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Starting from the adiabatic time-dependent Hartree-Fock approximation (ATDHF), we propose an efficient method to calculate the Thouless-Valatin moments of inertia for the nuclear system. The method is based on the rapid convergence of the expansion of the inertia matrix. The accuracy of the proposed method is verified in the rotational case by comparing the results with the exact Thouless-Valatin moments of inertia calculated using the self-consistent cranking model. The proposed method is computationally much more efficient than the full ATDHF calculation, yet it retains a high accuracy of the order of 1%.

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I. INTRODUCTION

The variation of nuclear ground-state shapes is governed by the modification of the shell structure of single-nucleon orbitals. Far from the valley of β stability, the energy spacings between single-nucleon levels change considerably with the number of neutrons and/or protons. The reduction of spherical shell closure is often associated with the occurrence of deformed ground states and, in many cases, with the phenomenon of coexistence of different shapes in a single nucleus. A quantitative description of the evolution of nuclear shapes, including regions of short-lived exotic nuclei that are becoming accessible in experiments at radioactive-beam facilities, necessitate accurate modeling of the underlying microscopic nucleonic dynamics. Major advances in nuclear theory have recently been made in studies of complex shapes and the corresponding excitation spectra and electromagnetic decay patterns, especially in the framework of nuclear energy density functionals (EDFs) [1–5].

A microscopic, EDF-based description of complex collective excitation spectra usually starts from a constrained Hartree-Fock plus BCS (HFBCS) or Hartree-Fock-Bogoliubov (HFB) calculation of the binding energy surface with the mass multipole moments as constrained quantities. The static nuclear mean-field is characterized by symmetry breaking: translational, rotational, and particle number. Even though symmetry breaking incorporates important static correlations (e.g., deformations and pairing), the static self-consistent solution can only provide an approximate description of bulk ground-state properties such as masses and radii. Modeling excitation spectra and transition rates in the EDF framework necessitates a systematic treatment of dynamical effects related to restoration of broken symmetries and fluctuations in collective coordinates.

One possible approach to five-dimensional quadrupole dynamics that restores rotational symmetry and allows for fluctuations around triaxial mean-field minima is to formulate a collective Hamiltonian, with deformation-dependent inertia parameters determined by microscopic self-consistent mean-field calculations. The dynamics of the collective Bohr Hamiltonian is governed by the vibrational inertial functions and the moments of inertia [6]. For these quantities either the Gaussian overlap approximation of the generator coordinate method (GCM-GOA) (Yoccoz masses [7]) or the adiabatic time-dependent Hartree-Fock-Bogoliubov (ATDHFB) expressions (Thouless-Valatin masses [8]) can be used. The Thouless-Valatin masses have the advantage that they also include the time-odd components of the self-consistent mean field and, in this sense, the full dynamics of a nuclear system. This can be seen most clearly in the case of translational motion, where the Thouless-Valatin mass corresponds to the exact mass $A \cdot m$ of A nucleons [9], whereas the GCM produces the exact value only when the center of the mass velocity is also included as the generator coordinate [10]. The calculation of the Thouless-Valatin masses is often simplified by adopting the cranking formulas [11,12] that neglect the residual interaction. The Thouless-Valatin corrections are then usually taken into account by scaling the inertia parameters with an empirical factor ($\approx$1.2–1.4) [13–15].

In this work we present an efficient method to calculate the Thouless-Valatin moments of inertia for the nuclear system. The method is based on the rapid convergence of the expansion of the inertia matrix. The accuracy of the proposed method is verified in the rotational case by comparing the results with the exact Thouless-Valatin moments of inertia calculated using the self-consistent cranking model. The proposed method is computationally much more efficient than the full ATDHF calculation, yet it retains a high accuracy of the order of 1%.

II. THEORETICAL FRAMEWORK

We begin with a brief review of the adiabatic time-dependent Hartree-Fock theory. A more detailed exposition of this formalism can be found, for instance, in Refs. [16,17]. The aim of the ATDHF theory is to derive in a fully microscopic and consistent way a Hamiltonian for the description of collective phenomena in which many nucleons act coherently. The theory is based on two approximations: (i) in the TDHF one assumes that the many-body time-dependent wave

function of the system is a Slater determinant at all times; and (ii) in the adiabatic approximation the collective motion is slow compared to single-particle motion and, therefore, the collective kinetic energy is a quadratic function of the velocities.

To identify the components of the density matrix that correspond to the coordinates and momenta of the collective Hamiltonian, we recall that the coordinates are even and the momenta are odd under time-reversal, and decompose the density matrix in the following way:

$$\rho(t) = e^{i\chi(t)/\hbar}\rho_0(t)e^{-i\chi(t)/\hbar}. \tag{1}$$

Both matrices, $\rho_0(t)$ and $\chi(t)$, are Hermitian and time-even. $\rho_0(t)$ represents the coordinates of the collective Hamiltonian, and $\chi(t)$ is the "adiabaticity parameter" that must be small compared to unity. At all times $\rho(t)$ is a Slater determinant, that is, $\rho_0(t)^2 = \rho_0(t)$ and $\mathrm{Tr}\rho_0 = N$, N being the particle number. In the following we work in the basis in which ρ_0 is diagonal, and consequently the operators ρ_0 and $\sigma_0 = 1 - \rho_0$ project onto hole and particle states, respectively. This basis depends on time because $\rho_0(t)$ is a function of time.

In the adiabatic approximation it is assumed that the total density $\rho(t)$ of the system is always close to the density $\rho_0(t)$, that is, the matrix χ that introduces the time-odd components remains small at all times. Expanding the density matrix to second order in the operator χ, the following expression is obtained:

$$\begin{aligned}\rho &\approx \left(1 + \frac{i}{\hbar}\chi - \frac{1}{\hbar^2}\chi^2\right)\rho_0\left(1 - \frac{i}{\hbar}\chi - \frac{1}{\hbar^2}\chi^2\right)\\ &\approx \rho_0 + \rho_1 + \rho_2,\end{aligned} \tag{2}$$

where

$$\rho_1 = \frac{i}{\hbar}[\chi, \rho_0] = \frac{i}{\hbar}(\chi\rho_0 - \rho_0\chi), \tag{3}$$

$$\rho_2 = -\frac{1}{2\hbar^2}[\chi, [\chi, \rho_0]] = \frac{1}{\hbar^2}\chi\rho_0\chi - \frac{1}{2\hbar^2}(\chi^2\rho_0 + \rho_0\chi^2). \tag{4}$$

ρ_1 is linear in χ, time-odd, and has only ph and hp nonvanishing matrix elements. ρ_2 is quadratic in χ, therefore time-even, and has only hh and pp matrix elements. The many-body Hamiltonian can also be expanded to second order in the operator χ:

$$\begin{aligned}h_{ab}(\rho) &= t_{ab} + \sum_{cd} V_{adbc}\rho_{cd}\\ &= t_{ab} + \sum_{cd} V_{adbc}(\rho_0)_{cd} + \sum_{cd} V_{adbc}(\rho_1)_{cd}\\ &\quad + \sum_{cd} V_{adbc}(\rho_2)_{cd},\end{aligned} \tag{5}$$

where t is the kinetic energy operator, and V denotes a generic two-body interaction. The Hamiltonian contains time-even (h_0 and Γ_2) and time-odd parts (Γ_1)

$$h(\rho) = h_0 + \Gamma_1 + \Gamma_2. \tag{6}$$

Consequently the time-dependent Hartree-Fock equation $i\hbar\dot{\rho} = [h, \rho]$ also decomposes into two equations:

$$i\hbar\dot{\rho}_0 = [h_0, \rho_1] + [\Gamma_1, \rho_0], \tag{7}$$

$$i\hbar\dot{\rho}_1 = [h_0, \rho_0] + [\Gamma_1, \rho_1] + [\Gamma_2, \rho_0]. \tag{8}$$

In Eq. (8) the term $[h_0, \rho_2]$ has been neglected because the ph and hp components are small, and the pp and hh parts vanish [17]. The total energy of the system

$$E = \sum_{ab} t_{ab}\rho_{ba} + \frac{1}{2}\sum_{abcd} \rho_{ba}V_{adbc}\rho_{cd}, \tag{9}$$

can be expressed in terms of the variables ρ_0 and ρ_1, or ρ_0 and χ. Terms which depend on the velocity in second order build the kinetic energy of the collective Hamiltonian:

$$K = \sum_{ab} (h_0)_{ab}(\rho_2)_{ba} + \frac{1}{2}\sum_{abcd} (\rho_1)_{ba}V_{adbc}(\rho_1)_{cd}. \tag{10}$$

We recall that the matrix ρ_0 projects onto the hole states and, inserting Eqs. (3) and (4) in the expression above, the kinetic energy can be written

$$K = \frac{1}{2\hbar^2}\begin{pmatrix}\chi^* & \chi\end{pmatrix}\begin{pmatrix}A & -B\\ -B^* & A\end{pmatrix}\begin{pmatrix}\chi\\ \chi^*\end{pmatrix}, \tag{11}$$

where the matrix A is Hermitian, and B is symmetric

$$A_{php'h'} = (\epsilon_p - \epsilon_h)\delta_{pp'}\delta_{hh'} + V_{phh'p'}, \quad B_{php'h'} = V_{php'h'}. \tag{12}$$

The effective interaction V_{adbc} can often be written as a sum of separable terms

$$V_{adbc} = \sum_r Q^r_{ab}V_r Q^{r*}_{cd}, \tag{13}$$

where Q^r denotes the single-particle operator characteristic for the channel index r. As discussed in Ref. [18], this is particulary the case for the relativistic point-coupling models, but the statement holds also for the meson-exchange relativistic Hartree models. The single-particle operators Q^r can be either even or odd under time reversal. The time-odd operators correspond to the isoscalar and isovector currents $\boldsymbol{j}(\boldsymbol{r})$ and $\vec{\tau}\,\boldsymbol{j}(\boldsymbol{r})$. By inserting the decomposition (13) into the Eq. (10), we obtain the following expression:

$$\frac{1}{2}\sum_{abcd} (\rho_1)_{ba}V_{adbc}(\rho_1)_{cd} = \sum_r \mathrm{Tr}(Q^r\rho_1)V_r\mathrm{Tr}(Q^r\rho_1)^*. \tag{14}$$

Since the matrix ρ_1 is time-odd, the traces vanish for the time-even operators Q^r, i.e., only the time-odd components of the residual interaction contribute to the kinetic energy of the collective Hamiltonian.

The equation of motion (7) can be written into the following form:

$$\begin{pmatrix}\dot{\rho}_0\\ \dot{\rho}_0^*\end{pmatrix} = \frac{1}{\hbar^2}\begin{pmatrix}A & -B\\ -B^* & A^*\end{pmatrix}\begin{pmatrix}\chi\\ \chi^*\end{pmatrix} \equiv \mathcal{M}^{-1}\begin{pmatrix}\chi\\ \chi^*\end{pmatrix}. \tag{15}$$

To perform realistic calculations the dimension of the problem has to be reduced, that is, one has to select a small number of active degrees of freedom $q_1, \ldots, q_f$. This means that we are able to generate a subset of time-even Slater determinants, characterized by the parameters $\mathbf{q}$, with the following property: the solution of the ATDHF problem will always remain within this subset of Slater determinants. In other words, we have found a path $\rho_0(t) = \rho_0[\mathbf{q}(t)]$ from which we can calculate the velocity

$$\dot{\rho}_0(t) = \dot{\mathbf{q}}(t)\frac{\partial \rho_0}{\partial \mathbf{q}}. \tag{16}$$

Next we define the operator $\mathbf{P}$ with the relation:

$$\frac{\partial \rho_0}{\partial \mathbf{q}} = -\frac{i}{\hbar}[\mathbf{P}, \rho_0] \,, \tag{17}$$

and obtain the following expression for the kinetic energy:

$$K = \frac{1}{2}\sum_{\mu,\nu=1}^{f} M_{\mu\nu}(\mathbf{q})\dot{q}_\mu \dot{q}_\nu \,, \tag{18}$$

where $M_{\mu\mu'}(\mathbf{q})$ denotes the real collective mass tensor

$$M_{\mu\mu'}(\mathbf{q}) = \frac{1}{\hbar^2}\begin{pmatrix} P^* & -P \end{pmatrix}_\mu \mathcal{M}\begin{pmatrix} P \\ -P^* \end{pmatrix}_{\mu'}. \tag{19}$$

To evaluate $\mathcal{M}$, we have to invert the matrix

$$\mathcal{M}^{-1} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix} = \mathcal{M}_0^{-1} + \mathcal{V} \tag{20}$$

in Eq. (15). For this purpose we decompose the matrix into a diagonal part containing the energies of particle and hole states

$$\left(\mathcal{M}_0^{-1}\right)_{php'h'} = (\epsilon_p - \epsilon_h)\delta_{pp'}\delta_{hh'} \,, \tag{21}$$

and the residual interaction $\mathcal{V}$, and use the fact that the interaction matrix elements are in most cases much smaller than the ph energies. This is because only the time-odd components of the residual interaction contribute. Therefore the matrix $\mathcal{M}$ can be written in the following form:

$$\mathcal{M} = \left[\mathcal{M}_0^{-1} + \mathcal{V}\right]^{-1} = \mathcal{M}_0[\mathbb{1} + \mathcal{V}\mathcal{M}_0]^{-1}. \tag{22}$$

We expand the factor in the square bracket and obtain

$$\mathcal{M} = \mathcal{M}_0 - \mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \mathcal{M}_0\mathcal{V}\mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \cdots. \tag{23}$$

Since $\mathcal{M}_0^{-1}$ is diagonal, inverting this matrix is trivial and the problem is reduced to simple matrix multiplications. The zero-order term, of course, yields the Inglis-Belyaev formula:

$$M^0_{\mu\mu'}(\mathbf{q}) = \frac{1}{\hbar^2}\begin{pmatrix} P^* & -P \end{pmatrix}_\mu \mathcal{M}_0 \begin{pmatrix} P \\ -P^* \end{pmatrix}_{\mu'} = \frac{2}{\hbar^2}\sum_{ph}\frac{|\hat{P}_{ph}|^2}{\epsilon_p - \epsilon_h}. \tag{24}$$

The first- and the second-order terms

$$\mathcal{M}_1 = -\mathcal{M}_0\mathcal{V}\mathcal{M}_0, \quad \mathcal{M}_2 = \mathcal{M}_0\mathcal{V}\mathcal{M}_0\mathcal{V}\mathcal{M}_0 \tag{25}$$

represent the leading corrections to the Inglis-Belyaev formula. The purpose of this exploratory study is to determine the convergence of the expansion (23), as well as the level of agreement with the Thouless-Valatin formula. In this work we only consider the moments of inertia for collective rotation, that is, the operator $\hat{P}$ corresponds to the components of the angular momentum vector.

It has to be noted that the deformed RPA equation built on top of the stationary ground-state solution (i.e., without the external quadrupole constraint) exhibits a Goldstone mode. As discussed in Chap. 8 of Ref. [17], the rotational invariance of the Hamiltonian $[H, J_x] = 0$ leads to the zero-frequency spurious solution for the operator $P = J_x$,

$$\mathcal{M}^{-1}\begin{pmatrix} P \\ P^* \end{pmatrix} = \begin{pmatrix} A & -B \\ -B^* & A^* \end{pmatrix}\begin{pmatrix} P \\ P^* \end{pmatrix} = 0. \tag{26}$$

The explicit inversion of the matrix $\mathcal{M}^{-1}$ is technically complicated because it has to be carried out in the space orthogonal to the Goldstone mode. However, the method proposed in this work avoids this difficulty. In each order of the expansion of the matrix $\mathcal{M}$ [see Eq. (19)], we multiply the vector

$$\begin{pmatrix} P \\ -P^* \end{pmatrix}, \tag{27}$$

which is orthogonal to the Goldstone mode, thus eliminating all spurious contributions. It also has to be emphasized that the problem of the Goldstone mode occurs only at the stationary points of the energy surface, where the quadrupole constraint vanishes. For all other points, the quadrupole constraint is finite and since it does not commute with the angular momentum operator, the Goldstone mode does not exist.

As a specific example of the nuclear energy density functional we consider the point-coupling implementation of a relativistic EDF—the functional PC-F1 [19]:

$$\begin{aligned} E_{\mathrm{RMF}} &= \int d\mathbf{r}\mathcal{E}_{\mathrm{RMF}}(\mathbf{r}) \\ &= \sum_{i=1}^{A}\int d\mathbf{r}\bar{\psi}_i(\mathbf{r})(-i\gamma\nabla + m)\psi_i(\mathbf{r}) + \int d\mathbf{r}\left[\frac{1}{2}\alpha_S\rho_S^2 + \frac{1}{3}\beta_S\rho_S^3 + \frac{1}{4}\beta_S\rho_S^4 + \delta_S\rho_S\triangle\rho_S + \frac{1}{2}\alpha_V j_\mu j^\mu + \frac{1}{4}\gamma_V(j_\mu j^\mu)^2\right. \\ &\quad \left. + \frac{1}{2}\delta_V j_\mu\Delta j^\mu + \frac{1}{2}\alpha_{TV}(j_{TV})_\mu(j_{TV})^\mu + \frac{1}{2}\delta_{TV}(j_{TV})_\mu\Delta(j_{TV})^\mu + \frac{1}{2}\alpha_{TS}\rho_{TS}^2 + \frac{1}{2}\delta_{TS}\rho_{TS}\Delta\rho_{TS} + \frac{e}{2}\rho_p A^0\right], \end{aligned} \tag{28}$$

where ψ denotes the Dirac spinor field of a nucleon, and the local isoscalar and isovector densities and currents

$$\rho_S(\mathbf{r}) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\psi_i(\mathbf{r}), \tag{29}$$

$$\rho_{TS}(\mathbf{r}) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\tau_3\psi_i(\mathbf{r}), \tag{30}$$

$$j^{\mu}(\mathbf{r}) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\gamma^{\mu}\psi_i(\mathbf{r}), \tag{31}$$

$$j^{\mu}_{TV}(\mathbf{r}) = \sum_{i=1}^{A} \bar{\psi}_i(\mathbf{r})\gamma^{\mu}\tau_3\psi_i(\mathbf{r}), \tag{32}$$

are calculated in the *no-sea* approximation: the summation runs over all occupied states in the Fermi sea. This means that only occupied single-nucleon states with positive energy explicitly contribute to the nucleon self-energies. In Eq. (28) ρ_p is the proton density, and A^0 denotes the Coulomb potential.

The matrix elements of the residual interaction are derived from the EDF Eq. (28)

$$V_{adbc} = \frac{\partial^2 E_{\mathrm{RMF}}}{\partial\rho_{ba}\partial\rho_{cd}}, \tag{33}$$

where generic indices $(a, b, c, d, \ldots)$ denote quantum numbers that specify the single-nucleon state $\{\psi_a\}$. These belong to three distinct sets: the index p (particle) denotes unoccupied states above the Fermi sea, the index h (hole) is for occupied states in the Fermi sea, and with α we denote the unoccupied negative-energy states in the Dirac sea. The calculation of the moments of inertia involves only the time-odd terms of the residual interaction, for which the isoscalar-vector channel plays the dominant role. The time-odd contributions of the isovector-vector and the electromagnetic fields are omitted because the corresponding couplings are small in comparison to the isoscalar-vector coupling. Here we make a further simplification by assuming that the nonlinear and the derivative terms can be neglected, that is, it is sufficient to retain only the linear isoscalar-vector term (see Fig. 1 and Table I):

$$V_{adbc} = -\alpha_V \int [\psi^{\dagger}_a \boldsymbol{\alpha}\psi_b][\psi^{\dagger}_d \boldsymbol{\alpha}\psi_c]d^3r\ . \tag{34}$$

III. NUMERICAL TEST

To verify our assumption that the time-odd part of the residual interaction can be approximated by the linear vector term, we have analyzed the contributions of the different time-odd terms to the moments of inertia by performing a self-consistent cranking calculation (see Refs. [3,20], and references cited therein). In the cranking framework there are two types of moments of inertia: the kinematic (or static) moment of inertia $\mathcal{I}^{(1)}$, and the dynamic moment of inertia $\mathcal{I}^{(2)}$. They are defined as

$$\mathcal{I}^{(1)}(\Omega) = \frac{J}{\Omega}, \quad \mathcal{I}^{(2)}(\Omega) = \frac{dJ}{d\Omega}. \tag{35}$$

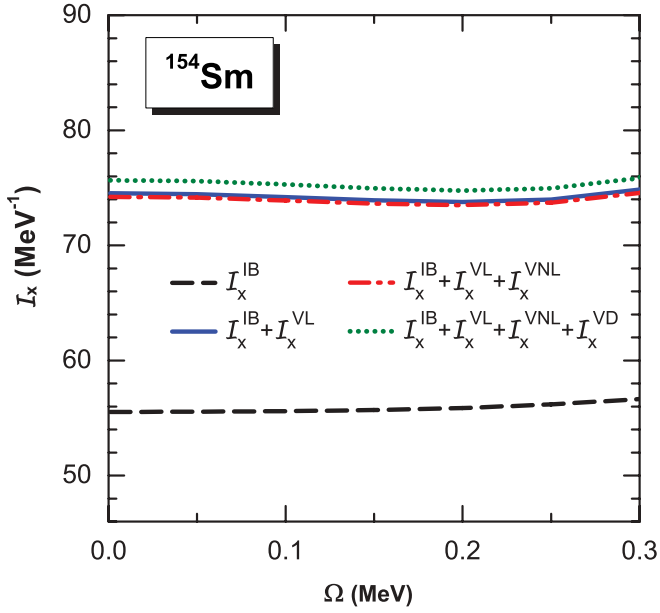

FIG. 1. (Color online) The moment of inertia $\mathcal{I}_x$ of ^{154}Sm computed using the cranking RMF framework. The various curves correspond to calculations that successively include the following terms of the residual interaction: the time-even part (Inglis-Belyaev formula denoted by IB), the linear (VL), nonlinear (VNL), and derivative (VD) time-odd terms in the isoscalar-vector channel.

In a self-consistent calculation with very small values of the rotational frequency, $\mathcal{J}^{(2)}(\Omega)$ is identical to the Thouless-Valatin moment of inertia, the linear response to the external Coriolis field. At the band-head in even-even nuclei the two quantities $\mathcal{J}^{(1)}$ and $\mathcal{J}^{(2)}$ coincide and we use in the figures the character $\mathcal{I}$ for this quantity. Calculations that neglect the time-odd fields and take into account only the Coriolis operator $\Omega\hat{J}_x$ in the Dirac equation, underestimate the empirical moments of inertia by roughly 30% [21]. As an illustrative example, in Fig. 1 we plot the dynamic moment of inertia for the ground state band in ^{154}Sm. By including only the linear time-odd term (VL) in isoscalar-vector channel the moment of inertia is enhanced by 34%, while the remaining two contributions: the nonlinear term (VNL) and the derivative term (VD) yield less than 3%. The results are summarized in Table I, where we list the contributions of the linear vector, nonlinear vector and vector derivative terms to the moment of inertia. Thus in the remaining calculations the model includes only the linear time-odd term.

TABLE I. Contributions to the moment of inertia $\mathcal{I}_x$ of different terms of the residual interaction: the time-even part (Inglis-Belyaev formula denoted by IB), the linear (VL), nonlinear (VNL), and derivative (VD) time-odd terms in the isoscalar-vector channel. The calculation is performed using the cranking RMF framework with the PC-F1 interaction, and the cranking frequency is $\Omega = 0.001$ MeV.

$\mathcal{I}_x^{\mathrm{IB}}$	$\mathcal{I}_x^{\mathrm{VL}}$	$\mathcal{I}_x^{\mathrm{VNL}}$	$\mathcal{I}_x^{\mathrm{VD}}$
55.53	18.99	−0.31	1.44

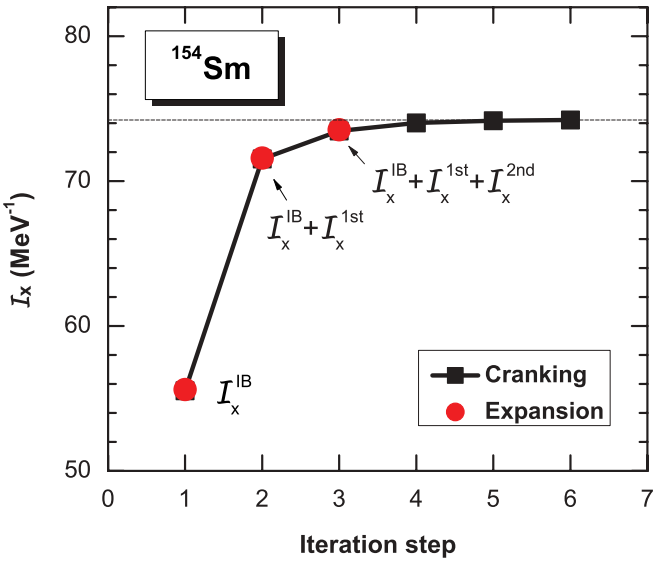

FIG. 2. (Color online) The moment of inertia $\mathcal{I}_x$ of ^{154}Sm computed at the zeroth-, first-, and second-order in the expansion Eq. (23) based on the PC-F1 density functional, and compared with the values obtained at the corresponding iteration steps in the cranking RMF based on the same density functional.

To estimate the convergence of the expansion formula (23), we have used it to calculate the moment of inertia $\mathcal{I}_x$ for the ^{154}Sm isotope, in comparison with the exact Thouless-Valatin moment of inertia computed with the cranking code. In Fig. 2 the latter is compared with the zeroth-, first-, and second-order in the expansion Eq. (23). Moreover, we also display the cranking results for each iteration step in the self-consistent cranking calculation, starting from the stationary solution without the cranking term (cf. Appendix). As one expects, the moment of inertia obtained after the first iteration is equal to the Inglis-Belyaev moment of inertia. The next two iterations are compared to the first and second order in the expansion formula (23). We note that the values obtained after the second and third iteration steps are in complete agreement with the first- and the second-order corrections, respectively. In the Appendix we demonstrate that these values have to be identical, thus the results displayed in Fig. 2 provide a crucial test for the numerical implementation of the expansion Eq. (23). Further iteration steps contribute to the value of the moment of inertia by less than 1%, that is, the convergence is quite rapid. We also emphasize that it is necessary to include the contributions from the negative-energy single-nucleon Dirac states in the calculation of the matrix $\mathcal{M}$. Omitting the negative energy states leads to a significant overestimation of the second-order correction to the moment of inertia.

Finally, in Fig. 3 we display the moments of inertia $\mathcal{I}_x$ for the sequence of even-even isotopes $^{152-164}$Sm. The values computed at the zeroth-, first-, and second-order in the expansion Eq. (23) are compared with the exact Thouless-Valatin moment of inertia calculated using the RMF cranking model. Through the whole isotopic chain the expansion method, truncated to second order, yields values very close to the exact Thouless-Valatin moments of inertia, with the relative deviation ∼1%. We note that the enhancement of the moment

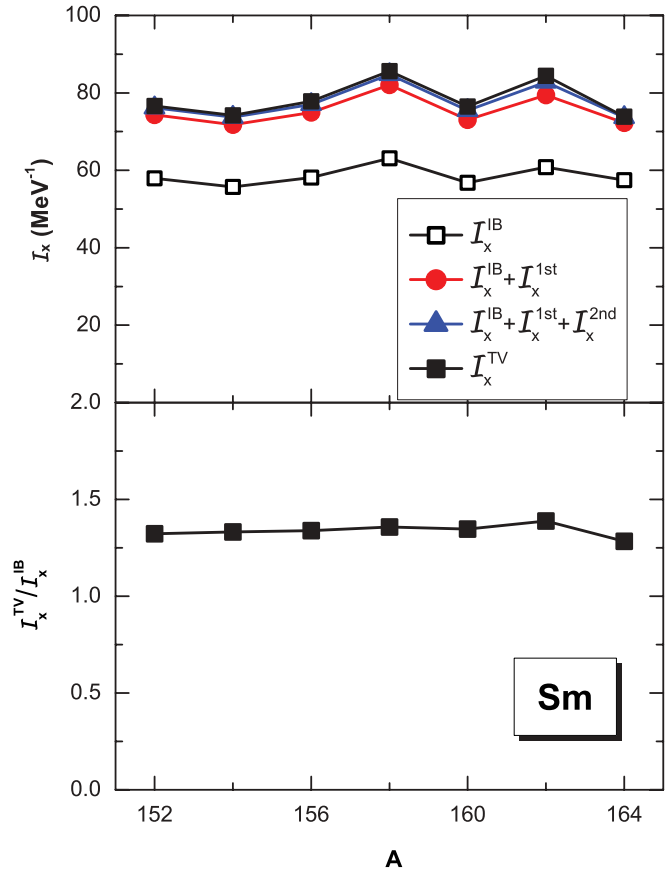

FIG. 3. (Color online) The moments of inertia $\mathcal{I}_x$ of $^{152-164}$Sm. The values computed at the zeroth-, first-, and second-order in the expansion Eq. (23) are compared with the exact Thouless-Valatin moment of inertia calculated using the RMF cranking model (upper panel). For the same nuclei the ratio of the Thouless-Valatin and Inglis-Belyaev moments of inertia (lower panel).

of inertia in comparison to the Inglis-Belyaev value ranges of 1.28∼1.39.

IV. SUMMARY AND OUTLOOK

Starting from the adiabatic time-dependent Hartree-Fock theory, we have introduced an efficient approximate method to calculate the Thouless-Valatin moments of inertia for the nuclear system. The method is based on the fact that the expansion of the inertial parameters converges rapidly because the matrix elements of the time-odd components of the residual interaction are usually small in comparison to the *ph* energies. This approximation is computationally much less demanding than the full ATDHF calculation, yet it retains high accuracy of the order of 1%. The accuracy of this method has been verified by comparing the results to the exact Thouless-Valatin rotational moments of inertia calculated within the cranking model.

One might, of course, encounter problems in regions of level crossings, where the *ph* energies are no longer necessarily small compared to the matrix elements of the residual interaction $\mathcal{V}$. In that case the matrix $\mathcal{M}^{-1}$ in Eq. (20)

has to be decomposed in a different way as, for instance, by shifting the diagonal elements of $\mathcal{V}$ to $\mathcal{M}_0^{-1}$, or by adding and subtracting complex diagonal elements.

The present investigation has been restricted to the rotational moments of inertia, only one specific energy density functional has been considered and the pairing correlations have been neglected. Further studies will include the calculations of the vibrational masses. As compared to the rotational moments of inertia, the main complication comes from the fact that the momentum operator is not known a priori. Several methods have already been proposed to tackle this problem [13,22,23] and we hope to solve it by the expansion method, similar to the one described in the manuscript. The described method can be used with other energy density functionals by simply replacing the time-odd residual interaction and the pairing correlations can easily be included by expanding the inverse of the QRPA instead of the RPA matrix. Work along these lines is already in progress.

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APPENDIX: ITERATIVE SOLUTION OF THE CRANKING EQUATION

In this Appendix it is demonstrated that the moment of inertia calculated at each step of the iterative solution of the cranking equation, coincides with the corresponding order of the expansion introduced in Sec. II. We assume that the cranking frequency in the equation of motion

$$[h(\rho) - \Omega j_x, \rho] = 0, \tag{A1}$$

is an infinitesimal quantity, that is, second and higher order terms in Ω can be safely neglected. As the initial point we choose the self-consistent solution ρ_0 for frequency $\Omega = 0$. The corresponding equation of motion reads

$$[h_0, \rho_0] = 0. \tag{A2}$$

In the first step of the iteration we diagonalize the operator $h_0 - \Omega j_x$, and compute the density $\rho_0 + \delta\rho_0$ determined by the following relation:

$$[h_0, \delta\rho_0] = \Omega\,[j_x, \rho_0]\,. \tag{A3}$$

In the basis which diagonalizes h_0, the only nonvanishing matrix elements of $\delta\rho_0$ are ph and hp. Using the definition of the matrix $\mathcal{M}_0$ Eq. (21), we obtain

$$\begin{pmatrix} \delta\rho_0 \\ \delta\rho_0^* \end{pmatrix} = \Omega\mathcal{M}_0 \begin{pmatrix} j_x \\ j_x^* \end{pmatrix}. \tag{A4}$$

In the following the shorthand notation is used:

$$\delta\tilde{\rho}_0 \equiv \begin{pmatrix} \delta\rho_0 \\ \delta\rho_0^* \end{pmatrix} \quad \text{and} \quad \tilde{j}_x \equiv \begin{pmatrix} j_x \\ j_x^* \end{pmatrix}, \tag{A5}$$

that is, $\delta\tilde{\rho}_0 = \Omega\mathcal{M}_0\tilde{j}_x$. After the first iteration we obtain the Inglis-Belyaev moment of inertia:

$$\mathcal{I}_0 = \frac{1}{\Omega}\mathrm{Tr}(j_x\delta\rho_0) = \frac{1}{\Omega}\,(j_x^* \quad j_x)\begin{pmatrix} \delta\rho_0 \\ \delta\rho_0^* \end{pmatrix} = \tilde{j}_x^\dagger\mathcal{M}_0\tilde{j}_x \equiv \mathcal{I}^{\mathrm{IB}}. \tag{A6}$$

In the second iteration we diagonalize the operator:

$$\begin{aligned} h_1 - \Omega j_x &= h(\rho_0 + \delta\rho_0) - \Omega j_x = h_0 + \mathcal{V}\delta\rho_0 - \Omega j_x \\ &= h_0 - \Omega(j_x - \mathcal{V}\mathcal{M}_0\tilde{j}_x), \end{aligned} \tag{A7}$$

where $\mathcal{V}\mathcal{M}_0\tilde{j}_x$ denotes the matrix

$$(\mathcal{V}\mathcal{M}_0\tilde{j}_x)_{ab} = \sum_{php'h'} \mathcal{V}_{ahbp}\mathcal{M}_{0php'h'}(j_x)_{p'h'} + \mathcal{V}_{apbh}\mathcal{M}_{0hph'p'}(j_x)^*_{p'h'}. \tag{A8}$$

The density $\rho_0 + \delta\rho_1$ is the solution of the equation of motion

$$[h_0 - \Omega(j_x - \mathcal{V}\mathcal{M}_0\tilde{j}_x), \rho_0 + \delta\rho_1] = 0\,. \tag{A9}$$

Again, $\delta\rho_1$ has only ph-matrix elements and, therefore, we need only these elements of the matrix (A8) and find

$$\delta\tilde{\rho}_1 = \Omega\mathcal{M}_0(\mathbb{1} - \mathcal{V}\mathcal{M}_0)\tilde{j}_x. \tag{A10}$$

The moment of inertia obtained in the second iteration coincides with that defined by Eq. (25)

$$\begin{aligned} \mathcal{I}_2 &= \frac{1}{\Omega}\mathrm{Tr}(j_x\delta\rho_1) = \begin{pmatrix} j_x^* & j_x \end{pmatrix}\begin{pmatrix} \delta\rho_1 \\ \delta\rho_1^* \end{pmatrix} \\ &= \tilde{j}_x^\dagger\mathcal{M}_0\,(\mathbb{1} - \mathcal{V}\mathcal{M}_0)\,\tilde{j}_x. \end{aligned} \tag{A11}$$

Obviously this can be continued, and finally we obtain the expansion for the full moment of inertia

$$\mathcal{I} = \tilde{j}_x^\dagger\,(\mathcal{M}_0 - \mathcal{M}_0\mathcal{V}\mathcal{M}_0 + \mathcal{M}_0\mathcal{V}\mathcal{M}_0\mathcal{V}\mathcal{M}_0 - \cdots)\,\tilde{j}_x, \tag{A12}$$

which is equivalent to the expansion of the matrix $\mathcal{M}$ in Eq. (23).

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