Energy-weighted sum rule for nuclear density functional theory

Nobuo Hinohara\textsuperscript{1,2}

\textsuperscript{1}Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan
\textsuperscript{2}Faculty of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

(Dated: March 1, 2019)

The expressions for the energy-weighted sum rule of the isoscalar and isovector coordinate operators are derived based on the second-order fluctuation of the local densities. Conventional derivation of the Thouless theorem for energy-weighted sum rule is based on the double commutator of the Hamiltonian, while the present derivation does not assume a Hamiltonian operator and is applicable to nuclear energy density functionals. The expressions include the contribution of the local gauge symmetry breaking of the energy density functional. It is shown that the local gauge invariance of the kinetic and current densities and kinetic pair density is important, while all the other local densities do not contribute to the energy-weighted sum rule of the coordinate operators. The finite-amplitude method calculations are performed and the expressions for the energy-weighted sum rule are numerically examined for the isoscalar and isovector multipole operators up to $L = 3$ for selected spherical and axially deformed nuclei.

I. INTRODUCTION

In atomic nuclei there are numerous excited states that are originated from the single-particle and collective motion of the constituent nucleons. Thus it is useful to have a few representative quantities of the excited states. The sum rule [1, 2] is a quantity which involves all the excited states, and contains important collective aspects of the properties of the excited states, such as the giant resonances [3] and the Nambu-Goldstone modes [4, 5].

The energy-weighted sum rule is the most commonly used one among various energy moment of the sum rules. Although it is a summation over all the excited states, the Thouless theorem [6] allows us to evaluate the sum-rule value that is the summation over all the excited states computed through the random-phase approximation (RPA) using the expectation value of the double commutator of the Hamiltonian at the ground state computed within the self-consistent Hartree-Fock (HF) theory. The theorem has been proven also for the Hartree-Fock-Bogoliubov (HFB) + quasiparticle RPA (QRPA) [7], and the second RPA [8, 9]. The double commutator of the Hamiltonian becomes simple for the isoscalar and isovector coordinate operators. In the zero-range Skyrme force, only the kinetic-energy term in the Hamiltonian contributes to the energy-weighted sum for an isoscalar coordinate operator, and the kinetic-energy term and momentum-dependent terms in the interaction contribute to the energy-weighted sum rule of an isovector coordinate operator. Therefore, the Thouless theorem significantly reduces the computational costs of the energy-weighted sum rule, and is also useful for verifying the accuracy of the QRPA calculation.

Nuclear density functional theory (DFT) can be regarded as a starting point of the mean-field models [10, 11]. In nuclear DFT, the form of the energy density functional (EDF) is not given a priori. Several EDFs based on the non-relativistic Skyrme and Gogny forces, and relativistic theory are widely used. The EDF of these types can be derived from the corresponding effective interaction. In that case one can go back to the Hamiltonian (effective interaction) starting from the EDF. However in general, there is no direct correspondence to the effective interaction in the nuclear DFT, if the EDF and its coupling constants are constructed directly by reproducing a representative set of the experimental observables. The existence of the Hamiltonian operator is not guaranteed.

Although the Thouless theorem has been applied widely within the framework of the nuclear DFT, to the best of our knowledge, it has not been proven for the nuclear DFT where the EDF does not correspond to a Hamiltonian operator, and thus the double-commutator expression cannot be justified. This includes the case when the EDF is constructed independent of the interactions (such as UNEDF functionals [12–15]). Even the standard Skyrme HFB calculation is not carried out within the two-body and three-body Skyrme effective interaction. Prescriptions used in the spin-orbit and tensor functional may break the correspondence with the Hamiltonian. The standard Skyrme spin-orbit interaction has a single interaction strength $W_0$ and it determines the isoscalar and isovector coupling constants of the spin-orbit functional. In several Skyrme EDFs, additional parameter $b_4'$ is introduced to control the isovector property of the spin-orbit functional [16]. The tensor-density (spin-current density) terms appear from the momentum-dependent $t_1$ and $t_2$ terms of the Skyrme effective interaction even without including the tensor effective interactions ($t_c$ and $t_o$ terms). However, because of the complicated treatment of the tensor-density terms in deformed nuclei, the contribution from this term is often neglected except for a few parameter sets such as SLy5 [17] and SkP [18]. Moreover, the existence of the two-body density-dependent term will also lose the connection to the Hamiltonian operator (However the density-dependent force has been shown not to contribute on the Thouless theorem [1]). Another issue is the treatment of the pairing interaction. Except for the SkP interaction, the pairing interaction used in the standard Skyrme
HFB calculation has a simple form and density dependence, and is independent with the particle-hole interaction, while in the mean-field approach starting from an effective interaction, the same interaction should provide the Hartree-Fock potential and pairing potential.

In our previous work [19], it has been numerically shown that in SLy4 EDF, the inclusion of the time-odd current terms is necessary to recover the energy-weighted sum-rule values of the Thouless theorem, and that other terms in the time-odd functional do not impact the values of the energy-weighted sum rule at all. The time-odd current terms are necessary in order to satisfy the Galilean invariance of the EDF. More generalized form of the EDF could be used in the future, and thus it is desired to understand the applicability of the Thouless theorem in the nuclear DFT. We note that Kerman-Onishi condition can be derived to the HFB state, and within the nuclear DFT [22–24].

In this paper we consider a fluctuation to the HFB state, and compare the fluctuation of the energy in two ways to derive the expression of the energy-weighted sum rule. This derivation can be applied to the nuclear EDF which does not have a corresponding Hamiltonian operator [20, 21], and note that the lack of the relation with the Hamiltonian formalism can cause problems when evaluating the energy of the quantum-number projected state within the nuclear DFT [22–24].

The aim of this paper is to derive the expression for the energy-weighted sum rule within the nuclear DFT without using the double commutator of the Hamiltonian. We consider a fluctuation to the HFB state, and compare the fluctuation of the energy in two ways to derive the expression of the energy-weighted sum rule. This derivation can be applied to the nuclear EDF which does not have a corresponding Hamiltonian operator.

This paper is organized as follows. In Sec. II, the nuclear EDF is introduced. Section III recapitulates the conventional derivation of the Thouless theorem based on the double commutator of the Hamiltonian, then presents the derivation for the nuclear EDF. Section IV summarizes the energy-weighted sum rule calculation based on complex-energy finite-amplitude method. In Sec. V, energy-weighted sum-rule values of various multipole operators are numerically calculated using the complex-energy finite-amplitude method, and are compared with the values of the Thouless theorem derived for general nuclear EDFs. Conclusions are given in Sec. VI.

II. NUCLEAR EDF

We consider a general form of the nuclear EDF of the Skyrme type that is quadratic in local densities (except for the density-dependent terms) and can contain up to two spacial derivatives but without neutron-proton mixing [25, 26]. The nuclear EDF has the following form

\[ E[\rho, \tilde{\rho}] = \int dr E(r), \]

\[ E(r) = \frac{\hbar^2}{2m} \tau_0(r) + \sum_{k=0} \chi_k(r) + E_{\text{Coul}}(r) + \sum_{t=n,p} \tilde{\chi}_t(r), \]

where the first term in Eq. (2) is the isoscalar kinetic energy, \( \chi_k \) is the isoscalar \((k = 0)\) and isovector \((k = 1)\) particle-hole EDF, \( E_{\text{Coul}} \) is the Coulomb energy functional, and \( \tilde{\chi}_t \) are the neutron \((t = n = 1/2)\) and proton \((t = p = -1/2)\) pairing EDF. Throughout this paper, we use the index \( k \) to specify the isoscalar or isovector character, and the index \( t \) for neutrons or protons.

The particle-hole EDF is given by its time-even and time-odd parts

\[ \chi_k(r) = \chi_k^{\text{even}}(r) + \chi_k^{\text{odd}}(r), \]

\[ \chi_k^{\text{even}}(r) = C_k^{\rho\rho}[\rho_0] \rho_k^2 + C_k^{\rho\Delta} \rho_k \Delta \rho_k + C_k^{\rho\tau} \rho_k \tau_k + C_k^{\rho J} J_k^2 + C_k^{\rho J^2} J_k^2, \]

\[ \chi_k^{\text{odd}}(r) = C_k^{s\rho}[\rho_0] s_k^2 + C_k^{s\Delta} s_k \Delta s_k + C_k^{s\tau} s_k \tau_k + C_k^{s J} s_k \cdot (\nabla \times J_k) + C_k^{s J^2} s_k \cdot (\nabla \times s_k) \]

\[ + C_k^{s J^2} s_k \cdot F_k. \]

The time-even part is composed with the particle-hole density \( \rho_k \), kinetic density \( \tau_k \), pseudoscalar, pseudovector, and pseudotensor densities \( J_k, J_k' \), and \( J_k \). The time-odd parts are described with the spin density \( s_k \), spin-kinetic density \( T_k \), current density \( j_k \), and tensor-kinetic density \( F_k \). Definitions of these local densities are summarized in Appendix A. Some of the coupling constants \( C_k^s \) and \( C_k^{J^2} \) have isoscalar-density dependence. In the Skyrme force, all the coupling constants are basically derived from the effective interactions, while in the UNEDF optimizations [12–15], only the time-even coupling constants are determined. For the even-even systems with the time-reversal symmetry, the time-odd functionals turn on only in the linear response calculation. The Coulomb functional is composed of the direct and exchange terms, and are functionals of the proton particle-hole density only \( [\rho_p = (\rho_0 - \rho_1)/2] \)

\[ E_{\text{Coul}}(r) = E_{\text{dir}}(r) + E_{\text{ex}}(r), \]

\[ E_{\text{dir}}(r) = \frac{1}{2} \frac{\hbar^2}{2m} \rho_p(r) \int dr' \frac{\rho_p(r')}{|r - r'|}, \]

\[ E_{\text{ex}}(r) = -\frac{e^2}{4} \frac{3}{\pi} \left( \frac{3}{5} \right) \rho_p(r)^{\frac{3}{2}}. \]

The general form of the pairing EDF that is quadratic in local pair densities is given by

\[ \tilde{\chi}_t(r) = \tilde{C}_t^\rho \rho_0 \rho_1 |\tilde{\rho}_t|^2 + \tilde{C}_t^{2\rho\rho} \rho_0 \rho_1 |\tilde{\rho}_t| |\tilde{\rho}_t| + \tilde{C}_t^{2\rho J} \rho_0 \rho_1 |\tilde{\rho}_t| J_t^2 + \tilde{C}_t^{2\rho J^2} \rho_0 \rho_1 J_t^2 \]

\[ + \tilde{C}_t^{2\rho J^2} \rho_0 \rho_1 (\nabla \times J_t) \]

with the pair density \( \tilde{\rho}_t \), kinetic pair density \( \tau_t \), and tensor pair densities \( J_t, J_t' \), and \( J_t \). In most of the Skyrme EDFs, only the first term with an isoscalar-density dependence is used in the pairing EDF

\[ \tilde{C}_t^\rho \rho_0 = \frac{V_t}{4} \left( 1 - \eta \frac{\rho_0(r)}{\rho_c} \right), \]

where \( V_t \) is the strength and \( \eta \) controls the isoscalar-density dependence.
III. THOULESS THEOREM FOR ENERGY-WEIGHTED SUM RULE

A. Operator derivation

First we recapitulate the conventional derivation of the Thouless theorem [6] based on the discussion in Ref. [1]. We consider a system described by a Hamiltonian of the Skyrme interaction

\[ \hat{H} = \hat{T} + \hat{V}, \]  
\[ \hat{T} = \frac{1}{2m} \sum_{i=1}^{A} \hat{p}_i^2, \]  
\[ \hat{V} = \sum_{i<j} t_0 (1 + x_0 \hat{P}^o) \delta(\hat{r}_{ij}) \]

where \( \hat{r}_{ij} = \hat{r}_i - \hat{r}_j, \hat{P}^o = (1 + \hat{\sigma}_i \cdot \hat{\sigma}_j)/2 \) is the spin-exchange operator, \( \hat{\Sigma} = 3(\hat{\sigma}_i \cdot \hat{e}_r)(\hat{\sigma}_j \cdot \hat{e}_r) - \hat{\sigma}_i \cdot \hat{\sigma}_j \) is the tensor operator, and

\[ \hat{k} = \frac{1}{2i} (\nabla_i - \nabla_j), \]
\[ \hat{k}' = -\frac{1}{2i} (\nabla_i - \nabla_j). \]

The energy-weighted sum rule of an operator \( \hat{F} \) is expressed in terms of the double commutator of the Hamiltonian

\[ m_1(\hat{F}^{IS}) = \sum_{\lambda, \Omega_\lambda > 0} \Omega_\lambda |\langle \lambda | \hat{F} | 0 \rangle|^2 \]
\[ = -\frac{1}{2} (\langle \Psi_{\text{HFB}} | [\hat{H}, \hat{F}] | \Psi_{\text{HFB}} \rangle), \]  

where \( |\Psi_{\text{HFB}}\rangle \) is the HFB state, \( |0\rangle \) is the QRPA correlated ground state, \( |\lambda\rangle \) is the QRPA-\( \lambda \)-th excited state with an excitation energy \( \Omega_\lambda = E_\lambda - E_0 \). When the operator \( \hat{F} \) is an isoscalar-coordinate type

\[ \hat{F}^{IS} = \alpha \sum_{i=1}^{A} f(\hat{r}_i), \]  

it can be shown that the double commutator of the interaction term cancels, and the contribution to the energy-weighted sum rule is from the momentum operator in the kinetic-energy term in the Skyrme interaction

\[ m_1(\hat{F}^{IV}) = \frac{1}{2} \langle [\hat{T} + \hat{V}, \hat{F}^{IV}] | \hat{F}^{IV} \rangle \]
\[ = \alpha^2 \frac{\hbar^2}{2m} \int dr |\nabla f(\hat{r})|^2 \rho_0(\hat{r}). \]

The momentum-independent terms with \( t_0 \) and \( t_3 \) are shown to commute with the coordinate operator. The \( t_1 \) and \( t_2 \) terms can be written as

\[ \hat{V}_{t_1,t_2} = \frac{1}{2} \sum_{i,j=1}^{A} \left( \frac{t_1}{8\hbar^2} [\hat{p}_{ij}^2, \delta(\hat{r}_{ij})] + \frac{t_2}{4\hbar^2} \hat{p}_{ij} \delta(\hat{r}_{ij}) \hat{p}_{ij} \right), \]

where \( \hat{p}_{ij} = \hat{p}_i - \hat{p}_j \). The first term is the second derivative of the \( \delta \) function, and commutes with any coordinate operator. The commutator with the second term is shown to be

\[ [\hat{V}_{t_1,t_2}, \hat{F}^{IS}] = \frac{1}{8\hbar^2} (t_1 + t_2) \sum_{i,j,k=1}^{A} [\hat{p}_{ij} \delta(\hat{r}_{ij}) \hat{p}_{ik}, f(\hat{r}_k)] \]
\[ = \frac{t_1 + t_2}{8\hbar^2} \sum_{i,j,k=1}^{A} \{ \hat{p}_{ij} \hat{p}_{ik}, f(\hat{r}_k) \} \]
\[ = -\frac{t_1 + t_2}{4\hbar} \sum_{i,j=1}^{A} \{ \hat{p}_{ij}, [\nabla f(\hat{r}_i), \delta(\hat{r}_{ij})] \}
\[ = 0, \]

as interchanging \( i \) and \( j \) changes the sign. In the same way, one can derive that the commutators with the \( t_e \), \( t_o \), and \( W_0 \) terms become zero.

For the isovector operator

\[ \hat{F}^{IV} = \sum_{i=1}^{A} \alpha_i f(\hat{r}_i) r_3(t_i), \]

where \( r_3(t_i) = 2t_i \), generally both the kinetic and interaction parts of the Hamiltonian contribute to the energy-weighted sum rule [2]

\[ m_1(\hat{F}^{IV}) = -\frac{1}{2} \langle [\hat{T} + \hat{V}, \hat{F}^{IV}] | \hat{F}^{IV} \rangle \]
\[ = m_1^{\text{kin}}(\hat{F}^{IV}) \left[ 1 + \kappa(\hat{F}^{IV}) \right], \]  

where \( m_1^{\text{kin}}(\hat{F}^{IV}) \) is the contribution from the kinetic en-
where we note that the contribution with the enhancement factor $\kappa(\hat{F}^{\text{IV}})$ shows the relative contribution of the interaction-energy term with respect to the kinetic part to the energy-weighted sum rule. The potential contribution is from the second term in Eq. (19). The spin-exchange parts with $x_1$ and $x_2$ also contribute with $\frac{1}{2}$ factor from $\hat{F}^{\text{IV}}$ operator, as the $\sigma_i \cdot \sigma_j$ part produces the spin density which is zero for even-even systems.

\begin{align}
m^{\text{kin}}_1(\hat{F}^{\text{IV}}) &= \frac{1}{2}\langle[[\hat{T}, \hat{F}^{\text{IV}}], \hat{F}^{\text{IV}}]\rangle \\
&= \frac{\hbar^2}{2m} \sum_{i=1}^{A} \alpha_i \frac{2}{2} \left\langle \left[ \nabla f(\hat{r}_i) \right]^2 \right\rangle \\
&= \frac{\hbar^2}{2m} \int d\rho \left[ \nabla f(r) \right]^2 [\alpha_n \rho_n(r) + \alpha_p \rho_p(r)],
\end{align}

(23)

and the enhancement factor $\kappa(\hat{F}^{\text{IV}})$ is given by

\begin{equation}
\kappa(\hat{F}^{\text{IV}}) = \frac{1}{\kappa(\hat{F}^{\text{HFB}})}.
\end{equation}

(24)

These expressions for the energy-weighted sum rule are based on the operator expressions of the kinetic and interaction terms. Strictly speaking in the nuclear EDF, because there is no correspondence between the EDF and the Hamiltonian operator $H$, we cannot derive Eqs. (18), (23), and (25) in the same manner. In the next subsection the expressions for the energy-weighted sum rule are derived without assuming the Hamiltonian operator.

### B. Derivation for nuclear EDF

We consider a small fluctuation starting from an HFB state $|\Psi_{\text{HFB}}\rangle$. As the HFB state is a vacuum of quasiparticles, $\hat{a}_\mu |\Psi_{\text{HFB}}\rangle = 0$, following the discussion in Sec. 10.2 of Ref. [27], such a fluctuation from the HFB state can be described by a quasiparticle-quasihole, quasiparticle-quasiparticle, and quasihole-quasihole densities. The quasihole-quasihole and quasiparticle-quasihole densities are given by

\begin{equation}
\bar{\pi}_{\mu \nu} = \langle \Phi'| \hat{a}_\mu \hat{a}_\nu | \Phi' \rangle,
\end{equation}

(26)

\begin{equation}
\bar{\pi}_{\mu \nu}' = \langle \Phi'| \hat{a}_\mu^\dagger \hat{a}_\nu | \Phi' \rangle,
\end{equation}

(27)

where the state $|\Phi'\rangle$ includes a small fluctuation. The coherent state representation of the state $|\Phi'\rangle$ gives that $\tilde{\rho}$ is shown to be a higher order in $\kappa$, $\tilde{\rho} \sim (\kappa \hat{\kappa})$. The small-amplitude expansion of the energy from the HFB state is given as an expansion with respect to $\kappa$ and $\kappa^*$

\begin{equation}
E'[\kappa, \kappa^*] = E_0 + \frac{1}{2} (\kappa^*) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \kappa \kappa^* \end{pmatrix} + O(|\kappa|^3),
\end{equation}

(28)

where $E'$ is the HFB value of the EDF (with particle-number constraint term), $A$ and $B$ are the QRPA matrices given by

\begin{equation}
A_{\rho \sigma, \mu \nu} = \delta_{\rho \mu} \delta_{\sigma \nu} (E_\mu + E_\nu) + \frac{\partial^2 E'}{\partial \kappa^* \partial \kappa_{\mu \nu}},
\end{equation}

(29)

\begin{equation}
B_{\rho \sigma, \mu \nu} = \frac{\partial^2 E'}{\partial \kappa_{\mu \nu} \partial \kappa_{\rho \sigma}},
\end{equation}

(30)

with the quasiparticle energies $E$.

Let us suppose that this small fluctuation is given with a Hermitian operator $\hat{F}$

\begin{equation}
|\Phi'\rangle = e^{i\eta \hat{F}} |\Psi_{\text{HFB}}\rangle,
\end{equation}

(31)

where $\eta$ is a small real parameter. The operator $\hat{F}$ is written in the quasiparticle representation as

\begin{equation}
\hat{F} = (\Psi_{\text{HFB}} | \hat{F} | \Psi_{\text{HFB}}\rangle
\end{equation}

(32)

where $F^{02} = F^{20}$. From Eqs. (31) and (32) we can express the quasihole-quasihole densities $\kappa$ in Eq. (26) in terms of the matrix element $F^{20}$ and $F^{02}$ as

\begin{equation}
\bar{\pi}_{\mu \nu} = \langle \Psi_{\text{HFB}} | e^{-i\eta \hat{F}} \hat{a}_\mu \hat{a}_\nu | \Psi_{\text{HFB}}\rangle = -i\eta F^{20}_{\mu \nu},
\end{equation}

(33)

\begin{equation}
\bar{\pi}_{\mu \nu}' = \langle \Psi_{\text{HFB}} | e^{-i\eta \hat{F}} \hat{a}_\mu^\dagger \hat{a}_\nu^\dagger | \Psi_{\text{HFB}}\rangle = i\eta F^{02}_{\mu \nu}.
\end{equation}

(34)

The energy of this state with the fluctuation $|\Phi'\rangle$ is given by

\begin{equation}
E'[-i\eta F^{20}, i\eta F^{02}] = E_0 + \eta^2 m_1(\hat{F}) + O(\eta^3),
\end{equation}

(35)

where

\begin{equation}
m_1(\hat{F}) = \frac{1}{2} \begin{pmatrix} F^{02} & -F^{20} \\ F^{20} & -F^{02} \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} F^{20} \end{pmatrix}.
\end{equation}

(36)

Equation (36) is derived by applying the QRPA equations

\begin{equation}
\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\lambda \\ Y^\lambda \end{pmatrix} = \Omega_{\lambda} \begin{pmatrix} X^\lambda \\ Y^\lambda \end{pmatrix}
\end{equation}

(37)
The local densities in the EDF transform as
\[
\rho'_k = \rho_k, \\
\tau'_k = \tau_k + 2p \cdot j_k + p^2 \rho_k, \\
s'_k = s_k, \\
T'_k = T_k + 2p \cdot J_k + p^2 s_k, \\
\tilde{j}'_k = j_k + p \rho_k, \\
F'_k = F_k + p J_k + J_k \cdot p + p (p \cdot s_k), \\
\tilde{\rho}'_t = e^{2i\eta\alpha} \tilde{\rho}_t, \\
\tilde{\tau}'_t = e^{2i\eta\alpha} (\tilde{\tau}_t + ip \cdot \nabla \tilde{\rho}_t - p^2 \tilde{\rho}_t), \\
\tilde{\gamma}'_t = e^{2i\eta\alpha} \gamma_t.
\]

For the local gauge invariant EDF, the transformation above does not change the EDF in Eq. (2), except for the kinetic-energy term. From Eq. (49), the kinetic-energy term transforms as
\[
E'_\text{kin} = \frac{\hbar^2}{2m} \int dr r'_0 = \frac{\hbar^2}{2m} \int dr [\tau_0 + 2\eta\alpha (\nabla f) \cdot j_0 + \eta^2 \alpha^2 (\nabla f)^2 \rho_0].
\]

The term proportional to $\eta^2$ contributes to the energy-weighted sum rule of the isoscalar operator. Then we have
\[
m_1(\tilde{F}^{\text{IS}}) = \frac{\hbar^2}{2m} \alpha^2 \int dr [\nabla f(r)]^2 \rho_0(r)
\]
for the local gauge invariant EDF.

This is the derivation of the Thouless theorem without using the Hamiltonian operator and double commutator. Only the local gauge invariance property of the EDF is imposed in the derivation, and thus the existence or absence of the spin, spin-orbit, and density-dependent terms both in the particle-hole and pairing channels does not contribute to the energy-weighted sum rule as long as the EDF is local gauge invariant. As for the pairing channel, local gauge invariant pairing EDF does not contribute to the energy-weighted sum rule. Such local gauge invariant EDFs are not limited to the ones with the isoscalar density dependence considered in Eq. (10), but including isovector density dependence [32] and Fayans functional with particle-hole density-gradient dependence [33].

We can consider a general EDF that does not hold the local gauge invariance. Without the local gauge invariance, the transformation introduces additional terms, but when computing the energy of the transformed state, the densities of an even-even nucleus are used. Therefore any time-odd densities included in the transformed EDF vanish. The contribution from the spin-orbit and tensor terms produce terms proportional to the spin density $s$, and thus they do not contribute to the energy-weighted
sum as well. The Coulomb functionals are written with the proton local densities only, and they are local gauge invariant. Thus the possible contributions are from the $\rho_k \tau_k$ and $\bar{\rho}_k^2$ terms in the particle-hole EDF, and Re$\bar{\rho}_k^2 \tau_k$ and Re$\bar{\rho}_k \Delta \rho_k$ terms in the pairing EDF. The particle-hole part and pairing part of the EDF transformations as

$$\int d\mathbf{r} \chi_k[\rho'_k, \tau'_k, \cdots] = \int d\mathbf{r} \left\{ \chi_k[\rho_k, \tau_k, \cdots] + (C_k^T + C_k^\dagger)p^2 \rho_k^2 \right\} + (C_k^T + C_k^\dagger)p^2 \rho_k^2,$$

$$\int d\mathbf{r} \tilde{\chi}_k[\rho'_k, \bar{\rho}'_k, \tau'_k, \cdots, \rho'_0] = \int d\mathbf{r} \left\{ \tilde{\chi}_k[\rho_k, \bar{\rho}_k, \tau_k, \cdots, \rho_0] - (4\tilde{C}_k^\Delta \rho + \tilde{C}_k^\tau)|\rho_k|^2 \right\} + (4\tilde{C}_k^\Delta \rho + \tilde{C}_k^\tau)|\rho_k|^2,$$

where we kept terms which are non-zero in time-reversal symmetric even-even systems.

The combinations of the coefficients ($C_k^T + C_k^\dagger$) and ($4\tilde{C}_k^\Delta \rho + \tilde{C}_k^\tau$) show that these additional terms exist only when the local gauge symmetry of $\rho_k \tau_k - \bar{\rho}_k^2$ and/or Re($4\tilde{C}_k^\Delta \bar{\rho}_k - \tilde{C}_k^\tau \bar{\tau}_k$) is broken. By taking the terms that are second order in $\eta$ and performing the integration, the Thouless theorem for the isoscalar operator in the nuclear EDF is derived

$$m_1^{(\text{FS})} = \alpha^2 \int d\mathbf{r} |\nabla f(r)|^2 \left\{ \frac{\hbar^2}{2m} \rho_0(r) \right\} + \sum_{k=0}^{1} (C_k^T + C_k^\dagger)\rho_k(r)^2 - \sum_{t=n,p}(4\tilde{C}_t^\Delta \rho + \tilde{C}_t^\tau)|\rho_t(r)|^2 \right\}.$$

We note that in Ref. [2] it is discussed that the sum rule is obtained by the exact cancellation of the potential contribution to the effective mass (\rho-$\eta$-term) and the isoscalar current-current interaction in the RPA level for the system with $N = Z$ and without spin-orbit interaction. The present derivation based on the local gauge transformation gives a unified view, including the contribution from the local gauge symmetry breaking of the isovector current terms and pairing EDF, and that the local gauge symmetry breaking in the spin-orbit and tensor functionals are shown not to play any role for the energy-weighted sum rule of the isoscalar coordinate operators.

### D. Isovector operator

The energy-weighted sum rule of the isovector operator for nuclear EDF can be derived by generating the fluctuation using the isovector operator in Eq. (21). Let us consider a corresponding transformation with the isovector operator

$$|\Psi'\rangle = \exp \left\{ i\eta \sum_{t=1}^A \alpha_t f(\hat{r}_t) \tau_3(t_i) \right\} |\Psi_{\text{HFB}}\rangle.$$

Because this transformation is not a local gauge transformation, even the local gauge invariant EDF is not invariant under this transformation.

The density matrices transform with Eq. (63) as

$$\tilde{\rho}'(rs, s's'; t) = e^{i(2t)\eta(\alpha_t[f(r) - f(r')])} \tilde{\rho}(rs, s's'; t),$$

$$\tilde{s}'(rs, s's'; t) = e^{i(2t)\eta(\alpha_t[f(r) + f(r')])} \tilde{s}(rs, s's'; t).$$

Then non-local densities of neutrons and protons transform as

$$\rho'_t(r, r') = e^{i(2t)\eta(\alpha_t[f(r) - f(r')])} \rho_t(r, r'),$$

$$s'_t(r, r') = e^{i(2t)\eta(\alpha_t[f(r) + f(r')])} s_t(r, r'),$$

$$\tilde{\rho}'(r, r') = e^{i(2t)\eta(\alpha_t[f(r) - f(r')])} \tilde{\rho}(r, r'),$$

$$\tilde{s}'(r, r') = e^{i(2t)\eta(\alpha_t[f(r) + f(r')])} \tilde{s}(r, r').$$

Note that the indices in Eqs. (66) and (67) are $t$. We define local momentum fields of neutron and proton

$$p_t(r) = (2t)\eta \alpha_t \nabla f(r).$$

The transformation in Eq. (63) does not mix the neutron and proton phase. Therefore the isoscalar and isovector
local densities transform as

\[
p'_k = \rho_k,
\]
\[
\tau'_0 = \tau_0 + (p_n + p_p) \cdot j_0 + \frac{1}{2} (p_n^2 + p_p^2) \rho_0
\]
\[
+ (p_n - p_p) \cdot j_1 + \frac{1}{2} (p_n^2 - p_p^2) \rho_1,
\]
\[
\tau'_1 = \tau_1 + (p_n + p_p) \cdot j_1 + \frac{1}{2} (p_n^2 + p_p^2) \rho_1
\]
\[
+ (p_n - p_p) \cdot j_0 + \frac{1}{2} (p_n^2 - p_p^2) \rho_0,
\]
\[
s'_k = s_k,
\]
\[
T'_0 = T_0 + (p_n + p_p) \cdot j_0 + \frac{1}{2} (p_n^2 + p_p^2) s_0
\]
\[
+ (p_n - p_p) \cdot j_1 + \frac{1}{2} (p_n^2 - p_p^2) s_1,
\]
\[
T'_1 = T_1 + (p_n + p_p) \cdot j_1 + \frac{1}{2} (p_n^2 + p_p^2) s_1
\]
\[
+ (p_n - p_p) \cdot j_0 + \frac{1}{2} (p_n^2 - p_p^2) s_0,
\]
\[
J'_0 = j_0 + \frac{1}{2} (p_n + p_p) p_0 + \frac{1}{2} (p_n - p_p) p_1,
\]
\[
J'_1 = j_1 + \frac{1}{2} (p_n + p_p) p_1 + \frac{1}{2} (p_n - p_p) p_0,
\]
\[
F'_0 = F_0 + \frac{1}{2} (p_n + p_p) j_0 + \frac{1}{2} (p_n - p_p) j_1
\]
\[
+ \frac{1}{2} j_0 \cdot (p_n + p_p) + \frac{1}{2} j_1 \cdot (p_n - p_p)
\]
\[
+ \frac{1}{2} (p_n \cdot s_0) p_n + (p_p \cdot s_0) p_p
\]
\[
+ (p_n \cdot s_1) p_n - (p_p \cdot s_1) p_p,
\]
\[
F'_1 = F_1 + \frac{1}{2} (p_n + p_p) j_1 + \frac{1}{2} (p_n - p_p) j_0
\]
\[
+ \frac{1}{2} j_1 \cdot (p_n + p_p) + \frac{1}{2} j_0 \cdot (p_n - p_p)
\]
\[
+ \frac{1}{2} (p_n \cdot s_1) p_n + (p_p \cdot s_1) p_p
\]
\[
+ (p_n \cdot s_0) p_n - (p_p \cdot s_0) p_p,
\]
\[
J'_0 = J_0 + \frac{1}{2} (p_n + p_p) \otimes s_0 + \frac{1}{2} (p_n - p_p) \otimes s_1,
\]
\[
J'_1 = J_1 + \frac{1}{2} (p_n + p_p) \otimes s_1 + \frac{1}{2} (p_n - p_p) \otimes s_0,
\]
\[
\tilde{\rho}'_k = \tilde{\rho}_k e^{2i(2 \tau' + \varphi)} f \tilde{\rho}_k,
\]
\[
\tilde{\tau}'_k = e^{2i(2 \tau' + \varphi)} (\tilde{\tau}_k + i \tilde{p}_k \cdot \nabla \tilde{\rho}_k - \tilde{p}_k^2 \tilde{\rho}_k),
\]
\[
\tilde{J}'_k = e^{2i(2 \tau' + \varphi)} \tilde{J}_k.
\]

We then consider an EDF transformed with Eq. (63)

\[
E'[-i\eta F^{20}, i\eta F^{02}] = \int dr \left\{ \frac{\hbar^2}{2m} \tau'_0 + \frac{1}{2} \sum_{k=0}^{1} \chi_k [\rho'_k, \tau'_k, \cdots] \right. 
\]
\[
+ \sum_{l=m,n,p} \bar{\chi}_l [\rho'_l, \tilde{\rho}'_l, \tilde{\tau}'_l, \cdots, \rho_0] \right\}
\]
\[
+ O(\eta^3).
\]

The kinetic-energy term transforms as

\[
\frac{\hbar^2}{2m} \tau'_0 = \frac{\hbar^2}{2m} \left[ \tau_0 + (p_n + p_p) \cdot j_0 + \frac{1}{2} (p_n^2 + p_p^2) \rho_0 \right. 
\]
\[
+ (p_n - p_p) \cdot j_1 + \frac{1}{2} (p_n^2 - p_p^2) \rho_1 \right]
\]
\[
+ \left. (p_n - p_p) \cdot j_0 + \frac{1}{2} (p_n^2 - p_p^2) \rho_0 \right].
\]

The kinetic-energy term transforms as

\[
\int dr \sum_{k=0}^{1} \chi_k [\rho'_k, \tau'_k, \cdots]
\]
\[
= \int dr \sum_{k=0}^{1} \left\{ \chi_k [\rho_k, \tau_k, \cdots] \right. 
\]
\[
+ C_0^+ \left[ (\rho'_k \tau'_k - j'_k^2) - (\rho_k \tau_k - j_k^2) \right] \left. \right\}
\]
\[
= \int dr \left\{ \sum_{k=0}^{1} \chi_k [\rho_k, \tau_k, \cdots] \right. 
\]
\[
+ \frac{1}{4} (C_0^+ - C_1^+) (p_n - p_p)^2 (\rho_0^2 - \rho_1^2) \left. \right\}
\]
\[
= m_1^{\text{kin}} (\tilde{F}^{IV}) \left[ 1 + \kappa (\tilde{F}^{IV}) \right].
\]

The fluctuation of the pairing EDF does not contribute because the neutron and proton terms are independent in the pairing EDF. By taking the terms proportional to \( \eta^2 \) from Eqs. (87) and (88), we have

\[
m_1^{\text{kin}} (\tilde{F}^{IV}) = \int dr [\nabla f(r)]^2 \left\{ \frac{\hbar^2}{2m} \left[ \alpha_n^2 \rho_n(r) + \alpha_p^2 \rho_p(r) \right] 
\]
\[
+ (C_0^+ - C_1^+) (\alpha_n + \alpha_p)^2 \rho_n(r) \rho_p(r) \right\}
\]
\[
= m_1^{\text{kin}} (\tilde{F}^{IV}) \left[ 1 + \kappa (\tilde{F}^{IV}) \right].
\]

The first term is the kinetic-energy contribution, and the ratio to the second term defines the isovector enhancement factor \( \kappa (\tilde{F}^{IV}) \)

\[
m_1^{\text{kin}} (\tilde{F}^{IV}) = \frac{\hbar^2}{2m} \int dr [\nabla f(r)]^2 \left[ \alpha_n^2 \rho_n(r) + \alpha_p^2 \rho_p(r) \right],
\]
\[
\kappa (\tilde{F}^{IV}) = \frac{2m}{\hbar^2} (C_0^+ - C_1^+) (\alpha_n + \alpha_p)^2
\]
\[
\times \frac{\int dr [\nabla f(r)]^2 \rho_n(r) \rho_p(r)}{\int dr [\nabla f(r)]^2 \left[ \alpha_n^2 \rho_n(r) + \alpha_p^2 \rho_p(r) \right]}.
\]

\( \alpha_n = \alpha_p = 1 \) produces Eqs. (6.32) and (6.38) in Ref. [2]

\[
m_1^{\text{kin}} (\tilde{F}^{IV}) = \frac{\hbar^2}{2m} \int dr [\nabla f(r)]^2 \rho_0(r),
\]
\[ \kappa = \frac{8m}{\hbar^2} (C_0^R - C_1^R) \frac{\int dr |\nabla f(r)|^2 \rho_n(r) \rho_p(r)}{\int dr |\nabla f(r)|^2 \rho_0(r)}. \]  
(93)

We often use \( \alpha_n = Z/A, \alpha_p = N/A \), especially for the dipole operator to remove the contribution of the center of mass motion. In the case of the isovector dipole operators \( f(r) = f_{1K}^{IV}(r)(K = 0, 1) \), we have a model-independent kinetic contribution (Thomas-Reiche-Kuhn sum rule [34-36]):

\[ m_{1K}^{\text{kin}}(f_{1K}^{IV}) = \frac{\hbar^2}{2m} \frac{3}{4\pi} \frac{NZ}{A}. \]  
(94)

\[ \kappa_{1K}^{IV} = \frac{2m A}{\hbar^2} \frac{NZ}{(C_0^R - C_1^R)} \int dr \rho_n(r) \rho_p(r). \]  
(95)

If the EDF does not hold the local gauge invariance, again all the additional terms to the energy-weighted sum rule in the particle-hole channel come from \( \rho_k \tau_k \) and \( \vec{j}_k \) terms, 

\[ \int dr \sum_{k=0}^{1} \left( C_k^R \rho_k \tau_k + C_k^I \vec{j}_k \right)^2 \]

\[ = \int dr \left\{ \sum_{k=0}^{1} C_k^R \rho_k \tau_k + (C_0^R - C_1^R)(\rho_n - \rho_p)^2 \rho_n \rho_p + (C_0^I + C_0^I + C_1^I)(\rho_n^2 \rho_p^2 + \rho_p^2 \rho_n^2) + 2(C_0^I + C_1^I - C_1^I - C_1^I) \rho_n \cdot \rho_p \rho_n \rho_p \right\}. \]  
(96)

The second term in the right hand side of Eq. (96) is the contribution to the enhancement factor. The third and fourth terms vanish when the EDF is local gauge invariant for \( \rho_k \tau_k \) and \( \vec{j}_k \) terms \( (C_k^I = -C_k^I) \).

The pairing EDF transforms as

\[ \tilde{\chi}_1 [\tilde{\rho}_n \tilde{\rho}_p, \tau^0_i, \cdots, \rho^0_0] = \tilde{\chi}_1 [\tilde{\rho}_n \tilde{\rho}_p, \tau^0_i, \cdots, \rho^0_0] - (4 \tilde{C}_1^{\Delta p} + \tilde{C}_1^{I}) \rho_n^2 |\tilde{\rho}_n|^2, \]  
(97)

and produces contributions from the local gauge symmetry breaking. The energy-weighted sum rule of an isovector operator for the nuclear EDF is then given by

\[ m_{11}(\tilde{F}^{IV}) = \int dr |\nabla f(r)|^2 \left\{ \frac{\hbar^2}{2m} \left[ \alpha_n^2 \rho_n(r) + \alpha_p^2 \rho_p(r) \right] + (C_0^R - C_1^R)(\alpha_n + \alpha_p)^2 \rho_n(r) \rho_p(r) \right. \]  

\[ + \sum_{k=0}^{1} \left( C_k^R + C_k^I \right) \left[ \alpha_n \rho_n(r) + (-1)^{k+1} \alpha_p \rho_p(r) \right]^2 \]  

\[ - \sum_{l=n,p} \left( 4 \tilde{C}_1^{\Delta p} + \tilde{C}_1^{I} \right) \alpha_l^2 |\tilde{\rho}_l(r)|^2 \right\}. \]  
(98)

IV. FINITE-AMPLITUDE METHOD

To check the expressions for the energy-weighted sum rules for nuclear EDF derived in the previous section, QPRA calculations based on the linear-response theory have been performed. In this section the procedure to calculate the energy-weighted sum rule from the linear response theory is summarized.

The finite-amplitude method (FAM) for computing the linear response is performed [37, 38]. The FAM allows to perform a linear response within nuclear DFT for a given external field \( \tilde{F} \) with a complex frequency \( \omega \). By solving the linearized time-dependent Hartree-Fock-Bogoliubov equations, the strength function \( S(\tilde{F}, \omega) \) can be numerically evaluated by an iterative method. The strength function is written in terms of the QRPA energies and strengths as

\[ S(\tilde{F}, \omega) = - \sum_{\lambda(\Omega_{\lambda} > 0)} \left\{ \frac{|\langle \lambda | \tilde{F} | 0 \rangle|^2}{\Omega_{\lambda} - \omega} + \frac{|\langle 0 | \tilde{F} | \lambda \rangle|^2}{\Omega_{\lambda} + \omega} \right\}. \]  
(99)

We perform a contour integration in the complex-energy plane to evaluate the energy-weighted sum rule numerically

\[ m_1(\tilde{F}) = \frac{1}{2\pi i} \int_{A_1} \omega S(\tilde{F}, \omega) d\omega, \]  
(100)

where the integration path is taken to include all the positive-energy poles in the strength function. We set the half counterclockwise arc \( A_1 \) from \( \omega = -iR_{A_1} \) to \( iR_{A_1} \) centered at the origin, and a line on the imaginary axis from \( \omega = iR_{A_1} \) to \( \omega = -iR_{A_1} \) to encircle all the poles in the range of \( 0 < \Omega_{\lambda} < R_{A_1} \). For a Hermitian operator \( \tilde{F} \) the integration along the imaginary axis vanishes, and Eq. (100) is derived. We refer Ref. [19] for more detailed discussion on the complex-energy FAM for the sum rules.

V. COMPARISON OF SUM-RULE VALUES

In the numerical comparison, we use the functionals based on the UNEDF1-HFB [15] which contains only the time-even coupling constants in the particle-hole channel. In the present calculation, we do not include the time-odd coupling constants in the particle-hole channel. Therefore the functional does not correspond to a specific Hamiltonian operator, and breaks the local gauge invariance in the spin-orbit terms.

For the comparison of the sum-rule values, we consider four EDFs with the isoscalar and isovector current terms.

1. isoscalar and isovector current terms in the local gauge invariant form \((C_0^R = -C_0^I\) and \(C_1^R = -C_1^I\)

2. isovector current term only \((C_0^R = 0, C_1^R = C_1^I)\)

3. isoscalar current term only \((C_0^R = C_0^I, C_1^R = 0)\)

4. no current terms \((C_0^R = C_1^I = 0)\)

We compute the energy-weighted sum rule of the monopole \((K = 0)\), dipole \((K = 0 \text{ and } 1)\), quadrupole
(\(K = 0, 1, \) and \(2\)), and octupole \((K = 0, 1, 2, \) and \(3\)) operators of the isoscalar and isovector type. Expressions for the energy-weighted sum rule of these operators in the cylindrical coordinate system are summarized in Appendix B. We use \(\alpha = Z/A\) for the isoscalar operators and \(\alpha_n = Z/A\) and \(\alpha_p = N/A\) for the isovector operators.

The calculations are performed with the HFBTHO code [39–41] and its FAM extension for the non-axial finite \(K\) modes [42]. This version of the code uses linearized densities explicitly, and thus \(\eta\) parameter in the FAM is not necessary in the numerical calculation. \(N_{\text{sh}} = 20\) harmonic-oscillator shells are used as the single-particle model space, and \(N_{\text{GH}} = 40, N_{\text{GL}} = 40,\) and \(N_{\text{leg}} = 80\) points are used for the Gauss quadratures. 60 MeV pairing window is employed. In the FAM calculation the integration radius is set to \(R_{\text{A}} = 200\) MeV, and the half arc \(A_1\) is discretized with 300 points.

We compute \(^{208}\text{Pb}\) ground state as a representative case of the spherical state without pairing, and \(^{166}\text{Dy}\) as a case with prolate deformation and pairing \((\beta = 0.33, \Delta_n = 0.64\ \text{MeV}, \) and \(\Delta_p = 0.58\ \text{MeV})\). Tables I and II compare energy-weighted sum rule of \(^{208}\text{Pb}\) from the Thouless theorem [Eqs. (62) and (98)] with Eq. (100) of the complex-energy FAM, while Tables III and IV are the same comparison but of \(^{166}\text{Dy}\). In \(^{208}\text{Pb}\), the sum rule of different \(K\) value gives the same value because of the spherical symmetry, while in \(^{166}\text{Dy}\), the sum-rule values depend on \(K\) for the same multipole \(L\) due to the ground-state deformation. The agreement between the expressions from the Thouless theorem and the values from the complex-energy FAM is excellent. From the ratio of the sum rules of the FAM to the value from the Thouless theorem, the maximum discrepancy is about 0.7% and 0.4% for \(^{208}\text{Pb}\) of the isoscalar and isovector operators, and 1.2% and 0.5% in \(^{166}\text{Dy}\), respectively. Because the current terms do not change the HFB state, the difference in the energy-weighted sum-rule value between the calculations with/without the current terms show the actual contribution of the local gauge symmetry breaking. The effect of the isoscalar (isovector) current is much larger than the other in the sum rule of the isoscalar (isovector) multipole operator. This is because the contribution of the isoscalar (isovector) current term to the energy-weighted sum rule of the isoscalar operator is proportional to the isoscalar (isovector) density squared in Eq. (62), and the isoscalar density is generally much larger than the isovector density. For the isovector multipole operator, as seen in Eq. (98), the contribution of the isovector current term is from an isoscalar-type density squared (in-phase with \(\alpha_n\) and \(\alpha_p\) weight factors), while that of the isoscalar current term is from an isovector-type (out of phase) density squared.

We then analyze the effect of the local gauge symmetry breaking of the pairing EDF on the energy-weighted sum rule using the EDF which was discussed in Ref. [43]. The particle-hole part of the EDF is UNEDF1-HFB with the local gauge invariant current terms \((C_0 = -C_6^\tau, \) \(C_1 = -C_1^\tau)\) and for the neutron pairing channel, in addition to a volume pairing term \(\tilde{C}_n^\rho = V_n/4 = -148.25\ \text{MeV}\ \text{fm}^3\). We include \(\tilde{C}_n^{\Delta \rho} \text{Re}(\tau_n^* \Delta \rho_n)\) and \(\tilde{C}_n^\tau \text{Re}(\tilde{\tau}_n^* \tilde{\rho}_n)\) terms. Three cases are considered:

1. local gauge invariant pairing functional with \(\tilde{C}_n^{\Delta \rho} = -20\ \text{MeV}\ \text{fm}^5\) and \(\tilde{C}_n^\tau = 80\ \text{MeV}\ \text{fm}^5\).
2. \(\tilde{C}_n^{\Delta \rho} = 0\) and \(\tilde{C}_n^\tau = 80\ \text{MeV}\ \text{fm}^5\).
3. \(\tilde{C}_n^{\Delta \rho} = -20\ \text{MeV}\ \text{fm}^5\) and \(\tilde{C}_n^\tau = 60\ \text{MeV}\ \text{fm}^5\).

Because of the low accuracy of the FAM strength function at high excitation energy with large pairing strength, we set a smaller integration radius \(R_{\text{A}} = 100\ \text{MeV}\) in this calculation. In Table V, the energy-weighted sum rule for \(^{120}\text{Sn}\) for \(K = 0\) modes are compared. The agreement is generally good. The maximum discrepancy is about 2.4% seen in the sum rule of the isovector monopole operator, indicating the high-energy contribution to the energy-weighted sum rule above 100 MeV. Comparing with the large effect of the local gauge symmetry breaking in the current terms, the effect of the local gauge symmetry breaking of the pairing EDF is just about 1% of the energy-weighted sum rule. This is because the pairing contribution to the energy-weighted sum rule in Eqs. (62) and (98) is proportional to the pair density squared, while the same contribution from the local gauge symmetry breaking in the particle-hole EDF is proportional to the density squared. The pairing density is about one order smaller than the particle-hole density, as we see that the contribution of the pairing energy to the total binding energy is much smaller than that of the particle-hole part. Thus considering the accuracy of the calculation, it is not easy to detect the local gauge symmetry breaking of the pairing EDF from the isoscalar and isovector coordinate operators. We note that the property of the HFB state (such as particle-hole and pair densities) changes with the pairing functionals, while they remain the same when we turn on and off the time-odd current coupling constants. The difference between, for example, the energy-weighted sum rule values computed with \(\tilde{C}_n^{\Delta \rho} = -C_1^\tau/4\) and \(\tilde{C}_n^{\Delta \rho} = 0\) is not only from the direct contribution from the local gauge symmetry breaking of the pairing EDF.

VI. CONCLUSIONS

The expressions for the energy-weighted sum rule of the isoscalar and isovector coordinate operators are derived for the case of the nuclear DFT where the EDF does not correspond to a Hamiltonian.

The importance of the local gauge invariance of the nuclear EDF for evaluating the energy-weighted sum rule of these operators is discussed. For time-reversal symmetric even-even systems, the local gauge invariance of \(\rho_k \tau_k - j_k^2\) term in the particle-hole channel and \(\text{Re}(\tau_k \Delta \rho_k - \rho_k^* \tau_k)\) in the pairing channel is responsible to obtain the energy-weighted sum-rule value of the conventional Thouless
employed. Four choices for the isoscalar and isovector current coupling constants are listed. The units are in MeV fm\(^4\) where \(x = 4, 2, 4\), and 6 for \(L = 0, 1, 2\), and 3 modes, respectively.

| \(x\) | ISM(K = 0) | ISD(K = 0) | ISQ(K = 0) | ISO(K = 0) | ISM(K = 1) | ISD(K = 1) | ISQ(K = 1) | ISO(K = 1) |
|---|---|---|---|---|---|---|---|---|
| \(C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) | \(+C_0\) | \(+C_0\) | \(+C_0\) | \(+C_0\) |
| \(C_2\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \(C_2\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \(C_4\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| \(C_6\) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

TABLE II. Energy-weighted sum rule of the isovector multipole operators for \(^{208}\)Pb. The HFB value are evaluated using Eq. (98).

| \(K\) | IVM(K = 0) | IVD(K = 0) | IVD(K = 1) | IVQ(K = 0) | IVQ(K = 1) |
|---|---|---|---|---|---|
| \(C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) |
| \(C_2\) | 0 | 0 | 0 | 0 | 0 |
| \(C_4\) | 0 | 0 | 0 | 0 | 0 |
| \(C_6\) | 0 | 0 | 0 | 0 | 0 |

TABLE III. Energy-weighted sum rule of the isoscalar multipole operators for \(^{166}\)Dy.

| \(K\) | ISM(K = 0) | ISD(K = 0) | ISQ(K = 0) | ISO(K = 0) |
|---|---|---|---|---|
| \(C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) | \(-C_0\) |
| \(C_2\) | 0 | 0 | 0 | 0 |
| \(C_4\) | 0 | 0 | 0 | 0 |
| \(C_6\) | 0 | 0 | 0 | 0 |
theorem, while the local gauge invariance of the other terms such as spin-orbit and tensor does not play any role for the energy-weighted sum rule of the multipole operators. The expressions for the energy-weighted sum-rule values are compared with the QRPA calculations with the complex-energy FAM, and expressions we derived are both analytically and numerically justified.

The ratio of energy-weighted and inverse-energy-weighted sum rule is useful for estimating the giant resonance energy. The present derivation establishes the efficient evaluation of the sum-rule ratio for nuclear EDF that does not correspond to a Hamiltonian, as the dielectric theorem is available for the nuclear EDF to evaluate the inverse-energy-weighted sum rule \cite{29}.

The local gauge invariance of $\rho_k r - \vec{J}_k^2$ is related to the Galilean invariance, and thus almost all the practical nuclear EDFs should hold it. However, the present derivation of the Thouless theorem is also applicable to other kinds of operators such as spin and isospin. The energy-weighted sum rule of the spin operators is related to the spin-orbit and tensor energy terms \cite{44, 45}. It will be very useful to derive the expression for the energy-weighted sum rule of the spin and spin-multipole operators for better understanding of the spin-orbit and tensor terms in nuclear EDFs.

Extensions to non-Hermitian operators such as charge-exchange and pair transfer excitation, and the derivation of the cubic energy-weighted sum rule within the nuclear DFT are another challenging future subjects.

**ACKNOWLEDGMENTS**

Discussions with Markus Kortelainen and Witold Nazarewicz are acknowledged. This work is supported by the JSPS KAKENHI Grant Number 16K17680 and 17H05194. Numerical calculations were performed at the COMA (PACS-IX) and Oakforest-PACS Systems through the Multidisciplinary Cooperative Research Program in Center for Computational Sciences, University of Tsukuba.

**Appendix A: Densities**

The particle-hole and particle-particle density matrices are given by

\[
\hat{\rho}(rs, r's'; t) = \langle \hat{c}_{r's'}^\dagger \hat{c}_{rst} \rangle, \quad \hat{\rho}(rs, r's'; t) = -2s' \langle \hat{c}_{r's'} \hat{c}_{rst} \rangle, \tag{A1}
\]

where $\hat{c}^\dagger$ and $\hat{c}$ are nucleon creation and annihilation operators. The non-local densities are expressed in terms of the density matrices as

\[
\rho_k(r, r') = \sum_{st} \hat{\rho}(rs, r's; t) \tau^k(t), \tag{A3}
\]

\[
s_k(r, r') = \sum_{s't'} \hat{s}(rs, r's; t) \sigma_{s't'}, \tag{A4}
\]

\[
\tilde{\rho}_k(r, r') = \sum_s \hat{\tilde{\rho}}(rs, r's; t), \tag{A5}
\]

\[
\tilde{s}_k(r, r') = \sum_{s't'} \hat{\tilde{s}}(rs, r's; t) \sigma_{s't'}, \tag{A6}
\]

where $\tau^k(t) = 1$ for $k = 0$, and $2t$ for $k = 1$.

All the local densities appear in the nuclear EDF are derived from non-local densities as

\[
\rho_k(r) = \rho_k(r, r), \tag{A7}
\]

\[
\tau_k(r) = [(\nabla \cdot \nabla') \rho_k(r, r')]_{r'=r}, \tag{A8}
\]

\[
J_k(r) = \frac{1}{2t} [(\nabla \times \nabla') \otimes \sigma_k(r, r')]_{r'=r}, \tag{A9}
\]

\[
s_k(r) = s_k(r, r), \tag{A10}
\]

\[
T_k(r) = [(\nabla \cdot \nabla') s_k(r, r')]_{r'=r}, \tag{A11}
\]

\[
j_k(r) = \frac{1}{2t} [(\nabla \times \nabla') \rho_k(r, r')]_{r'=r}, \tag{A12}
\]

\[
F_k(r) = \frac{1}{2} [(\nabla \otimes \nabla + \nabla' \otimes \nabla') \cdot \sigma_k(r, r')]_{r'=r}, \tag{A13}
\]

\[
\tilde{\rho}_k(r) = \tilde{\rho}_k(r, r'), \tag{A14}
\]

\[
\tilde{s}_k(r) = [(\nabla \times \nabla') \tilde{\rho}_k(r, r')]_{r'=r'}, \tag{A15}
\]

\[
\tilde{j}_k(r) = \frac{1}{2t} [(\nabla \times \nabla') \otimes \tilde{s}_k(r, r')]_{r'=r'}, \tag{A16}
\]

and tensor densities can be decomposed into

\[
J_k(r) = \sum_a J_{kaa}(r), \tag{A17}
\]

\[
J_k(r) = \sum_{bc} \varepsilon_{abc} J_{kbca}(r), \tag{A18}
\]

\[
J_{kab}(r) = \frac{1}{2} J_{kab}(r) + \frac{1}{2} J_{kba}(r) - \frac{1}{3} J_k(r) \delta_{ab}, \tag{A19}
\]

\[
J_k(r) = \sum_a J_{kaa}(r), \tag{A20}
\]

\[
J_k(r) = \sum_{bc} \varepsilon_{abc} J_{kbca}(r), \tag{A21}
\]

\[
J_{kab}(r) = \frac{1}{2} J_{kab}(r) + \frac{1}{2} J_{kba}(r) - \frac{1}{3} J_k(r) \delta_{ab}. \tag{A22}
\]

**Appendix B: Energy-weighted sum rule expressions for multipole operators**

The expressions for the energy-weighted sum rule of the multipole operators up to $L = 3$ in cylindrical coordinates are summarized in this section. The multipole
TABLE IV. Energy-weighted sum rule of the isovector monopole (IVM), dipole (IVD), quadrupole (IVQ), and octupole (IVO) operators for $^{166}$Dy.

| IVM($K = 0$) | IVD($K = 0$) | IVD($K = 1$) | IVQ($K = 0$) | IVQ($K = 1$) |
|--------------|--------------|--------------|--------------|--------------|
| $C_0^I = -C_0^T$ | $C_1^I = -C_1^T$ | 105723 | 106141 | 234.288 | 234.797 | 234.599 | 25581.9 | 25628.4 | 23307.5 | 23349.6 |
| $C_0^T = 0$ | $C_1^T = -C_1^T$ | 105734 | 106154 | 234.306 | 234.815 | 234.618 | 25584.5 | 25631.2 | 23309.8 | 23352.0 |
| $C_0^T = -C_0^T$ | $C_1^T = 0$ | 95552.1 | 95979.6 | 208.108 | 208.912 | 208.758 | 23075.0 | 23125.3 | 21042.2 | 21085.9 |
| $C_0^T = 0$ | $C_1^T = 0$ | 95562.4 | 95991.8 | 208.126 | 208.930 | 208.777 | 23077.5 | 23128.0 | 21044.5 | 21088.4 |

TABLE V. Energy-weighted sum rule of $K = 0$ isoscalar and isovector operators computed for $^{120}$Sn. The HFB values are evaluated using Eqs. (62) and (98). UNEDF1-HFB functional is used in the particle-hole channel, and three pairing functionals are employed.

| ISM | ISD | ISQ | ISO |
|-----|-----|-----|-----|
| HFB | FAM | HFB | FAM | HFB | FAM | HFB | FAM |
| $C_0^I = -4\tilde{C}_n^{\Delta \rho }$ | 37612.3 | 37525.5 | 97823.2 | 98732.1 | 7482.72 | 7494.26 | 445873 | 447563 |
| $C_0^{\Delta \rho } = 0$ | 37247.0 | 37085.9 | 97401.9 | 97633.7 | 7410.05 | 7415.64 | 440527 | 442097 |
| $C_0^{\Delta \rho } = -3\tilde{C}_n^{\Delta \rho }$ | 37807.7 | 37700.9 | 97261.3 | 98883.0 | 7521.59 | 7536.32 | 447205 | 449376 |

| IVM | IVD | IVQ | IVO |
|-----|-----|-----|-----|
| HFB | FAM | HFB | FAM | HFB | FAM | HFB | FAM |
| $C_0^I = -4\tilde{C}_n^{\Delta \rho }$ | 59979.3 | 58634.3 | 171.491 | 171.583 | 11932.5 | 11859.2 | 679415 | 675736 |
| $C_0^{\Delta \rho } = 0$ | 59627.8 | 58220.1 | 170.723 | 170.711 | 11862.6 | 11785.1 | 674162 | 670461 |
| $C_0^{\Delta \rho } = -3\tilde{C}_n^{\Delta \rho }$ | 60208.2 | 58798.6 | 171.957 | 172.069 | 11978.0 | 11907.4 | 681180 | 677783 |
operators are expressed using \( x = \rho \cos \phi, y = \rho \sin \phi \) as

\[
f_{00}(r) = r^2 = \rho^2 + z^2, \quad (B1)
\]

\[
f_{10}^{IS}(r) = r^3 Y_{10} - \eta_{10} r Y_{10} = \sqrt{\frac{3}{4\pi}} (z^3 + \rho^2 z - \eta_{10} z), \quad (B2)
\]

\[
f_{10}^{IV}(r) = r Y_{30} = \sqrt{\frac{3}{4\pi}} z, \quad (B3)
\]

\[
f_{11}^{IS}(r) = (r^3 - \eta_{11} r) \frac{Y_{11} - Y_{1-1}}{\sqrt{2}}
\]

\[
= -\sqrt{\frac{3}{16\pi}} \rho (\rho^2 + z^2 - \eta_{11}) (e^{i\phi} + e^{-i\phi}), \quad (B4)
\]

\[
f_{11}^{IV}(r) = r (Y_{11} - Y_{1-1}) = -\sqrt{\frac{3}{16\pi}} \rho (e^{i\phi} + e^{-i\phi}), \quad (B5)
\]

\[
f_{20}(r) = r^2 Y_{20} = \sqrt{\frac{5}{16\pi}} (2z^2 - \rho^2), \quad (B6)
\]

\[
f_{21}(r) = -r^2 (Y_{21} - Y_{2-1}) = \sqrt{\frac{15}{64\pi}} z \rho (e^{i\phi} + e^{-i\phi}), \quad (B7)
\]

\[
f_{22}(r) = r^2 (Y_{22} + Y_{2-2}) = \sqrt{\frac{15}{64\pi}} \rho^2 (e^{2i\phi} + e^{-2i\phi}), \quad (B8)
\]

\[
f_{30}^{IS}(r) = r^3 Y_{30} - \eta_{30} r Y_{10}
\]

\[
= \sqrt{\frac{7}{16\pi}} (2z^3 - 3\rho^2 z - \eta_{30} z), \quad (B9)
\]

\[
f_{30}^{IV}(r) = r^3 Y_{30} = \sqrt{\frac{7}{16\pi}} z (2z^2 - 3\rho^2), \quad (B10)
\]

\[
f_{31}^{IS}(r) = r^3 Y_{31} - \eta_{31} r Y_{11}
\]

\[
= \sqrt{\frac{21}{128\pi}} [-4z^2 \rho + \rho^3 + \eta_{31} \rho] (e^{i\phi} + e^{-i\phi}), \quad (B11)
\]

\[
f_{31}^{IV}(r) = r^3 (Y_{31} - Y_{3-1}) = -\sqrt{\frac{21}{128\pi}} (4z^2 - \rho^2) (e^{i\phi} + e^{-i\phi}), \quad (B12)
\]

\[
f_{32}(r) = r^3 (Y_{32} + Y_{3-2}) = \sqrt{\frac{105}{64\pi}} z \rho^2 (e^{2i\phi} + e^{-2i\phi}), \quad (B13)
\]

\[
f_{33}(r) = r^3 (Y_{33} - Y_{3-3}) = -\sqrt{\frac{35}{128\pi}} \rho^3 (e^{3i\phi} + e^{-3i\phi}). \quad (B14)
\]

The parameters \( \eta_{lm} \) in the isoscalar dipole and octupole operators are given by \([46–48]\)

\[
\eta_{10} = \frac{1}{A} \int dr (3z^2 + \rho^2) \rho_0(r), \quad (B15)
\]

\[
\eta_{11} = \frac{1}{A} \int dr (z^2 + 2\rho^2) \rho_0(r), \quad (B16)
\]

\[
\eta_{30} = \sqrt{\frac{12}{7}} \eta_{30} = \frac{1}{A} \int dr (6z^2 - 3\rho^2) \rho_0(r), \quad (B17)
\]

\[
\eta_{31} = \sqrt{\frac{8}{7}} \eta_{31} = \frac{1}{A} \int dr (4z^2 - 2\rho^2) \rho_0(r). \quad (B18)
\]

The sum rules are written using the root-mean-square radius and deformation parameters

\[
\langle r_2^2 \rangle = \frac{1}{N_t} \int dr (\rho^2 + z^2) \rho_t(r), \quad (B19)
\]

\[
\langle r_{\text{tot}}^2 \rangle = \frac{1}{N_t} \int dr (\rho^2 + z^2) \rho_0(r) = \frac{N_t \langle r_2^2 \rangle + Z \langle r_{\text{tot}}^2 \rangle}{A}, \quad (B20)
\]

\[
\beta_{2t} = \sqrt{\frac{\pi}{5}} \int \frac{dr (2z^2 - \rho^2) \rho_t(r)}{dr \rho_t(r)} \int dr (2z^2 - \rho^2) \rho_t(r), \quad (B21)
\]

\[
\beta_{4t} = \sqrt{\frac{\pi}{32}} \int \frac{dr (35z^2 - 30z^2 \rho^2 + 3\rho^2) \rho_t(r)}{dr \rho_t(r)} \int dr (8z^2 - 24z^2 \rho^2 + 3\rho^2) \rho_t(r), \quad (B22)
\]

\[
\langle r_4^2 \rangle = \frac{1}{N_t} \int dr (\rho^2 + z^2)^2 \rho_t(r) = \frac{1}{N_t} \int dr (\rho^2 + z^2)^2 \rho_t(r), \quad (B23)
\]

The energy-weighted sum rules of isoscalar multipole operators are written as

\[
m_1(F^{IS}) = m_1^{\text{kin}}(F^{IS}) + m_1^{\text{LGSB}}(F^{IS}), \quad (B24)
\]

where the first term is from the kinetic-energy term, and the second term is from the local gauge symmetry breaking of the particle-hole and pairing EDF. The expressions
for each multipole operator are

\begin{equation}
\mathcal{F}_{00}^{1\text{kin}} = 4 \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} A \langle r_{\text{tot}}^2 \rangle,
\end{equation}

\begin{equation}
\mathcal{F}_{00}^{1\text{LGSB}} = 4 \left( \frac{Z}{A} \right)^2 \int dr (\rho^2 + z^2) G_{\text{IS}}^{1\text{LGSB}}(r),
\end{equation}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{10}) &= 3 \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \times \left[ \int dr (\rho^4 + 10 \rho^2 z^2 + 9 z^4) \rho_0(r) - \eta_{10}^2 \right], \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{10}) &= \frac{3}{4\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \int dr [\rho^4 + 10 \rho^2 z^2 + 9 z^4 \\
&\quad + \eta_{10}^2 - 2 \eta_0 (2 \rho^2 + 3 z^2)] G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{11}) &= 3 \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \times \left[ \int dr (5 \rho^4 + 6 \rho^2 z^2 + 4 z^4) \rho_0(r) - \eta_{11}^2 \right], \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{11}) &= \frac{3}{4\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \int dr [5 \rho^4 + 6 \rho^2 z^2 + 4 z^4 \\
&\quad + \eta_{11}^2 - 2 \eta_1 (2 \rho^2 + 3 z^2)] G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{20}) &= \frac{5}{2\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} A \langle r_{\text{tot}}^2 \rangle \left(1 + \sqrt{\frac{5}{4\pi}} \beta_2 \right), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{20}) &= \frac{5}{4\pi} \left( \frac{Z}{A} \right)^2 \int dr (\rho^2 + 4 z^2) G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{21}) &= \frac{5}{2\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} A \langle r_{\text{tot}}^2 \rangle \left(1 + \sqrt{\frac{5}{16\pi}} \beta_2 \right), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{21}) &= \frac{15}{8\pi} \left( \frac{Z}{A} \right)^2 \int dr (\rho^2 + 2 z^2) G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{22}) &= \frac{10}{4\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} A \langle r_{\text{tot}}^2 \rangle \left(1 - \sqrt{\frac{5}{4\pi}} \beta_2 \right), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{22}) &= \frac{15}{4\pi} \left( \frac{Z}{A} \right)^2 \int dr \rho^2 G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{30}) &= \frac{7}{16\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \times \left[ 9 \int dr (\rho^4 + 4 z^4) \rho_0(r) - \eta_{30}^2 \right], \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{30}) &= \frac{7}{16\pi} \left( \frac{Z}{A} \right)^2 \int dr [9 \rho^4 + 36 z^4 \\
&\quad + \eta_{30}^2 - 2 \eta_{30} (-3 \rho^2 + 6 z^2)] G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{31}) &= \frac{21}{32\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \times \left[ \int dr (5 \rho^4 + 16 \rho^2 z^2 + 16 z^4) \rho_0(r) - \eta_{31}^2 \right], \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{31}) &= \frac{21}{32\pi} \left( \frac{Z}{A} \right)^2 \int dr [5 \rho^4 + 16 \rho^2 z^2 + 16 z^4 \\
&\quad + \eta_{31}^2 - 2 \eta_{31} (-2 \rho^2 + 4 z^2)] G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{32}) &= \frac{105}{32\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \int dr (8 z^2 \rho^2 + \rho^4) \rho_0(r), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{32}) &= \frac{105}{32\pi} \left( \frac{Z}{A} \right)^2 \int dr (8 z^2 \rho^2 + \rho^4) G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{33}) &= \frac{315}{32\pi} \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \int dr \rho^4 \rho_0(r), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{33}) &= \frac{315}{32\pi} \left( \frac{Z}{A} \right)^2 \int dr \rho^4 G_{\text{IS}}^{1\text{LGSB}}(r),
\end{align}

where

\begin{equation}
G_{\text{IS}}^{1\text{LGSB}}(r) \equiv \frac{1}{k_0} \left( C_k^l + C_k^{-l} \right) \rho_0^2(r) \\
\quad - \sum_{t=n,p} (4 C_t^\Delta \rho + C_t^{-\Delta} \rho) |\hat{p}(r)|^2.
\end{equation}

The isovector sum rules are expressed as the sum of the kinetic term, enhancement factor, and the contribution from the local gauge symmetry breaking of the EDF

\begin{equation}
m_1(\mathcal{F}^{\text{IV}}) = m_1^{\text{kin}}(\mathcal{F}^{\text{IV}}) \left[ 1 + \kappa(\mathcal{F}^{\text{IV}}) \right] + m_1^{\text{LGSB}}(\mathcal{F}^{\text{IV}}).
\end{equation}

Each term for the multipole operators is given by

\begin{align}
m_{1}^{\text{kin}}(\mathcal{F}_{00}^{\text{IV}}) &= \frac{h^2}{2m} \frac{NZ}{A^2} \left( \langle r_n^2 \rangle + N \langle r_p^2 \rangle \right), \\
m_{1}^{\text{kin}}(\mathcal{F}_{00}^{\text{IV}}) &= 4 \left( C_0^l - C_1^{-l} \right) \int dr (\rho^2 + z^2) \rho_n(r) \rho_p(r), \\
m_{1}^{\text{LGSB}}(\mathcal{F}_{00}^{\text{IV}}) &= \frac{1}{A^2} \int dr (\rho^2 + z^2) G_{\text{IV}}^{1\text{LGSB}}(r),
\end{align}
\[
m_{1}^{\text{kin}}(\hat{F}_{10}) = \frac{3}{4\pi} \frac{h^2}{2m} A, \quad (B50) \\
m_{1}^{\text{kin}}(\hat{F}_{11}) = \frac{3}{4\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr \rho_{n}(r) \rho_{p}(r), \quad (B51) \\
m_{1}^{\text{LGBS}}(\hat{F}_{10}) = \frac{3}{4\pi} \frac{1}{A^2} \int dr G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B52) \\
m_{1}^{\text{kin}}(\hat{F}_{11}) = \frac{3}{4\pi} \frac{h^2}{2m} A, \quad (B53) \\
m_{1}^{\text{kin}}(\hat{F}_{11}) = \frac{3}{4\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr \rho_{n}(r) \rho_{p}(r), \quad (B54) \\
m_{1}^{\text{LGBS}}(\hat{F}_{11}) = \frac{3}{4\pi} \frac{1}{A^2} \int dr G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B55) \\
m_{1}^{\text{kin}}(\hat{F}_{20}) = \frac{5}{2\pi} \frac{h^2}{2m} A^2 \left[ Z(r_n^2) \left( 1 + \sqrt{\frac{5}{4\pi}} \beta_{2n} \right) \right] + N(r_p^2) \left( 1 + \sqrt{\frac{5}{4\pi}} \beta_{2p} \right), \quad (B56) \\
m_{1}^{\text{kin}}(\hat{F}_{20}) = \frac{5}{4\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr (\rho^2 + 4z^2) \rho_{n}(r) \rho_{p}(r), \quad (B57) \\
m_{1}^{\text{LGBS}}(\hat{F}_{20}) = \frac{5}{4\pi} \frac{1}{A^2} \int dr (\rho^2 + 4z^2) G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B58) \\
m_{1}^{\text{kin}}(\hat{F}_{21}) = \frac{5}{2\pi} \frac{h^2}{2m} A^2 \left[ Z(r_n^2) \left( 1 + \sqrt{\frac{5}{16\pi}} \beta_{2n} \right) \right] + N(r_p^2) \left( 1 + \sqrt{\frac{5}{16\pi}} \beta_{2p} \right), \quad (B59) \\
m_{1}^{\text{kin}}(\hat{F}_{21}) = \frac{15}{8\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr (\rho^2 + 2z^2) \rho_{n}(r) \rho_{p}(r), \quad (B60) \\
m_{1}^{\text{LGBS}}(\hat{F}_{21}) = \frac{15}{8\pi} \frac{1}{A^2} \int dr (\rho^2 + 2z^2) G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B61) \\
m_{1}^{\text{kin}}(\hat{F}_{22}) = \frac{5}{2\pi} \frac{h^2}{2m} A^2 \left[ Z(r_n^2) \left( 1 - \sqrt{\frac{5}{4\pi}} \beta_{2n} \right) \right] + N(r_p^2) \left( 1 - \sqrt{\frac{5}{4\pi}} \beta_{2p} \right), \quad (B62) \\
m_{1}^{\text{kin}}(\hat{F}_{22}) = \frac{15}{4\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr \rho^2 \rho_{n}(r) \rho_{p}(r), \quad (B63) \\
m_{1}^{\text{LGBS}}(\hat{F}_{22}) = \frac{15}{4\pi} \frac{1}{A^2} \int dr \rho^2 G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B64) \\
m_{1}^{\text{kin}}(\hat{F}_{30}) = \frac{63}{4\pi} \frac{h^2}{2m} A^2 \int dr (\rho^4 + 4z^4) \times \left[ Z^2 \rho_{n}(r) + N^2 \rho_{p}(r) \right], \quad (B65) \\
m_{1}^{\text{kin}}(\hat{F}_{30}) = \frac{63}{16\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr (\rho^4 + 4z^4) \times \rho_{n}(r) \rho_{p}(r), \quad (B66) \\
m_{1}^{\text{LGBS}}(\hat{F}_{30}) = \frac{63}{16\pi} \frac{1}{A^2} \int dr (\rho^2 + 4z^2) G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B67) \\
m_{1}^{\text{kin}}(\hat{F}_{31}) = \frac{21}{32\pi} \frac{h^2}{2m} A^2 \int dr (5\rho^4 + 16z^4 + 16\rho^2 z^2) \times \left[ Z^2 \rho_{n}(r) + N^2 \rho_{p}(r) \right], \quad (B68) \\
m_{1}^{\text{kin}}(\hat{F}_{31}) = \frac{21}{32\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr (5\rho^4 + 16z^4 + 16\rho^2 z^2) \times \rho_{n}(r) \rho_{p}(r), \quad (B69) \\
m_{1}^{\text{LGBS}}(\hat{F}_{31}) = \frac{21}{32\pi} \frac{1}{A^2} \int dr (5\rho^4 + 16z^4 + 16\rho^2 z^2) G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B70) \\
m_{1}^{\text{kin}}(\hat{F}_{32}) = \frac{105}{32\pi} \frac{h^2}{2m} A^2 \int dr (\rho^4 + 8\rho^2 z^2) \times \rho_{n}(r) \rho_{p}(r), \quad (B71) \\
m_{1}^{\text{LGBS}}(\hat{F}_{32}) = \frac{105}{32\pi} \frac{1}{A^2} \int dr (\rho^4 + 8\rho^2 z^2) G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B72) \\
m_{1}^{\text{kin}}(\hat{F}_{33}) = \frac{315}{32\pi} \frac{h^2}{2m} A^2 \int dr \rho^4 [Z^2 \rho_{n}(r) + N^2 \rho_{p}(r)], \quad (B73) \\
m_{1}^{\text{kin}}(\hat{F}_{33}) = \frac{315}{32\pi} \left( C_{0}^{T} - C_{1}^{T} \right) \int dr \rho^4 \rho_{n}(r) \rho_{p}(r), \quad (B74) \\
m_{1}^{\text{LGBS}}(\hat{F}_{33}) = \frac{315}{32\pi} \frac{1}{A^2} \int dr \rho^4 G_{1 \text{IV}}^{\text{LGBS}}(r), \quad (B75) \\
\text{where} \\
G_{1 \text{IV}}^{\text{LGBS}}(r) = \sum_{k=0}^{1} \left( C_{k}^{T} + C_{k}^{L} \right) \left[ Z \rho_{n}(r) + (-1)^{k+1} N \rho_{p}(r) \right]^2 - \left( 4 \hat{C}_{n}^{T} + \hat{C}_{n}^{L} \right) Z^2 |\rho_{n}(r)|^2 - \left( 4 \hat{C}_{p}^T + \hat{C}_{p}^L \right) N^2 |\rho_{p}(r)|^2. \quad (B76)
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