_q(\mathbf{r};\omega) = \tau_q(\mathbf{r};\omega) - \tau_q(\mathbf{r};\omega=0)$$
(26)

does not depend on simplex and provides a background that is an even function of ω . The simplex-dependent term in Eq. (25) is ω -odd; together with the time-odd component of $\rho_{q\check{\sigma}_y}(\mathbf{r};\omega)$ is responsible for the difference between the values of $C^{\tau}_{q\check{\sigma}_y}$ 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 $\Delta C_{q\breve{\sigma}_y}^{\tau}$, 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 $\Delta \tau^{\text{TF}}$ with ω . Similar to the CHO case discussed in Sec. III D, $\Delta \tau$ and $\Delta \tau^{\text{TF}}$ are in antiphase that results in a constructive interference when it comes to ΔC^{τ} . Furthermore, $\Delta \tau$, $\Delta \tau^{\text{TF}}$, and $\Delta C_{q\bar{\sigma}_y}$ of opposite values of $\bar{\sigma}_y$ change in the opposite direction with ω . That is, a ridge in $\Delta C_{q\uparrow}$ corresponds to a valley in $\Delta C_{q\downarrow}$. According to Eqs. (21), this is due to the contributions from time-odd densities which change sign between different values of $\bar{\sigma}_y$.

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-

-0.1

0.1

0

0

-5

-0.1



FIG. 17. Similar to Fig. 15, but for $\Delta \tau_{q\bar{\sigma}_y}$ (in fm⁻⁵). The reference value of $\tau_{a\bar{\sigma}_y}$ at $\omega = 0$ is shown in the first column.

cussion 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 $\Delta \tau_{a\check{\sigma}_v}^{\text{TF}}$ (in fm⁻⁵).



FIG. 19. Neutron (top) and proton (bottom) contributions to $\Delta \tau$ (in fm⁻⁵) in the *x*-*z* (*y* = 0) plane for different parity-signature blocks (π , r_y) in ¹⁵²Dy at $\hbar \omega = 0.1$ MeV.

Figure 19 shows $\Delta \tau$ at $\hbar \omega = 0.1$ MeV for different paritysignature 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- \mathcal{N} orbits 7₁ and 7₂. 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 $\mathcal{N} = 6$ states 6₁, 6₂, 6₃, and 6₄ (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



FIG. 20. Contributions to $\Delta \tau$ (in fm⁻⁵) in the *x*-*z* (*y* = 0) plane for different parity-signature blocks from individual s.p. Routhians in ¹⁵²Dy at $\hbar \omega = 0.1$ MeV: the four $\pi = +$, r = +i neutron levels [651]1/2, [642]5/2, [413]5/2, and [411]1/2 with (a) r = +i and (b) -i that appear below the N = 86 shell gap in Fig. 1 (see Fig. 1 of Ref. [45] for the asymptotic (Nilsson) quantum numbers $[\mathcal{N}n_z\Lambda]\Omega$ of s.p. levels in SD ¹⁵²Dy). The $\mathcal{N} = 7$ neutron intruder states (c) 7_1 and (d) 7_2 ; the $\mathcal{N} = 6$ proton intruder states (e) $6_2 + 6_4$ and (f) $6_1 + 6_3$; and the (g) [541]1/2₂ and (h) [541]1/2₁ proton states.

s.p. orbits with large N and n_z , 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 the general case of rotating deformed systems, three localization measures $C_{qs_{\mu}}(\mathbf{r})$, with $\mu = x, y, z$, which depend on the anisotropy of the spin distribution, can be defined.

We used the NLF to interpret the results of cranked Skyrme-HF calculations for rotating nuclei, especially to study the interplay between collective and s.p. motion. While the standard probabilistic interpretation of the NLF cannot be easily extended to the case of self-consistent symmetries associated with point groups, such as signature or simplex, 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 \mathbf{j} , density gradient $\nabla \rho$, and spin-current tensor density \mathbb{J} are appreciable only in the surface region. If one neglects these surface terms, one can define a simplified localization measure C^{τ} , which involves only the kinetic-energy density τ and the Thomas-Fermi kineticenergy density τ^{TF} . We argue that C^{τ} is amplified by the out-of-phase spatial oscillation of τ and τ^{TF} attributed to the specific nodal structure of high- \mathcal{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 ¹⁵²Dy. As the rotational frequency increases, rotationally aligned s.p. states with high- \mathcal{N} and high- n_z 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^{τ} 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^{τ} 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 \mathbb{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 Og is believed to be a spin-saturated system (the whole 7p shell is filled), this is not the case for, e.g., Fl (Z = 114, $7p_{3/2}$ shell empty) for which \mathbb{J} and the resulting spin-orbit current should be consider when analyzing the corresponding ELF.

ACKNOWLEDGMENTS

Discussions with Jacek Dobaczewski, Samuel Giuliani, and Simin Wang are gratefully acknowledged. Computational resources were provided by the Institute for Cyber-Enabled Research at Michigan State University. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Awards No. DE-SC0013365 and No. DE-SC0018083 (NUCLEI SciDAC-4 Collaboration).

- A. Bohr and B. R. Mottelson, *Nuclear Structure* (W. A. Benjamin, Reading, 1975), Vol. II.
- [2] Z. Szymański, *Fast Nuclear Rotation* (Clarendon Press, Oxford, 1983).
- [3] W. Nazarewicz, The nuclear collective motion, in *An Advanced Course in Modern Nuclear Physics*, edited by J. M. Arias and M. Lozano (Springer, Berlin, Heidelberg, 2001), pp. 102–140.
- [4] S. Frauendorf, Spontaneous symmetry breaking in rotating nuclei, Rev. Mod. Phys. 73, 463 (2001).
- [5] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Self-consistent mean-field models for nuclear structure, Rev. Mod. Phys. 75, 121 (2003).
- [6] T. Duguet and J. Sadoudi, Breaking and restoring symmetries within the nuclear energy density functional method, J. Phys. G 37, 064009 (2010).
- [7] J. Drut, R. Furnstahl, and L. Platter, Toward *ab initio* density functional theory for nuclei, Prog. Part. Nucl. Phys. 64, 120 (2010).

- [8] T. Nakatsukasa, K. Matsuyanagi, M. Matsuo, and K. Yabana, Time-dependent density-functional description of nuclear dynamics, Rev. Mod. Phys. 88, 045004 (2016).
- [9] A. D. Becke and K. E. Edgecombe, A simple measure of electron localization in atomic and molecular systems, J. Chem. Phys. 92, 5397 (1990).
- [10] A. Savin, O. Jepsen, J. Flad, O. K. Andersen, H. Preuss, and H. G. von Schnering, Electron localization in solid-state structures of the elements: The diamond structure, Angew. Chem., Int. Ed. Engl. **31**, 187 (1992).
- [11] A. Savin, R. Nesper, S. Wengert, and T. F. Fässler, ELF: The electron localization function, Angew. Chem., Int. Ed. Engl. 36, 1808 (1997).
- [12] T. Burnus, M. A. L. Marques, and E. K. U. Gross, Timedependent electron localization function, Phys. Rev. A 71, 010501 (2005).
- [13] P. Fuentealba, E. Chamorro, and J. C. Santos, Understanding and using the electron localization function, in *Theoretical*

Aspects of Chemical Reactivity, edited by A. Toro-Labbé (Elsevier, Amsterdam, 2007), Vol. 19, Chap. 5, pp. 57–85.

- [14] P. Jerabek, B. Schuetrumpf, P. Schwerdtfeger, and W. Nazarewicz, Electron and Nucleon Localization Functions of Oganesson: Approaching the Thomas-Fermi Limit, Phys. Rev. Lett. **120**, 053001 (2018).
- [15] P.-G. Reinhard, J. A. Maruhn, A. S. Umar, and V. E. Oberacker, Localization in light nuclei, Phys. Rev. C 83, 034312 (2011).
- [16] B. Schuetrumpf, C. Zhang, and W. Nazarewicz, Clustering and pasta phases in nuclear density functional theory, in *Nuclear Particle Correlations and Cluster Physics*, edited by W.-U. Schröder (World Scientific, Singapore, 2017), pp. 135–153.
- [17] J.-P. Ebran, E. Khan, T. Nikšić, and D. Vretenar, Localization and clustering in atomic nuclei, J. Phys. G 44, 103001 (2017).
- [18] B. Schuetrumpf and W. Nazarewicz, Cluster formation in precompound nuclei in the time-dependent framework, Phys. Rev. C 96, 064608 (2017).
- [19] C. L. Zhang, B. Schuetrumpf, and W. Nazarewicz, Nucleon localization and fragment formation in nuclear fission, Phys. Rev. C 94, 064323 (2016).
- [20] G. Scamps and C. Simenel, Impact of pear-shaped fission fragments on mass-asymmetric fission in actinides, Nature (London) 564, 382 (2018).
- [21] G. Scamps and C. Simenel, Effect of shell structure on the fission of sub-lead nuclei, Phys. Rev. C 100, 041602 (2019).
- [22] Z. Matheson, S. A. Giuliani, W. Nazarewicz, J. Sadhukhan, and N. Schunck, Cluster radioactivity of ²⁹⁴₁₁₈Og₁₇₆, Phys. Rev. C 99, 041304 (2019).
- [23] J. Sadhukhan, S. A. Giuliani, Z. Matheson, and W. Nazarewicz, Efficient method for estimation of fission fragment yields of *r*process nuclei, Phys. Rev. C 101, 065803 (2020).
- [24] J. Dobaczewski and J. Dudek, Time-odd components in the mean field of rotating superdeformed nuclei, Phys. Rev. C 52, 1827 (1995).
- [25] W. Satuła, J. Dobaczewski, J. Dudek, and W. Nazarewicz, Additivity of Quadrupole Moments in Superdeformed Bands: Single-Particle Motion at Extreme Conditions, Phys. Rev. Lett. 77, 5182 (1996).
- [26] A. V. Afanasjev and H. Abusara, Time-odd mean fields in covariant density functional theory: Rotating systems, Phys. Rev. C 82, 034329 (2010).
- [27] Y. M. Engel, D. M. Brink, K. Goeke, S. J. Krieger, and D. Vautherin, Time-dependent Hartree-Fock theory with Skyrme's interaction, Nucl. Phys. A 249, 215 (1975).
- [28] E. Perlińska, S. G. Rohoziński, J. Dobaczewski, and W. Nazarewicz, Local density approximation for proton-neutron pairing correlations: Formalism, Phys. Rev. C 69, 014316 (2004).
- [29] J. W. Negele and D. Vautherin, Density-matrix expansion for an effective nuclear Hamiltonian, Phys. Rev. C 5, 1472 (1972).
- [30] J. Dobaczewski, B. G. Carlsson, and M. Kortelainen, The Negele–Vautherin density-matrix expansion applied to the Gogny force, J. Phys. G 37, 075106 (2010).
- [31] S. G. Rohoziński, J. Dobaczewski, and W. Nazarewicz, Self-consistent symmetries in the proton-neutron Hartree-Fock-Bogoliubov approach, Phys. Rev. C 81, 014313 (2010).
- [32] D. Vautherin and D. M. Brink, Hartree-Fock calculations with Skyrme's interaction. I. Spherical nuclei, Phys. Rev. C 5, 626 (1972).

- [33] T. Lesinski, M. Bender, K. Bennaceur, T. Duguet, and J. Meyer, Tensor part of the Skyrme energy density functional: Spherical nuclei, Phys. Rev. C 76, 014312 (2007).
- [34] M. Zalewski, J. Dobaczewski, W. Satuła, and T. R. Werner, Spin-orbit and tensor mean-field effects on spin-orbit splitting including self-consistent core polarizations, Phys. Rev. C 77, 024316 (2008).
- [35] M. Bender, K. Bennaceur, T. Duguet, P. H. Heenen, T. Lesinski, and J. Meyer, Tensor part of the Skyrme energy density functional. II. Deformation properties of magic and semi-magic nuclei, Phys. Rev. C 80, 064302 (2009).
- [36] Y. Iwata and J. A. Maruhn, Enhanced spin-current tensor contribution in collision dynamics, Phys. Rev. C 84, 014616 (2011).
- [37] C. F. v. Weizsäcker, Zur theorie der kernmassen, Eur. Phys. J. A 96, 431 (1935).
- [38] S. T. Clark, G. Hackman, R. V. F. Janssens, R. M. Clark, P. Fallon, S. N. Floor, G. J. Lane, A. O. Macchiavelli, J. Norris, S. J. Sanders, and C. E. Svensson, Empirical Investigation of Extreme Single-Particle Behavior of Nuclear Quadrupole Moments in Highly Collective A ~ 150 Superdeformed Bands, Phys. Rev. Lett. 87, 172503 (2001).
- [39] P. Bonche, H. Flocard, and P.-H. Heenen, Microscopic study of superdeformation in the A = 150 mass region, Nucl. Phys. A **598**, 169 (1996).
- [40] V. Hellemans, P.-H. Heenen, and M. Bender, Tensor part of the Skyrme energy density functional. III. Time-odd terms at high spin, Phys. Rev. C 85, 014326 (2012).
- [41] Y. Shimizu, E. Vigezzi, and R. Broglia, Role of static and dynamic pairing correlations in the superdeformed band of ¹⁵²Dy, Phys. Lett. B **198**, 33 (1987).
- [42] C. Baktash, B. Haas, and W. Nazarewicz, Identical bands in deformed and superdeformed nuclei, Annu. Rev. Nucl. Part. Sci. 45, 485 (1995).
- [43] J. Dobaczewski, W. Nazarewicz, and T. R. Werner, Closed shells at drip-line nuclei, Phys. Scr. **T56**, 15 (1995).
- [44] T. Bengtsson, I. Ragnarsson, and S. Åberg, The role of high-N orbits in superdeformed states, Phys. Lett. B 208, 39 (1988).
- [45] W. Nazarewicz, R. Wyss, and A. Johnson, Structure of superdeformed bands in the $A \approx 150$ mass region, Nucl. Phys. A 503, 285 (1989).
- [46] N. Schunck, J. Dobaczewski, J. McDonnell, W. Satuła, J. A. Sheikh, A. Staszczak, M. Stoitsov, and P. Toivanen, Solution of the Skyrme–Hartree–Fock–Bogolyubov equations in the Cartesian deformed harmonic-oscillator basis.: (VII) hfodd (v2.49t): A new version of the program, Comput. Phys. Commun. 183, 166 (2012).
- [47] J. Bartel, P. Quentin, M. Brack, C. Guet, and H. B. Håkansson, Towards a better parametrisation of Skyrme-like effective forces: A critical study of the SkM force, Nucl. Phys. A 386, 79 (1982).
- [48] M. Bender, J. Dobaczewski, J. Engel, and W. Nazarewicz, Gamow-Teller strength and the spin-isospin coupling constants of the Skyrme energy functional, Phys. Rev. C 65, 054322 (2002).
- [49] A. Goodman, Self-consistent symmetries of the Hartree-Fock-Bogoliubov equations in a rotating frame, Nucl. Phys. A 230, 466 (1974).
- [50] J. Dobaczewski and J. Dudek, Solution of the Skyrme-Hartree-Fock equations in the Cartesian deformed harmonic oscillator basis I. The method, Comput. Phys. Commun. **102**, 166 (1997).

- [51] J. Dobaczewski, J. Dudek, S. G. Rohoziński, and T. R. Werner, Point symmetries in the Hartree-Fock approach. I. Densities, shapes, and currents, Phys. Rev. C 62, 014310 (2000).
- [52] F. S. Stephens, Coriolis effects and rotation alignment in nuclei, Rev. Mod. Phys. 47, 43 (1975).
- [53] S. G. Nilsson and I. Ragnarsson, *Shapes and Shells in Nuclear Structure* (Cambridge University Press, Cambridge, 1995).
- [54] D. Glas, U. Mosel, and P. G. Zint, The cranked harmonic oscillator in coordinate space, Z. Phys. A: At. Nucl. (1975) 285, 83 (1978).
- [55] T. Troudet and R. Arvieu, Shapes of nuclear configurations in a cranked harmonic oscillator model, Ann. Phys. (NY) 134, 1 (1981).
- [56] W. Nazarewicz and J. Dobaczewski, Dynamical Symmetries, Multiclustering, and Octupole Susceptibility in Superdeformed and Hyperdeformed Nuclei, Phys. Rev. Lett. 68, 154 (1992).
- [57] Z. Szymański and W. Nazarewicz, Rotating pseudo-oscillator scheme: Pseudo-spin symmetry and identical bands, Phys. Lett. B 433, 229 (1998).
- [58] M. Radomski, Nuclear rotational current and velocity fields, the cranking model, and transverse electroexcitation of the first excited state of ¹²C, Phys. Rev. C 14, 1704 (1976).
- [59] P. Gulshani and D. J. Rowe, Quantum mechanics in rotating frames. II. The lattice structure of current circulations for a rotating single-particle fluid, Can. J. Phys. 56, 480 (1978).
- [60] J. Kunz and U. Mosel, Flow patterns for collective rotations in heavy nuclei, Nucl. Phys. A 323, 271 (1979).
- [61] J. Fleckner, J. Kunz, U. Mosel, and E. Wuest, Current distributions for rotating nuclei, Nucl. Phys. A 339, 227 (1980).
- [62] M. Durand, P. Schuck, and J. Kunz, Semiclassical description of currents in normal and superfluid rotating nuclei, Nucl. Phys. A 439, 263 (1985).

- [63] H. Laftchiev, D. Samsœn, P. Quentin, and I. N. Mikhailov, Equivalence of pairing correlations and intrinsic vortical currents in rotating nuclei, Phys. Rev. C 67, 014307 (2003).
- [64] J. Bartel, K. Bencheikh, and P. Quentin, Currents, spin densities and mean-field form factors in rotating nuclei: A semi-classical approach, Int. J. Mod. Phys. E 13, 225 (2004).
- [65] A. V. Afanasjev and H. Abusara, From cluster structures to nuclear molecules: The role of nodal structure of the singleparticle wave functions, Phys. Rev. C 97, 024329 (2018).
- [66] K. Petrík and M. Kortelainen, Thouless-Valatin rotational moment of inertia from linear response theory, Phys. Rev. C 97, 034321 (2018).
- [67] T. Dumitrescu and T. Suzuki, Spin distributions in the vibrational excitations of closed-shell nuclei, Nucl. Phys. A 423, 277 (1984).
- [68] J. Xu and B.-A. Li, Probing in-medium spin-orbit interaction with intermediate-energy heavy-ion collisions, Phys. Lett. B 724, 346 (2013).
- [69] Y. Xia, J. Xu, B.-A. Li, and W.-Q. Shen, Spin-orbit coupling and the up-down differential transverse flow in intermediate-energy heavy-ion collisions, Phys. Rev. C 89, 064606 (2014).
- [70] K. Godbey, A. S. Umar, and C. Simenel, Dependence of fusion on isospin dynamics, Phys. Rev. C 95, 011601 (2017).
- [71] V. O. Nesterenko, A. Repko, J. Kvasil, and P.-G. Reinhard, Individual Low-Energy Toroidal Dipole State in ²⁴Mg, Phys. Rev. Lett. **120**, 182501 (2018).
- [72] M. Gennari and P. Navrátil, Nuclear kinetic density from *ab initio* theory, Phys. Rev. C 99, 024305 (2019).
- [73] P. Schwerdtfeger, O. R. Smits, and P. Pyykkö, The periodic table and the physics that drives it, Nat. Rev. Chem. 4, 359 (2020).