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Complex-energy approach to sum rules within nuclear density functional theory

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Background: The linear response of the nucleus to an external field contains unique information about the effective interaction, the correlations governing the behavior of the many-body system, and the properties of its excited states. To characterize the response, it is useful to use its energy-weighted moments, or sum rules. By comparing computed sum rules with experimental values, the information content of the response can be utilized in the optimization process of the nuclear Hamiltonian or the nuclear energy density functional (EDF). But the additional information comes at a price: compared to the ground state, computation of excited states is more demanding.

Purpose: To establish an efficient framework to compute energy-weighted sum rules of the response that is adaptable to the optimization of the nuclear EDF and large-scale surveys of collective strength, we have developed a new technique within the complex-energy finite-amplitude method (FAM) based on the quasiparticle random-phase approximation (QRPA).

Methods: To compute sum rules, we carry out contour integration of the response function in the complex-energy plane. We benchmark our results against the conventional matrix formulation of the QRPA theory, the Thouless theorem for the energy-weighted sum rule, and the dielectric theorem for the inverse-energy-weighted sum rule. We demonstrate that calculated sum-rule values agree with those obtained from the matrix formulation of the QRPA. We also discuss the applicability of both the Thouless theorem about the energy-weighted sum rule and the dielectric theorem for the inverse-energy-weighted sum rule to nuclear density functional theory in cases when the EDF is not based on a Hamiltonian.

Conclusions: The proposed sum-rule technique based on the complex-energy FAM is a tool of choice when optimizing effective interactions or energy functionals. The method is very efficient and well-adaptable to parallel computing. The FAM formulation is especially useful when standard theorems based on commutation relations involving the nuclear Hamiltonian and the external field cannot be used.


I. INTRODUCTION

Atomic nuclei exhibit various kinds of collective excitations, with characteristics considerably different from simple nucleonic excitations [1,2]. Among those, giant resonances form a distinct class [3]. Although their excitation energies are relatively high compared to the low-energy collective modes, the main characteristics of giant resonances are understood in terms of the superposition of many nucleonic excitations. Experimentally, various types of giant resonances have been seen. Examples are shape vibrations, spin excitations, and charge-exchange excitations of various multipolarities and isospins. These modes carry rich information about basic nuclear properties.

There has been excellent progress in the modeling of atomic nuclei using nuclear density functional theory (DFT) [4]. State-of-the-art energy density functionals (EDFs), optimized to various classes of data [5–9], enable a quantitative description of global nuclear properties throughout the nuclear landscape [10–12]. Ground-state properties of nuclei, such as binding energies, charge radii, effective single-particle energies of doubly closed shell nuclei, and basic parameters characterizing the nuclear matter equation of state, are typically used as empirical inputs in EDF parameter optimization. However, properties of excited states, such as giant resonances, are seldom considered (see Refs. [5,13–19] for representative examples of work along those lines). This results in large uncertainties of EDF parameters sensitive to, and governing, low- and high-frequency nuclear excitations. The EDFs of the next generation are expected to overcome this deficiency by including selected properties of the giant resonances into the pool of observables used in the optimization.

To extract the information content of giant resonances, the sum-rule technique [20–24] has been widely used. For instance, mean giant resonance energies can be related to the ratio of the sum rules of different energy moments [22,25–28]. The inverse-energy-weighted sum rule provides...
information about the nuclear polarizability, which is the fundamental quantity characterizing the nuclear response. An important quantity, in the context of studies of neutron-rich matter, is the electric dipole polarizability, which is related to symmetry energy and its density dependence [29–31]. Various polarizabilities carry information about instabilities in nuclear matter [32–34]. In some cases, the Thouless theorem [35–37] provides a simple way to access sum rules directly from the Hartree-Fock-Bogoliubov (HFB) solution. Unfortunately, the Thouless theorem applies to positive-odd energy moments, and simple expressions can be derived only for simple operators (such as multipole moments). Moreover, the theorem is justified only if a Hamiltonian representation of the interaction is available, which is generally not the case for nuclear DFT where modern EDFs are usually not connected to an underlying Hamiltonian and often break local gauge invariance [38]. Therefore, an efficient technique to compute nuclear sum rules, regardless of the form of the operator, is desired.

The direct evaluation of sum rules from self-consistent quasiparticle random-phase approximation (QRPA) matrix solutions is computationally demanding because of the configuration spaces involved. A recent formulation of the sum rule in terms of QRPA matrices enables the computation of sum rules without diagonalizing the QRPA matrix [27]. Nevertheless, this method still requires knowledge of the QRPA matrix, which has large dimensions, especially when spherical symmetry is broken. Other recent developments include applications of the Lanczos algorithm to random-phase approximation (RPA) sum rules [39] and the use of the Lorentz integral transform method and the Lanczos technique [40].

The finite-amplitude method (FAM) [41], based on the linear-response approach, significantly reduces the computational cost of the QRPA problem. The residual two-body interaction is numerically computed from the finite-amplitude nucleonic fields induced by an external polarizing field. The FAM has been recently implemented in various self-consistent frameworks, including three-dimensional Hartree-Fock (HF) [41], spherical HFB [42], axially deformed Skyrme-HFB [43–45], and relativistic mean-field models [46,47]. The FAM has been applied to the description of giant resonances and low-energy dipole strength [48,49], and the computation of the QRPA matrix elements [50], and the description of discrete low-lying QRPA modes by means of the contour integration technique in the complex energy plane [51].

The objective of this study is to propose an efficient approach to sum rules by using the contour integration technique of Ref. [51]. Because of its inherently parallel structure, the new method is ideally suited to optimizations of next-generation nuclear EDFs, informed by experimental data on multipole and charge-exchange strength. This paper is organized as follows. Section II summarizes the basic expressions. In Sec. III, we present the formulation of the complex-energy FAM approach to sum rules. Section IV contains numerical tests, benchmarking examples, and applications to realistic cases. The conclusions and outlook are given in Sec. V.

II. BASIC EXPRESSIONS
A. Sum rule
The ground-state (g.s.) strength function \( S(E) \) for a one-body operator \( \hat{F} \) is defined as

\[
S(E) \equiv \sum_v \delta(E - E_v) \langle \nu | \hat{F} | 0 \rangle^2.
\]

where \(|0\rangle\) and \(|\nu\rangle\) denote, respectively, the ground state and excited state of the system with energies \( E_0 \) and \( E_v \). The \( k \)th moment of \( S(E) \),

\[
m_k(\hat{F}) \equiv \int (E - E_0)^k S(E) dE,
\]

is called the energy-weighted sum rule of order \( k \). In terms of the transition matrix elements of \( \hat{F} \), it is given by

\[
m_k(\hat{F}) \equiv \sum_v (E_v - E_0)^k |\langle \nu | \hat{F} | 0 \rangle|^2.
\]

As discussed in, e.g., Refs. [1,2], certain sum rules are independent of the specific many-body theory used to describe the ground state and the excited states. For example, the nuclear shell model and QRPA frameworks have been widely used to evaluate the sum rules. In QRPA, the excitation energy \( E_v - E_0 \) is replaced with the QRPA frequency \( \Omega_\nu \), which is the eigenvalue of the matrix equation:

\[
\begin{pmatrix}
A & B \\
-B^* & -A^*
\end{pmatrix}
\begin{pmatrix}
X^v \\
Y^v
\end{pmatrix}
= \Omega_\nu \begin{pmatrix}
X^v \\
Y^v
\end{pmatrix}.
\]

B. Finite-amplitude method
The FAM is an efficient technique to obtain the response function \( S(E) \) without explicitly computing the \( A \) and \( B \) QRPA matrices in Eq. (4). For the details pertaining to the FAM, we refer the reader to, e.g., Ref. [42]. The complex response function for a given operator \( \hat{F} \) at a given complex frequency \( \omega_\nu = \omega + i\gamma \), found as a solution of the FAM equations, is given as

\[
S(\hat{F},\omega_\nu) = -\sum_{\nu=0} \left[ \frac{|\langle \nu | \hat{F} | 0 \rangle|^2}{\Omega_\nu - \omega_\nu} + \frac{|\langle 0 | \hat{F} | \nu \rangle|^2}{\Omega_\nu + \omega_\nu} \right].
\]

The Lorentzian distribution of the strength function is obtained by taking the imaginary part of \( S \):

\[
\frac{1}{\pi} \text{Im} S(\hat{F},\omega_\nu) = \frac{\gamma}{\pi} \sum_{\nu=0} \left[ \frac{|\langle \nu | \hat{F} | 0 \rangle|^2}{(\Omega_\nu - \omega)^2 + \gamma^2} - \frac{|\langle 0 | \hat{F} | \nu \rangle|^2}{(\Omega_\nu + \omega)^2 + \gamma^2} \right].
\]
transition strength to state $|\nu\rangle$ \[1\]
\[
\frac{1}{2\pi i} \oint_{C_v} S(\hat{F},\omega_r)d\omega_r = |\langle \nu | \hat{F} | 0 \rangle|^2 \quad (\Omega_v > 0),
\]
(7)
or, alternatively, along $C_{-v}$,
\[
\frac{1}{2\pi i} \oint_{C_{-v}} S(\hat{F},\omega_r)d\omega_r = -|\langle 0 | \hat{F} | \nu \rangle|^2 = -|\langle \nu | \hat{F} | 0 \rangle|^2 \quad (\Omega_v < 0).
\]
(8)

For a small $\gamma \ll \omega$, the relation $1/(\omega + i\gamma) = P(1/\omega) - i\pi \delta(\omega)$ holds, and the sum rules can be formally calculated using
\[
m_k(\hat{F}) = -\frac{1}{\pi} \lim_{\gamma \to 0} \int_0^\infty \omega^k \text{Im} S(\hat{F},\omega + i\gamma)d\omega.
\]
(9)

An approximate value of the sum rules can be found from this expression from a finite value of $\gamma$ \[42,43,47,49\]. However, to guarantee sufficient numerical accuracy, a very fine mesh would be required for the integration \(9\) to take into account all the QRPA modes, whose locations are not known beforehand.

### III. SUM-RULE EXPRESSIONS IN THE FAM

In this section we introduce the sum-rule approach based on the contour integration of the FAM. For simplicity, we assume that the operator $\hat{F}$ cannot excite spurious modes and that all the QRPA energies $\Omega_v$ are nonzero. We also assume that the HFB state is stable with respect to small density variations; i.e., there are no imaginary-frequency QRPA solutions. This guarantees that all the QRPA poles $\Omega_v$ lie on the real axis. In the following, we adopt the notation $\omega$ for a complex frequency.

The basic idea behind the FAM approach to sum rules is to utilize the identity based on Cauchy’s integral theorem:
\[
\oint_D f(\omega)S(\hat{F},\omega)d\omega = \sum_{v>0} f(\Omega_v)|\langle \nu | \hat{F} | 0 \rangle|^2,
\]
(10)

where the contour $D$ encircles all the positive QRPA frequencies $\Omega_v > 0$ and excludes all the singularities of the complex function $f(\omega)$. By setting $f(\omega) = \omega^k$, we obtain the expressions for the sum rule $m_k(\hat{F})$.

In the following, we assume the operator $\hat{F}$ to be Hermitian for simplicity. In this case, positive and negative energy solutions are associated with the same transition strength:
\[
|\langle \nu | \hat{F} | 0 \rangle|^2 = |\langle 0 | \hat{F} | \nu \rangle|^2.
\]
(11)

The above equation does not hold when $\hat{F}$ is not Hermitian. However, Eq. (10) still can be used with an appropriately chosen contour $D$.

#### A. Laurent series of the FAM response function

By using the Laurent series expansion of $(1 - z)^{-1}$, we can derive the expansion of the FAM response function. The FAM response function has poles at $\omega = \Omega_v$ and $-\Omega_v$. In the inner region below the lowest QRPA pole, $|\omega| < \min_{v>0} \Omega_v$, $S(\hat{F},\omega)$ can be written as
\[
S(\hat{F},\omega) = -2 \sum_{n=0}^{\infty} m_{n+1}(\hat{F})\omega^{2n}.
\]
(12)

One can see that odd-$k$ sum rules can be simply related to the expansion coefficients of Eq. (12). The same is true in the outer region above the highest QRPA pole, $|\omega| > \max_{v>0} \Omega_v$, where the response function can be expanded as
\[
S(\hat{F},\omega) = 2 \sum_{n=0}^{\infty} \frac{m_{2n+1}(\hat{F})}{\omega^{2n+2}}.
\]
(13)

The expansions (12) and (13) are generalizations of expansions proposed in Ref. [23] to the full complex energy plane. We note that the inverse-energy-weighted sum rule ($k = -1$) is found by setting $\omega = 0$ in Eq. (12). This should be done with care, however. If spurious modes are present, they would produce a zero-frequency pole resulting in numerical instabilities near or at the pole. If we choose the semicircle $A_1$ (counterclockwise) and $A_2$ (clockwise) with the radii satisfying $0 < R_{A_1} < \min_{v>0} \Omega_v$ and $R_{A_2} > \max_{v>0} \Omega_v$, as in Fig. 1, we can apply the series (12) and (13) along the integration path. The odd-$k$ sum rules are then given as
\[
m_k(\hat{F}) = \begin{cases} 
\frac{1}{2\pi i} \oint_{A_1} \omega^k S(\hat{F},\omega)d\omega & (k > 0, \text{odd}), \\
\frac{1}{2\pi i} \oint_{A_2} \omega^k S(\hat{F},\omega)d\omega & (k < 0, \text{odd}).
\end{cases}
\]
(14)

To evaluate even-$k$ sum rules, we need to connect $A_1$ and $A_2$ to enclose the positive-energy poles. To this end, we consider contour $D$ of Fig. 1 composed of semicircles $A_1$ and $A_2$ connected by straight segments $I_1$ and $I_2$ on the imaginary axis.

In summary, regardless of the moment $k$, the sum rule is given by the integration along $D$:
\[
m_k(\hat{F}) = \frac{1}{2\pi i} \oint_D \omega^k S(\hat{F},\omega)d\omega = \sum_{v>0} \Omega_v^k |\langle \nu | \hat{F} | 0 \rangle|^2.
\]
(15)

However, for certain moments $k$, some parts of path $D$ do not contribute to the sum rule. For odd values of $k$, the
TABLE I. Portions of the contour $D$ required for computing various sum rules $m_k$. For sum rules with even $k$, the contributions from $I_1$ and $I_2$ are identical.

<table>
<thead>
<tr>
<th>$k$</th>
<th>Required portions of $D$</th>
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<tr>
<td>Negative, even</td>
<td>$A_2, I_1, I_2 (R_{A_1} \to \infty)$</td>
</tr>
<tr>
<td>Negative, odd</td>
<td>$A_2 (R_{A_1} \to \infty)$</td>
</tr>
<tr>
<td>0</td>
<td>$A_1, A_2, I_1, I_2$</td>
</tr>
<tr>
<td>Positive, odd</td>
<td>$A_1 (R_{A_1} \to 0)$</td>
</tr>
<tr>
<td>Positive, even</td>
<td>$A_1, I_1, I_2 (R_{A_1} \to 0)$</td>
</tr>
</tbody>
</table>

contributions from $I_1$ and $I_2$ cancel each other. Furthermore, for negative $k$, application of Jordan’s lemma, together with a limit of $R_{A_1} \to \infty$, allows for the removal of the contribution from $A_1$. For positive $k$, there is no pole at $\omega = 0$, and the limit $R_{A_1} \to 0$ can be taken. Table I lists the portions of the contour $D$ required for each $k$. Furthermore, for even $k$, the contributions from $I_1$ and $I_2$ are identical. Similar contours are considered in Refs. [52–54] to compute energy-weighted sum rules.

IV. RESULTS

A. Numerical checks and benchmarking against MQRPA

To check the FAM approach to sum rules, following Refs. [43,51] we consider the oblate configuration of $^{24}\text{Mg}$ computed with the SLy4 [55] Skyrme EDF. The HFB calculations were carried out with the DFT solver HFBTHO [56] in a model space of five harmonic oscillator shells by employing a volume pairing with the strength of $V_0 = -125.20$ MeV fm$^3$ and a 60 MeV quasiparticle energy cutoff. The resulting oblate minimum of $^{24}\text{Mg}$ has nonzero pairing in protons and neutrons. The small single-particle model space employed makes it possible to benchmark FAM results against the matrix formulation of the QRPA (MQRPA) [57] without any further truncation. To compute spatial integrals we used Gauss-Hermite ($N_{\text{GH}} = 30$), Gauss-Laguerre ($N_{\text{GL}} = 30$), and Gauss-Legendre ($N_{\text{LEG}} = 30$) quadratures. The finite-amplitude expansion parameter $\eta$ was set to $10^{-7}$, and the convergence criterion of the FAM was set such that the change of the individual FAM amplitudes from the previous iteration should be less than $10^{-5}$. This convergence criterion is chosen to be consistent with the accuracy obtained with a given value of $\eta$, as discussed in Ref. [43]. The integration along semicircles $A_1$ and $A_2$ was discretized with $N_{A_1}$ and $N_{A_2}$ points, respectively. In addition, the integration along $I_1$ was discretized with $N_{I_1}$ points and evaluated using the composite Simpson’s rule. As for negative-$k$ moments, the composite Simpson’s rule was applied to the variable $1/\omega$ to describe the divergent behavior of integrand around $\omega = 0$. In this particular test case, the smallest and largest energy MQRPA poles appear at 1.3 and 128.7 MeV, respectively. Consequently, the contour radii were set to $R_{A_1} = 1$ MeV and $R_{A_2} = 200$ MeV. To systematically assess our numerical procedure for different moments $k$, we used the same contour $D$ for all cases, without simplifications listed in Table I.

As far as the external field $\hat{F}$ is concerned, we considered the isoscalar (IS) and isovector (IV) monopole (M) and quadrupole (Q) operators:

$$\hat{F}_{\text{ISM}} = \frac{eZ}{A} \sum_{i=1}^{A} r_i^2 \hat{\tau}_i,$$

$$\hat{F}_{\text{IVM}} = \frac{e}{A} \sum_{i=1}^{A} e_{\text{eff}}(\tau_{3i}) r_i^2 \hat{\tau}_{3i},$$

$$\hat{F}_{\text{ISQ}} = \frac{eZ}{A} \sum_{i=1}^{A} r_i^2 Y_{20}(\theta_i, \phi_i),$$

$$\hat{F}_{\text{IVQ}} = \frac{e}{A} \sum_{i=1}^{A} e_{\text{eff}}(\tau_{3i}) r_i^2 Y_{20}(\theta_i, \phi_i) \hat{\tau}_{3i},$$

where $e_{\text{eff}}(n) = eZ/A$ and $e_{\text{eff}}(p) = -eN/A$.

It is worth noting that neutron and proton pairing-rotational spurieu modes, associated with the breaking of the particle number symmetry, are present in the $K^\pi = 0^+$ sector. Fortunately, these mode—generated by the neutron and proton particle number operators—cannot be excited by particle-hole operators (16)–(19). Therefore, the presence of pairing-rotational spurieu modes does not cause any additional difficulties [41,43].

TABLE II. The real part of the integral (15) for $-4 \leq k \leq 4$ and $\hat{F}_{\text{ISM}}$ (in MeV$^k c^2$ fm$^4$) along the semicircle $A_1$ with $R_{A_1} = 200$ MeV. The integral was discretized with $N_{A_1}$ points. The numbers in parentheses denote powers of 10.

<table>
<thead>
<tr>
<th>$N_{A_1}$</th>
<th>$k = -4$</th>
<th>$k = -3$</th>
<th>$k = -2$</th>
<th>$k = -1$</th>
<th>$k = 0$</th>
<th>$k = 1$</th>
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<td>$-2.6(-6)$</td>
<td>$-3.8(-4)$</td>
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<td>$14.4510$</td>
<td>$4195.31$</td>
<td>$608575$</td>
<td>$4318446$</td>
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</tr>
<tr>
<td>3</td>
<td>$9.0(-9)$</td>
<td>$6.8(-8)$</td>
<td>$1.7(-4)$</td>
<td>$1.1(-4)$</td>
<td>$13.8328$</td>
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<tr>
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<tr>
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<td>9</td>
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</table>
To begin with, we checked the convergence of the integral (15) along $A_1$, $A_2$, and $I_1$ with respect to the number of integration points. The results are presented in Tables II–IV for the isoscalar monopole operator. As seen in Table II, the integrals along $A_1$ are small for negative $k$. Analytically, these values should be zero for negative-odd values of $k$; hence, nonzero values in Table II reflect the numerical error of calculations. As far as the positive $k$ moments are concerned, the convergence is faster for odd-$k$ sum rules. In particular, the convergence for $k = 1$ is excellent, because a six-digit accuracy is achieved already with $N_{A_1} = 5$. The integration along $A_1$ captures the total $m_1$ and $m_3$ sum rules; the result in Table II indicates that these sum rules can be computed very efficiently. Moreover, because the semicircle $A_1$ is located very far from the QRPA poles, FAM calculations along $A_1$ converge very quickly, typically after six iterations. Furthermore, each FAM calculation at a given $\omega$ along the contour is easily parallelizable; this could significantly reduce the total computational time, although not so many points are required for the convergence of $m_1$ and $m_3$.

Table III shows the convergence of the integral (15) along $A_2$. This portion of the contour is required for the sum rules with negative $k$. Of most practical importance is the inverse-energy-weighted sum rule $m_{-1}$. The value of $m_{-1}$ converges here with $N_{A_2} = 16$ points. In general, as compared to integration along $A_1$, more FAM iterations are required to achieve reasonable convergence along $A_2$. In the case considered, typically 50 FAM iterations are necessary for each $\omega$. When choosing $R_{A_2}$, one has to keep in mind that its value should be smaller than the lowest QRPA pole, whose energy is not a priori known. At the same time, the convergence of FAM calculations for negative-$k$ moments deteriorates rapidly when $R_{A_2}$ gets too close to zero.

Table IV illustrates the convergence along the segment $I_1$ on the imaginary axis. As discussed, this integration should be nonzero only for even-$k$ moments. The convergence for $k = 0$ is reached rather slowly, especially when compared with the case of $k = 4$ and $-4$ cases. This is because the Simpson’s formula used approximates the integrand with quadratic functions, which is a poor ansatz for $k = 0$.

To benchmark our FAM approach, in Table V we display the values of sum rules for the isoscalar and isovector monopole operators; they are compared with the MQRPA results based on the direct evaluation of the right-hand side of Eq. (15). Overall, there is an excellent agreement between the two sets of calculations. This result indicates that the proposed FAM technique can be used to predict sum rules of interest in model spaces that are too large to be treated with MQRPA. The convergence of integration along $A_2$ is not sufficient in the case of $k = -4$; this sum rule is, however, less important than other moments discussed.

### Table III

<table>
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<tr>
<th>$N_{A_1}$</th>
<th>$k = -4$</th>
<th>$k = -3$</th>
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<th>$k = 0$</th>
<th>$k = 1$</th>
<th>$k = 2$</th>
<th>$k = 3$</th>
<th>$k = 4$</th>
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<td>3.2165</td>
<td>5.00438</td>
<td>3.23108</td>
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<td>-1.22915</td>
<td>2.2(-3)</td>
<td>0.996296</td>
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<tr>
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<td>5.00387</td>
<td>3.18902</td>
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<td>-1.09039</td>
<td>4.1(-5)</td>
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### Table IV

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<td>61.7093</td>
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<td>-1.477671</td>
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</table>
TABLE V. Sum rules (in MeV e^2 fm^4) for the isoscalar and isovector monopole operators calculated with the MQRPA and the FAM. The FAM calculations were performed by using \( N_{\text{sh}} = 301 \), \( N_{\text{sh}} = 101 \), and \( N_{\text{sh}} = 200 \) integration points.

<table>
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<tr>
<th>( S )</th>
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<th>( k = -1 )</th>
<th>( k = 0 )</th>
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<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td>MQRPA(ISM)</td>
<td></td>
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<td>0.013077</td>
<td>0.037815</td>
<td>0.253118</td>
<td>5.00072</td>
<td>139.825</td>
<td>240.028</td>
<td>131.368</td>
<td>1442.358</td>
<td>157906.09</td>
</tr>
<tr>
<td>( 10 )</td>
<td>0.012579</td>
<td>0.036992</td>
<td>0.253186</td>
<td>5.00385</td>
<td>139.844</td>
<td>4199.44</td>
<td>131.277</td>
<td>4336.644</td>
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</tr>
<tr>
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<td>0.00723782</td>
<td>0.0712949</td>
<td>2.78500</td>
<td>113.908</td>
<td>4735.03</td>
<td>199.525</td>
<td>8527.358</td>
<td>370625.216</td>
</tr>
<tr>
<td>( 20 )</td>
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<td>0.07133510</td>
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<td>113.908</td>
<td>4734.30</td>
<td>199.510</td>
<td>8524.830</td>
<td>368643.941</td>
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</table>

RPA [58,59]. In the case of HF + RPA, expression (20) also holds for the Skyrme force due to the \( \delta \)-character of the momentum-dependent terms [23,24]. However, as pointed out in Ref. [33], the theorem has not been proven for a generalized EDF, which is not explicitly related to an effective interaction. Deviations from relation (20) can be caused by, e.g., different assumptions about particle-hole and pairing channels, the Slater approximation to the Coulomb exchange operator \( \hat{C} \), approximations to spin-orbit and tensor terms [60], and generalized density dependence [61–63]. To the best of our knowledge, the Thouless theorem has not been proven in the case of generalized EDFs.

In the following, we refer to the value (20) as the “HFB value” of the energy-weighted sum rule. In Table VI the energy-weighted sum rules obtained in HFB and the FAM are compared for different model spaces given by \( N_{\text{sh}} \). In a small model space of \( N_{\text{sh}} = 5 \), the difference between FAM and HFB values is non-negligible but quickly becomes small with \( N_{\text{sh}} \). This can be attributed to a poor representation of the time-odd part (21) does not affect the HFB value (20).

TABLE VI. The energy weighted sum rule (in MeV e^2 fm^4) for the operators (16)–(19) at the oblate minimum of \( ^{24}\text{Mg} \) as a function of \( N_{\text{sh}} \). The FAM values were obtained by taking \( R_{\text{sh}} = 200 \) MeV and \( N_{\text{sh}} = 12 \); they are compared to HFB values (20). The results without time-odd terms except for the current-current coupling \( \mathcal{C}_L^0(\rho_0) = C_L^{\Delta} = C_L^{\chi} = C_L^T = 0 \) (a) and with the full time-odd functional except for the current-current and kinetic spin-spin couplings \( \mathcal{C}_L^0 = C_L^T = 0, C_L(\rho_0) \neq 0, C_L^{\Delta} \neq 0, C_L^{\chi} \neq 0 \) (b), obtained with \( N_{\text{sh}} = 20 \), are also listed.

<table>
<thead>
<tr>
<th>( N_{\text{sh}} )</th>
<th>FAM(ISM)</th>
<th>HFB(ISM)</th>
<th>FAM(ISM)</th>
<th>HFB(ISM)</th>
<th>FAM(ISQ)</th>
<th>HFB(ISQ)</th>
<th>FAM(ISQ)</th>
<th>HFB(ISQ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 5 )</td>
<td>4199.44</td>
<td>4303.67</td>
<td>4734.25</td>
<td>4752.37</td>
<td>762.638</td>
<td>767.933</td>
<td>848.110</td>
<td>845.235</td>
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<td>( 10 )</td>
<td>4524.39</td>
<td>4502.75</td>
<td>4970.34</td>
<td>4940.08</td>
<td>779.019</td>
<td>775.724</td>
<td>852.955</td>
<td>849.015</td>
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<td>( 15 )</td>
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<td>4523.80</td>
<td>4958.02</td>
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<td>776.587</td>
<td>776.161</td>
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<td>849.116</td>
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<tr>
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<td>4529.46</td>
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<td>4966.01</td>
<td>777.425</td>
<td>776.832</td>
<td>850.145</td>
<td>849.747</td>
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</table>

C. Dielectric theorem for the inverse-energy-weighted sum rule

The dielectric theorem connects the inverse-energy-weighted sum rule (related to nuclear polarizability) with the constrained potential energy surface. This theorem is proposed in Refs. [20,23] for the HF case and is proven in the HFB framework in Ref. [27]. Based on this theorem, the numerical results demonstrate that these do not affect the energy-weighted sum rule.
TABLE VII. Inverse-energy-weighted sum rule (in MeV$^{-1}e^2$ fm$^4$) computed using the dielectric theorem (HFB) and the FAM for various sizes of the model space given by $N_{\text{sh}}$. FAM calculations were performed using $N_{A_2} = 22$ and $R_2 = 1.0$ MeV.

<table>
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<th>FAM(ISM)</th>
<th>HFB(ISM)</th>
<th>FAM(IVM)</th>
<th>HFB(IVM)</th>
<th>FAM(ISQ)</th>
<th>HFB(ISQ)</th>
<th>FAM(IVQ)</th>
<th>HFB(IVQ)</th>
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</thead>
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<tr>
<td>5</td>
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<td>5.00 375</td>
<td>2.78 615</td>
<td>2.78 614</td>
<td>4.44 830</td>
<td>4.44 765</td>
<td>0.798 680</td>
<td>0.798 680</td>
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<tr>
<td>10</td>
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<td>5.21 586</td>
<td>1.075 516</td>
<td>1.075 524</td>
</tr>
<tr>
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<td>5.71 960</td>
<td>5.31 250</td>
<td>5.31 268</td>
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<tr>
<td>20</td>
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<td>5.35 730</td>
<td>1.157 448</td>
<td>1.157 771</td>
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</tbody>
</table>

Table VIII summarizes the results. The calculated ground-state properties show a gradual spherical-to-deformed shape transition with increasing neutron number. Moreover, in some of the isotopes we predict pairing collapse. For that reason, the chosen set of nuclei is representative of a realistic situation encountered in global surveys across the nuclear landscape, where deformations and pairing may vary rapidly as a function of proton and neutron number.

D. Example of systematic calculations

As an illustrative example, we discuss the energy-weighted $K^\pi = 0^+$ sum rules in the shape transitional region of $^{142-152}$Nd and $^{144-154}$Sm. The calculations were carried out by using the SLy4 EDF parametrization with the volume pairing strength $V_0 = V_p = -190$ MeV fm$^3$ in the model space of $N_{\text{sh}} = 20$ oscillator shells. The pairing strength was adjusted to reproduce the experimental proton pairing gap of 1.23 MeV in $^{142}$Nd. In this realistic calculation we use $N_{\text{GH}} = N_{\text{GL}} = 40$ and $N_{\text{Leg}} = 80$, which are the recommended values based on recent analysis [56]. The FAM contour integration was carried out using a semicircle with $R_A = 200$ MeV, discretized with $N_{A_1} = 12$ points.

Table VIII summarizes the results. The calculated ground-state properties show a gradual spherical-to-deformed shape transition with increasing neutron number. Moreover, in some of the isotopes we predict pairing collapse. For that reason, the chosen set of nuclei is representative of a realistic situation encountered in global surveys across the nuclear landscape, where deformations and pairing may vary rapidly as a function of proton and neutron number.

The energy-weighted sum rules computed with the FAM agree well with the HFB expressions in the Appendix. This agreement holds regardless of nuclear shape or pairing. As expected, the energy-weighted sum rule for the isoscalar monopole operator increases with $N$ in the region of the shape transition; this is attributed to an increase of the rms radius due to deformation. Similarly, the isoscalar quadrupole operator increases even more rapidly with increasing quadrupole deformation.

Next, we consider the energy-weighted sum rules in constrained HFB states. The constrained HFB potential energy curve as a function of quadrupole moment was obtained using the quadratic constraint. The contribution from the quadratic constraining potential to the residual field in the FAM was included consistently. This kind of calculation represents the local QRPA on top of the constrained HFB [67], it contains dynamical information about nonequilibrium configurations in the deformation space.

TABLE VIII. Isoscalar monopole and quadrupole energy-weighted $K^\pi = 0^+$ sum rules in units of MeV$e^2$ fm$^4$ computed with the FAM and the HFB techniques for $^{142-152}$Nd and $^{144-154}$Sm isotopes. The quadrupole deformation $\beta$, neutron and proton pairing gaps ($\Delta_n$ and $\Delta_p$, respectively), and total rms radius $\sqrt{\langle r^2 \rangle}$ are also shown.

<table>
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<th>$^{142}$Nd</th>
<th>$^{144}$Nd</th>
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<th>$^{148}$Nd</th>
<th>$^{150}$Nd</th>
<th>$^{152}$Nd</th>
<th>$^{144}$Sm</th>
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<td>$\Delta_p$ (MeV)</td>
<td>$\sqrt{\langle r^2 \rangle}$ (fm)</td>
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<td>FAM(ISM)</td>
<td>HFB(ISQ)</td>
<td>FAM(ISQ)</td>
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<td>0.00</td>
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<td>0.00</td>
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<td>54.849</td>
<td>13.071</td>
<td>13.084</td>
<td>13.084</td>
<td>13.084</td>
<td>13.084</td>
</tr>
</tbody>
</table>
The energy-weighted sum rule of the isoscalar quadrupole operator as a function of quadrupole deformation is shown in Fig. 2. The sum rule increases monotonically with β and agrees very well with HFB values. This, together with results presented in Table VIII, indicates that the Thouless theorem provides a good approximation to the energy-weighted sum rule within the Skyrme-EDF picture, which is not based on the underlying Hamiltonian.

In passing, we should note that when departing from the HFB minimum, there is a possibility of imaginary energy QRPA solutions; in such cases, a pair of QRPA poles would appear on the imaginary axis. Although one expects no contribution to odd-κ sum rules from such a pair, a careful consideration needs to be given to the choice of integration contour in the FAM. A general extension of the complex FAM formalism to the case of the local QRPA will be an interesting avenue for future studies.

V. CONCLUSIONS

We propose an efficient formalism to compute sum rules by using the contour integration formalism within the complex-energy finite-amplitude method. In particular, when the order of the moment is odd, the obtained expression becomes extremely simple, because the sum rules appear as expansion coefficients of the Laurent series of the response function. The new formalism has been successfully benchmarked against the matrix diagonalization method of the QRPA.

We compare the energy-weighted sum rule obtained in the FAM with those based on the Thouless theorem. Although the double commutator cannot be evaluated for general EDFs, the theorem provides a very good approximation to the obtained expression as a function of quadrupole deformation for the constrained HFB solutions.

Our results suggest that sum rules can be computed efficiently in the FAM even in cases when other methods are not easily available (e.g., the Thouless theorem cannot be applied or constrained calculations cannot be carried out because of self-consistent symmetries assumed). Of particular interest is the systematic analysis of the isovector dipole sum rule and neutron skins. The extension of the FAM formalism to non-Hermitian operators is also straightforward, because it has already been applied to the β-decay rates [44]. Extension of the complex-energy FAM to weakly-bound systems near the drip line, e.g., within the framework of Ref. [45], is also an interesting future avenue.

The FAM approach to sum rules promises to add new functionality to the EDF optimization framework of Refs. [6–8] because it will allow adding new kinds of data on multipole- and charge-exchange strength to the set of fit observables defining the objective function. The new FAM technique can be very useful when studying the nuclear response to nontrivial operators such as the nuclear Schiff moment, which is closely related to the isoscalar dipole operator [68,69].

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APPENDIX: THOULESS THEOREM FOR MONOPOLE AND QUADRUPOLE OPERATORS

According to the Thouless theorem (20), the energy-weighted sum rules for isoscalar monopole and quadrupole operators of an axially deformed nucleus are

\[ m_1(\text{ISM}) = 4e^2 \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} A(r^2), \]

\[ m_1(\text{ISQ}) = e^2 \left( \frac{Z}{A} \right)^2 \frac{\hbar^2}{2m} \frac{5}{2\pi} A(r^2) \left( 1 + \sqrt{\frac{5}{4\pi}} \beta \right), \]

where \( r^2 \) is the total rms radius and \( \beta \) is the mass quadrupole deformation parameter:

\[ \beta = \sqrt{\frac{\pi}{5}} \frac{1}{A(r^2)} \int (3z^2 - r^2) \rho(r) d\mathbf{r}. \]
For isovector operators, an enhancement factor appears,

\[ \kappa = \frac{8m}{\hbar^2} (C_0^* - C_1^*) \frac{\int [\nabla f(r) \rho_n(r) \rho_p(r)] d\mathbf{r}}{\int [\nabla f(r)^2] \rho(r) d\mathbf{r}}, \]  

where \( C_i \) is the coupling constant of the term \( \rho_i \tau_i \) in the EDF in the notation of Ref. [64]. The expressions for the isovector monopole and quadrupole operators are

\[ m_1(IVM) = 4e^2 \frac{\hbar^2}{2m} \frac{N Z}{A^2} [Z(r^2)_n + N(r^2)_p] (1 + \kappa_{IVM}) \],

\[ \kappa_{IVM} = \frac{8m}{\hbar^2} (C_0^* - C_1^*) \frac{1}{A(r^2)} \int r^2 \rho_n(r) \rho_p(r) d\mathbf{r}, \]

and

\[ m_1(IVQ) = e^2 \frac{\hbar^2}{2m} \frac{N Z}{A^2} \frac{5}{2\pi} \left[ Z(r^2)_n \left(1 + \sqrt{\frac{5}{4\pi} \beta_p} \right) + N(r^2)_p \left(1 + \sqrt{\frac{5}{4\pi} \beta_p} \right) \right] (1 + \kappa_{IVQ}), \]

\[ \kappa_{IVQ} = \frac{8m}{\hbar^2} (C_0^* - C_1^*) \frac{1}{2A(r^2)} \int (3z^2 + r^2) \rho_n(r) \rho_p(r) d\mathbf{r}, \]

where the subscripts \( n \) and \( p \) indicate neutron and proton expectation values, respectively.