Quadrupole collective inertia in nuclear fission: Cranking approximation

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(Received 21 July 2010; revised manuscript received 19 September 2011; published 28 November 2011)

A collective mass tensor derived from the cranking approximation to the adiabatic time-dependent Hartree-Fock-Bogoliubov (ATDHFB) approach is compared with that obtained in the Gaussian overlap approximation (GOA) to the generator coordinate method. Illustrative calculations are carried out for one-dimensional quadrupole fission pathways in ^{256}Fm. It is shown that the collective mass exhibits strong variations with the quadrupole collective coordinate. These variations are related to the changes in the intrinsic shell structure. The differences between collective inertia obtained in cranking and perturbative cranking approximations to ATDHFB, and within GOA, are discussed.

DOI: 10.1103/PhysRevC.84.054321 PACS number(s): 24.75.+i, 21.60.Jz, 21.60.Ev

I. INTRODUCTION

Microscopic understanding of nuclear collective dynamics is a long-term goal of low-energy nuclear theory. Large-amplitude collective motion (LACM), as seen in fission and fusion, provides a particularly important challenge. Those phenomena can be understood in terms of many-body tunneling involving the mixing of mean fields with different symmetries. We have yet to obtain a microscopic understanding of LACM that is comparable to what we have for ground states, excited states, and response functions.

For heavy, complex nuclei, the theoretical tool of choice is the self-consistent nuclear density-functional theory (DFT) [1,2]. The advantage of DFT is that, while treating the nucleus as a many-body system of fermions, it provides an avenue for identifying the essential collective degrees of freedom and provides an excellent starting point for time-dependent extensions. The time-dependent Hartree-Fock-Bogoliubov (TDHFB) theory appears, in principle, to provide a proper theoretical framework to describe the LACM. However, the main drawback of TDHFB, when applied to fission, is its inability to describe the quantum-mechanical motion under the collective barrier. (For description of fission from excited states above the barrier, time-dependent self-consistent approaches have been proven very successful [3].)

On the other hand, the adiabatic approximation to TDHFB (ATDHFB) has been successfully applied to the LACM [4–13]. The main assumption behind ATDHFB, well fulfilled in the context of spontaneous fission, is that the collective motion of the system is slow compared to the single-particle motion of individual nucleons [1,14]. According to the path formulation of the fission problem [15], ATDHFB provides the best framework to tackle the problem of nuclear dynamics under the barrier. Another advantage of ATDHFB is that it provides a connection between the microscopic many-body theory and phenomenological models based on collective shape variables.

The main theoretical input for an estimate of fission half-lives is collective inertia (mass tensor) and collective potential. ATDHFB provides the best framework to calculate the mass tensor [15]. However, in most applications, various approximations are adopted. In the commonly used cranking expression, for instance, the derivatives with respect to collective coordinates (i.e., collective momenta) are evaluated using the perturbation theory, and the Thouless-Valatin self-consistent terms yielding time-odd fields are neglected. The resulting collective masses are known to be too small [7,12]; hence it is imperative to go beyond the perturbative cranking treatment.

In the self-consistent investigations of Ref. [12], based on the Gogny energy density functional, collective masses were calculated by explicitly evaluating the collective-coordinate derivatives appearing in the ATDHFB mass expression. The resulting collective mass obtained in such an approach turned out to exhibit appreciable variations along the collective path, suppressed in the perturbative cranking treatment. Furthermore, they noted that ATDHFB cranking mass could be an order of magnitude greater than the perturbative cranking mass. As noted in Ref. [12], the enhanced masses obtained in the improved analysis can significantly impact the calculated fission lifetimes.

The main goal of this work is to investigate the ATDHFB cranking mass using the nuclear DFT approach with Skyrme energy functionals. The paper is organized as follows. Section II summarizes the basic ATDHFB expressions for collective inertia obtained in Ref. [7]. The approximate cranking, perturbative cranking, and Gaussian overlap approximation (GOA) formulations are given in Sec. III. Section IV describes the model and technical details of our calculations. The illustrative examples are contained in Sec. V, where the results are presented for ^{256}Fm. Finally, the main results are given in Sec. VI.

II. ATDHFB THEORY

This section contains a brief derivation of the collective mass tensor in the ATDHFB framework. Although some of the expressions are well documented in the literature [1,7], we

repeat them here for the sake of completeness with particular attention paid to various approximations involved.

A. Summary of Hartree-Fock-Bogoliubov

We begin with the Hartree-Fock-Bogoliubov (HFB) approach. In what follows, we use the same notation as in Ref. [16]. The HFB formalism can be conveniently expressed in terms of the generalized density matrix, $\mathcal{R}$, defined as

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}, \tag{1}$$

where ρ and κ are the particle and pairing densities and $\mathcal{R}^2 = \mathcal{R}$. The energy variation results in the HFB equation

$$[\mathcal{W}, \mathcal{R}] = 0, \tag{2}$$

which can be written as a nonlinear eigenvalue problem:

$$\mathcal{W}\begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix} = \begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix}\begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \tag{3}$$

where

$$\mathcal{W} = \begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}, \tag{4}$$

where E is a diagonal matrix of quasiparticle energies E_μ, λ is the chemical potential, and matrices h and Δ are the particle-hole and pairing mean-field potentials [1], respectively.

For the sake of comparison with the commonly used BCS formalism, it is quite useful to write the HFB equations in the canonical representation. The single-particle canonical wave function $|\mu\rangle$ can be expanded in the original single-particle (harmonic-oscillator) basis $|n\rangle$ as

$$|\mu\rangle = \sum_n D_{n\mu}|n\rangle, \tag{5}$$

where the unitary transformation D is obtained by diagonalizing the density matrix ρ. In the canonical basis, the HFB wave function is given in a BCS-like form:

$$\breve{A}_{\mu\nu} = u_\mu \delta_{\mu\nu}, \quad \breve{B}_{\mu\nu} = s^*_{\bar{\mu}} v_\mu \delta_{\bar{\mu}\nu}, \tag{6}$$

$$u_\mu = u_{\bar{\mu}} = u^*_\mu, \quad v_\mu = v_{\bar{\mu}} = v^*_\mu, \tag{7}$$

where the phase s_μ, for the time-even quasiparticle vacuum considered here, is defined through the time inversion of the single-particle states:

$$\hat{T}|\mu\rangle = s_\mu|\bar{\mu}\rangle, \quad s_{\bar{\mu}} = -s_\mu. \tag{8}$$

In Eq. (6) and in the following, the quantities in the canonical basis are denoted by symbols with breve accents [16].

The HFB energy matrix $\breve{E}$ in the canonical basis is nondiagonal and is given by

$$\breve{E}_{\mu\nu} = \xi^+_{\mu\nu}(\breve{h}-\lambda)_{\mu\nu} - \eta^+_{\mu\nu}\breve{\Delta}_{\mu\bar{\nu}}s^*_{\bar{\nu}}, \tag{9}$$

where

$$\eta^\pm_{\mu\nu} = u_\mu v_\nu \pm u_\nu v_\mu \quad \text{and} \quad \xi^\pm_{\mu\nu} = u_\mu u_\nu \mp v_\mu v_\nu. \tag{10}$$

The diagonal matrix elements of the matrix $\breve{E}_{\mu\nu}$ can be written as [1,16]

$$\breve{E}_\mu \equiv \breve{E}_{\mu\mu} = \sqrt{(\breve{h}_{\mu\mu}-\lambda)^2 + \breve{\Delta}^2_{\mu\bar{\mu}}}. \tag{11}$$

Even though the above equation resembles the BCS expression for quasiparticle energy, it involves $\breve{h}_{\mu\mu}$ and $\breve{\Delta}_{\mu\bar{\mu}}$, which are respectively obtained by transforming the HFB particle-hole and the pairing fields to the canonical basis via the transformation (5). It is only in the BCS approximation that these quantities can be associated with single-particle energies and the pairing gap.

B. Summary of ATDHFB

The ATDHFB approach is a theoretical method to treat the problem of the large-amplitude collective motion. In ATDHFB, the motion of the system can be described in terms of collective coordinates $\{q_i\}$ and canonically conjugated collective momenta $p_i = -i\partial/\partial q_i$. ATDHFB is an approximation to the time-dependent HFB theory; in its roots lies the adiabatic assumption that the collective motion is slow, i.e., the collective velocities of the system $\{\dot{q}_i\}$ is well below the average single-particle velocity of the nucleons [1,17]. The collective coordinates are expectation values of dynamic generator operators $\{\hat{Q}_i\}$ in the HFB vacuum:

$$q_i = \langle 0|\hat{Q}_i|0\rangle. \tag{12}$$

In practical applications, the collective subspace (or collective path) is determined by solving the constrained HFB problem by introducing the set of Lagrange multipliers λ_{Q_i} determined from Eqs. (12). In most applications, the generators $\{\hat{Q}_i\}$ are one-body operators; hence, the particle-hole field h is modified by adding a cranking term:

$$h \to h - \sum_i \lambda_{Q_i}\hat{Q}_i. \tag{13}$$

At present, sophisticated methods exist to reach solutions in which average values $\langle 0|\hat{Q}_i|0\rangle$ take arbitrary values and thus build continuous collective paths or potential-energy surfaces (see Ref. [18] for a review). Although Lagrange multipliers are usually complicated multivalued functions of collective coordinates q_i, around each point in the collective space the total energy is always stationary for some fixed values of λ_{Q_i}.

In the ATDHFB method, the generalized HFB density matrix is expanded around the quasistationary HFB solution $\mathcal{R}_0$ up to quadratic terms in the collective momentum:

$$\mathcal{R} = \mathcal{R}_0 + \mathcal{R}_1 + \mathcal{R}_2, \tag{14}$$

with $\mathcal{R}_1$ being time-odd and $\mathcal{R}_0$ and $\mathcal{R}_2$ being time-even densities. The corresponding expansion for the HFB Hamiltonian matrix reads

$$\mathcal{W} = \mathcal{W}_0 + \mathcal{W}_1 + \mathcal{W}_2. \tag{15}$$

Employing the density expansion (14), the HFB energy can be separated into the collective kinetic and the potential parts. In terms of the density expansion (14), the kinetic energy is given

by

$$\mathcal{K} = \frac{1}{2}\mathrm{Tr}(\mathcal{W}_0\mathcal{R}_2) + \frac{1}{4}\mathrm{Tr}(\mathcal{W}_1\mathcal{R}_1) = \frac{i}{4}\mathrm{Tr}\left(\dot{\mathcal{R}}_0[\mathcal{R}_0, \mathcal{R}_1]\right) - \frac{1}{2}\left([\mathcal{R}_2, \mathcal{R}_0][\mathcal{W}_0, \mathcal{R}_0]\right). \quad (16)$$

In the usual ATDHFB treatment, the second term involving $\mathcal{R}_2$ is neglected, and, in the case of one collective coordinate q, the kinetic energy can be written in the familiar form:

$$\mathcal{K} = \tfrac{1}{2}\dot{q}^2\mathcal{M}, \quad (17)$$

where the collective mass is given by

$$\mathcal{M} = \frac{i}{2\dot{q}^2}\mathrm{Tr}(\dot{\mathcal{R}}_0[\mathcal{R}_0, \mathcal{R}_1]) \quad (18)$$

$$= \frac{i}{2\dot{q}}\mathrm{Tr}\left(\frac{\partial\mathcal{R}_0}{\partial q}[\mathcal{R}_0, \mathcal{R}_1]\right). \quad (19)$$

The trace in the above expression can easily be evaluated in the quasiparticle basis. To this end, one can utilize the ATDHFB equation [4–7]:

$$i\dot{\mathcal{R}}_0 = [\mathcal{W}_0, \mathcal{R}_1] + [\mathcal{W}_1, \mathcal{R}_0]. \quad (20)$$

In the quasiparticle basis, the matrices $\mathcal{R}_0$, $\mathcal{W}_0$, $\mathcal{W}_1$, $\mathcal{R}_1$, and $\dot{\mathcal{R}}_0$ are represented by the matrices $\mathcal{G}$, $\mathcal{E}_0$, $\mathcal{E}_1$, $\mathcal{Z}$, and $\mathcal{F}$, respectively:

$$\mathcal{R}_0 = \mathcal{A}\mathcal{G}\mathcal{A}^\dagger, \quad (21)$$

$$\mathcal{W}_0 = \mathcal{A}\mathcal{E}_0\mathcal{A}^\dagger, \quad (22)$$

$$\mathcal{W}_1 = \mathcal{A}\mathcal{E}_1\mathcal{A}^\dagger, \quad (23)$$

$$\mathcal{R}_1 = \mathcal{A}\mathcal{Z}\mathcal{A}^\dagger, \quad (24)$$

$$\dot{\mathcal{R}}_0 = \mathcal{A}\mathcal{F}\mathcal{A}^\dagger, \quad (25)$$

where

$$\mathcal{A} = \begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix} \quad (26)$$

is the matrix of the Bogolyubov transformation, and

$$\mathcal{G} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathcal{E}_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}. \quad (27)$$

ATDHFB equation (20) can now be written in the quasiparticle basis as

$$i\mathcal{F} = [\mathcal{E}_0, \mathcal{Z}] + [\mathcal{E}_1, \mathcal{G}]. \quad (28)$$

This 2×2 matrix equation is, in fact, equivalent [7] to the following equation:

$$iF = EZ + ZE + E_1, \quad (29)$$

where the antisymmetric matrices F, Z, and E_1 are related to $\mathcal{F}$, $\mathcal{Z}$, and $\mathcal{E}_1$:

$$\mathcal{F} = \begin{pmatrix} 0 & F \\ -F^* & 0 \end{pmatrix}, \quad \mathcal{Z} = \begin{pmatrix} 0 & Z \\ -Z^* & 0 \end{pmatrix}, \quad (30)$$

$$[\mathcal{E}_1, \mathcal{G}] = \begin{pmatrix} 0 & E_1 \\ -E_1^* & 0 \end{pmatrix}. \quad (31)$$

In the case of several collective coordinates $\{q_i\}$, the ATDHFB equation (20) must be solved for each coordinate:

$$i\dot{q}_i\frac{\partial\mathcal{R}_0}{\partial q_i} = \left[\mathcal{W}_0, \mathcal{R}_1^i\right] + \left[\mathcal{W}_1^i, \mathcal{R}_0\right], \quad (32)$$

and the collective mass tensor becomes

$$\mathcal{M}_{ij} = \frac{i}{2\dot{q}_j}\mathrm{Tr}\left(\frac{\partial\mathcal{R}_0}{\partial q_i}\left[\mathcal{R}_0, \mathcal{R}_1^j\right]\right). \quad (33)$$

Then, in terms of the corresponding matrices F^i and Z^j, the collective mass tensor is given by

$$\mathcal{M}_{ij} = \frac{i}{2\dot{q}_i\dot{q}_j}\mathrm{Tr}(F^{i*}Z^j - F^iZ^{j*}). \quad (34)$$

The expression (34) for the mass tensor contains the matrix Z^i, which is associated with time-odd density matrix $\mathcal{R}_1^i$ and can, in principle, be obtained by solving the HFB equations with time-odd fields. The time-odd fields have been incorporated in mass-tensor calculations only in a limited number of cases. For instance, in Ref. [11], time-odd fields have been included in the HF study with a constraint of cylindrical symmetry. The time-odd fields have also been incorporated in the HFB study in an approximate iterative scheme with the collective path based on the Woods-Saxon potential [7].

III. APPROXIMATIONS TO ATDHFB

This section contains the summary of various commonly used approximations to the exact ATDHFB expression (34).

A. Cranking approximation

In most of the studies, the time-odd interaction matrix E_1 appearing in Eq. (29) is neglected. In the following, this approximation will be referred to as the cranking approximation (ATDHFB-C). In the absence of the term involving E_1, the Z matrix can be easily obtained in the quasiparticle basis from the equation

$$-iF^i_{\alpha\beta} = (E_\alpha + E_\beta)Z^i_{\alpha\beta}, \quad (35)$$

and the collective cranking mass tensor is given by

$$\mathcal{M}^C_{ij} = \frac{1}{2\dot{q}_i\dot{q}_j}\sum_{\alpha\beta}\frac{\left(F^{i*}_{\alpha\beta}F^j_{\alpha\beta} + F^i_{\alpha\beta}F^{j*}_{\alpha\beta}\right)}{E_\alpha + E_\beta}. \quad (36)$$

It should be noted that Eq. (35) is diagonal in the quasiparticle basis $|\alpha\rangle$ and not in the canonical basis $|\mu\rangle$. The essential input to the ATDHFB-C mass tensor (36) is the matrix F. In the following, F is evaluated in both the canonical and quasiparticle basis.

1. Canonical basis

To begin with, Eq. (25) can be written explicitly in terms of the HFB eigenvectors:

$$\dot{\mathcal{R}}_0 = \dot{q}\frac{\partial}{\partial q}\begin{pmatrix} \rho_0 & \kappa_0 \\ -\kappa_0^* & 1-\rho_0^* \end{pmatrix} = \begin{pmatrix} AFB^T - B^*F^*A^\dagger & AFA^T - B^*F^*B^\dagger \\ BFB^T - A^*F^*A^\dagger & BFA^T - A^*F^*B^\dagger \end{pmatrix}. \quad (37)$$

Evaluating the matrix elements of Eq. (37) in the canonical basis, we obtain

$$\check{F}^i_{\mu\bar{\nu}} = \frac{s_{\bar{\nu}}}{(u_\mu v_\nu + v_\mu u_\nu)} \dot{q}_i \left(\frac{\partial \rho_0}{\partial q_i}\right)_{\mu\nu}. \tag{38}$$

By differentiating the HFB equation $[\mathcal{W}_0, \mathcal{R}_0] = 0$ with respect to q_i, the derivative of the density matrix in Eq. (38) can be expressed in terms of the derivatives of the particle-hole and the pairing mean fields. The resulting 2×2 matrix equation is

$$\left[\mathcal{A}^\dagger \dot{q}_i \frac{\partial \mathcal{W}_0}{\partial q_i} \mathcal{A}, \mathcal{G}\right] + [\mathcal{E}_0, \mathcal{F}] = 0. \tag{39}$$

By employing the properties of h and Δ with respect to time reversal, we obtain

$$\left(\frac{\partial h^*}{\partial q_i}\right)_{\mu\nu} = s^*_\mu s_\nu \left(\frac{\partial h}{\partial q_i}\right)_{\bar{\mu}\bar{\nu}}, \tag{40}$$

$$\left(\frac{\partial \Delta^*}{\partial q_i}\right)_{\mu\nu} = s^*_\mu s^*_\nu \left(\frac{\partial \Delta}{\partial q_i}\right)_{\bar{\mu}\bar{\nu}}, \tag{41}$$

and, by approximating the HFB energy matrix in the canonical basis by its diagonal matrix elements,

$$\check{E}_{\mu\nu} \approx \delta_{\mu\nu} \check{E}_\mu, \tag{42}$$

one arrives at an approximate "BCS-equivalent" expression for the matrix elements of F in the canonical basis:

$$\check{F}^i_{\mu\nu} \approx \frac{-\dot{q}_i}{\check{E}_\mu + \check{E}_\nu} [s_\nu \eta^+_{\mu\nu}(\check{h}_{,i} - \lambda_{,i})_{\mu\bar{\nu}} + \xi^+_{\mu\nu}(\check{\Delta}_{,i})_{\mu\nu}], \tag{43}$$

where we applied the usual notation $x_{,i} \equiv \partial x/\partial q_i$ for $x = \check{h}$, $\check{\Delta}$, or λ. In the following, the results obtained by using this approximation will be called ATDHFB-C$^{\rm c}$.

Using relations (42) and (43), the collective mass tensor (36) can now be expressed in terms of the derivatives of the mean-field potentials with respect to the collective coordinates q_i and BCS-like quasiparticle energies (11):

$$\mathcal{M}^{C^{\rm c}}_{ij} \approx \frac{1}{2\dot{q}_i\dot{q}_j} \sum_{\mu\nu} \frac{(\check{F}^{i*}_{\mu\nu}\check{F}^j_{\mu\nu} + \check{F}^i_{\mu\nu}\check{F}^{j*}_{\mu\nu})}{\check{E}_\mu + \check{E}_\nu}. \tag{44}$$

In the one-dimensional case, the resulting expression agrees with that of Ref. [12].

2. *Quasiparticle basis*

In order to obtain the expression for matrix F in the quasiparticle basis, we invert Eq. (25) and write the matrix expression for $\mathcal{F} = \mathcal{A}^\dagger \dot{\mathcal{R}}_0 \mathcal{A}$:

$$\mathcal{F} = \begin{pmatrix} A^\dagger\dot{\rho}_0 A + A^\dagger\dot{\kappa}_0 B - B^\dagger\dot{\kappa}^*_0 A - B^\dagger\dot{\rho}^*_0 B & A^\dagger\dot{\rho}_0 B^* + A^\dagger\dot{\kappa}_0 A^* - B^\dagger\dot{\kappa}^*_0 B^* - B^\dagger\dot{\rho}^*_0 A^* \\ B^T\dot{\rho}_0 A + B^T\dot{\kappa}_0 B - A^T\dot{\kappa}^*_0 A - A^T\dot{\rho}^*_0 B & B^T\dot{\rho}_0 B^* + B^T\dot{\kappa}_0 A^* - A^T\dot{\kappa}^*_0 B^* - A^T\dot{\rho}^*_0 A^* \end{pmatrix}. \tag{45}$$

Elements (1,1) and (2,2) of $\mathcal{F}$ vanish because $\mathcal{R}_0$ is projective, $\mathcal{R}_0^2 = \mathcal{R}_0$. Equating the above expression with Eq. (30), we obtain

$$-F^* = B^T\dot{\rho}_0 A + B^T\dot{\kappa}_0 B - A^T\dot{\kappa}^*_0 A - A^T\dot{\rho}^*_0 B. \tag{46}$$

In the following, we evaluate the above expression in the simplex basis, as the mean-field analysis has been performed by imposing this symmetry. In this basis, the HFB wave function has the following structure:

$$B = \begin{pmatrix} B_+ & 0 \\ 0 & B_- \end{pmatrix} \text{ and } A = \begin{pmatrix} 0 & A_+ \\ A_- & 0 \end{pmatrix}. \tag{47}$$

The density matrices acquire the following forms in the simplex basis:

$$\rho = \begin{pmatrix} B^*_+ B^T_+ & 0 \\ 0 & B^*_- B^T_- \end{pmatrix} = \begin{pmatrix} \rho_+ & 0 \\ 0 & \rho_- \end{pmatrix}, \tag{48}$$

$$\kappa = \begin{pmatrix} 0 & B^*_+ A^T_- \\ B^*_- A^T_+ & 0 \end{pmatrix} = \begin{pmatrix} 0 & \kappa_+ \\ \kappa_- & 0 \end{pmatrix}. \tag{49}$$

The simplex structure of various terms in Eq. (46) is given by

$$\begin{aligned} B^T\dot{\rho}_0 A &= \begin{pmatrix} 0 & B^T_+\dot{\rho}_{0+}A_+ \\ B^T_-\dot{\rho}_{0-}A_- & 0 \end{pmatrix}, \\ A^T\dot{\rho}^*_0 B &= \begin{pmatrix} 0 & A^T_-\dot{\rho}^*_{0-}B_- \\ A^T_+\dot{\rho}^*_{0+}B_+ & 0 \end{pmatrix}, \\ B^T\dot{\kappa}_0 B &= \begin{pmatrix} 0 & B^T_+\dot{\kappa}_{0+}B_- \\ B^T_-\dot{\kappa}_{0-}B_+ & 0 \end{pmatrix}, \\ A^T\dot{\kappa}^*_0 A &= \begin{pmatrix} 0 & A^T_-\dot{\kappa}^*_{0-}A_+ \\ A^T_+\dot{\kappa}^*_{0+}A_- & 0 \end{pmatrix}. \end{aligned} \tag{50}$$

This yields

$$-F^* = \begin{pmatrix} 0 & F_+ \\ F_- & 0 \end{pmatrix}, \tag{51}$$

where

$$\begin{aligned} F_+ &= B^T_+\dot{\rho}_{0+}A_+ - A^T_-\dot{\rho}^*_{0-}B_- \\ &\quad + B^T_+\dot{\kappa}_{0+}B_- - A^T_-\dot{\kappa}^*_{0-}A_+, \end{aligned} \tag{52}$$

$$\begin{aligned} F_- &= B^T_-\dot{\rho}_{0-}A_- - A^T_+\dot{\rho}^*_{0+}B_+ \\ &\quad + B^T_-\dot{\kappa}_{0-}B_+ - A^T_+\dot{\kappa}^*_{0+}A_-. \end{aligned} \tag{53}$$

Since F is antisymmetric, we have obviously $F_+^T = -F_-$, which is fulfilled explicitly provided $\kappa_+^T = -\kappa_-$.

3. Calculation of derivatives

The collective mass involves either derivatives of the density matrices or the mean-field potentials. It should be stressed that these derivatives must be calculated in the original single-particle basis $|n\rangle$, as the canonical basis (5) varies with $\{q_i\}$. In the following, we show how to evaluate the collective derivatives in the one-dimensional case of a single collective coordinate, the quadrupole deformation q. To this end, we approximate the derivative of the density operator ρ or κ at a deformation point $q = q_0$ by means of the Lagrange three-point formula for unequally spaced points $q_0 - \delta q$, q_0, and $q_0 + \delta q'$ [11,12,19]:

$$\left(\frac{\partial\rho}{\partial q}\right)_{q=q_0} \approx \frac{-\delta q'}{\delta q(\delta q + \delta q')}\rho(q_0 - \delta q) + \frac{\delta q - \delta q'}{\delta q\,\delta q'}\rho(q_0) + \frac{\delta q}{\delta q'(\delta q + \delta q')}\rho(q_0 + \delta q'). \tag{54}$$

The corresponding matrix element in the canonical basis can be expressed through the matrices $D_{n\nu}$ of the canonical transformation (5):

$$\left(\frac{\partial\rho}{\partial q}\right)_{\mu\nu} \approx \frac{-\delta q'}{\delta q(\delta q + \delta q')}\sum_{n_1 n_2} D^*_{n_1\mu}[\rho(q_0 - \delta q)]_{n_1 n_2} D_{n_2\nu} + \frac{\delta q - \delta q'}{\delta q\,\delta q'} v_\mu^2 \delta_{\mu\nu} + \frac{\delta q}{\delta q'(\delta q + \delta q')}\sum_{n_1 n_2} D^*_{n_1\mu}[\rho(q_0 + \delta q')]_{n_1 n_2} D_{n_2\nu}. \tag{55}$$

It should be noted that the canonical matrix $D_{n\nu}$ in the above expression corresponds to the deformation point, q_0, at which the mass is evaluated. Furthermore, as mentioned above, the density matrices at the three deformation points in Eq. (54) need to be calculated using the single-particle basis $|n\rangle$ with the same basis deformation.

B. Perturbative cranking approximation

The perturbative cranking approximation (ATDHFB-C$^{\rm p}$) has been widely used for the evaluation of the collective mass tensor. In this approximation, apart from neglecting the time-odd interaction terms in the ATDHFB equation and off-diagonal matrix elements of the HFB energy matrix (42), the derivatives are not explicitly evaluated. Instead, they are obtained by using a perturbative approach, in which the collective derivatives of the particle-hole potential, $h_{,i}$, are approximated by terms proportional to generator operators $\hat{Q}_i$, rearrangement terms of the mean field are neglected [3], and derivatives $\Delta_{,i}$ and $\lambda_{,i}$ are neglected too [20]. A complete description of the perturbative cranking model as applied to the nuclear fission process can be found in Refs. [20–24].

The perturbative cranking expression for the mass tensor reads [3,25,26]

$$\mathcal{M}^{C^{\rm p}} = \frac{1}{4}[M^{(1)}]^{-1}M^{(3)}[M^{(1)}]^{-1}, \tag{56}$$

where the energy-weighted moment tensor

$$M_{ij}^{(K)} = \sum_{\alpha\beta}\frac{\langle 0|\hat{Q}_i|\alpha\beta\rangle\langle\alpha\beta|\hat{Q}_j^\dagger|0\rangle}{(E_\alpha + E_\beta)^K} \tag{57}$$

is written in the quasiparticle basis of HFB. In Eq. (57), $|\alpha\beta\rangle$ is a two-quasiparticle wave function. In the canonical approximation, one can express Eq. (57) by

$$M_{ij}^{(K)} \approx \sum_{\mu\nu}\frac{\langle\mu|\hat{Q}_i|\nu\rangle\langle\nu|\hat{Q}_j^\dagger|\mu\rangle}{(\breve{E}_\mu + \breve{E}_\nu)^K}(\eta_{\mu\nu}^+)^2, \tag{58}$$

where the sums run over the whole set of canonical states. This expression resembles the standard BCS cranking expression for the collective mass tensor [20–22,24], originally derived for a phenomenological mean-field potential. In the following, the corresponding mass tensor is denoted as $\mathcal{M}^{C^{\rm pc}}$.

The above expressions for the mass tensor are valid for one kind of fermions only. In the case of the cranking approximation, the total mass tensor is a sum of neutron and proton contributions:

$$\mathcal{M}^C_{\rm total} = \mathcal{M}^C_n + \mathcal{M}^C_p. \tag{59}$$

C. Gaussian overlap approximation

To compare cranking expressions with those obtained within the GOA, it is convenient to introduce the $\mathcal{S}$ matrices [27]:

$$\mathcal{S}^{(K)} = \frac{1}{4}[M^{(1)}]^{-1}M^{(K)}[M^{(1)}]^{-1}. \tag{60}$$

It is immediately seen that one has $\mathcal{M}^{C^{\rm p}} = \mathcal{S}^{(3)}$. The GOA mass tensor is given by [27,28]

$$\mathcal{M}^{\rm GOA} = \mathcal{S}^{(2)}[\mathcal{S}^{(1)}]^{-1}\mathcal{S}^{(2)}. \tag{61}$$

In the GOA, the total inverse inertia $(\mathcal{M}^{\rm GOA}_{\rm total})^{-1}$ for a composite system is given as a sum of proton and neutron inverse covariant inertia tensors [28]:

$$\left(\mathcal{M}^{\rm GOA}_{\rm total}\right)^{-1} = \left(\mathcal{M}^{\rm GOA}_n\right)^{-1} + \left(\mathcal{M}^{\rm GOA}_p\right)^{-1}. \tag{62}$$

IV. THE MODEL

The calculations presented in this paper were performed by using the SkM* energy density functional [29] in the particle-hole channel. In the particle-particle channel we employed the density-dependent pairing interaction in the mixed variant of Refs. [30,31]:

$$V_\tau(\vec{r}) = V_{\tau 0}[1 - \rho(\vec{r})/2\rho_0]\delta(\vec{r}), \tag{63}$$

where $\tau = n$, p and $\rho_0 = 0.16$ fm^{-1}. To test the sensitivity of results on pairing, we carried out both HF+BCS and HFB calculations. The pairing interaction strengths were adjusted

to reproduce the neutron and proton ground-state pairing gaps in ^{252}Fm [32]. In HFB, to truncate the quasiparticle space, we adopted the commonly used quasiparticle-cutoff value of 60 MeV in the equivalent energy spectrum [33]. As discussed in Refs. [34,35], such a large value of cutoff together with the appropriate renormalization of pairing strength guarantees the stability of HFB results. The resulting pairing strengths (in MeV fm^3) are $V_{n0} = -268.9$ and $V_{p0} = -332.5$. In the HF+BCS variant, we took the lowest Z (or N) single-particle HF levels in pairing calculations with $V_{n0} = -372.0$ and $V_{p0} = -438.0$ [36].

The one-dimensional collective pathway, determined by the axial mass quadrupole moment $q = Q_{20}$, was obtained by means of the self-consistent constrained calculations with the symmetry-unrestricted HFB solver HFODD [37] capable of treating simultaneously all the possible collective degrees of freedom that might appear on the way to fission. We stress here that the self-consistent method guarantees that all other deformations $Q_{\lambda\mu}$ for $\lambda\mu \neq 20$ correspond always to a minimized total energy and take values depending on the shape of the optimum collective path. The driving quadrupole moment $q = Q_{20}$ is used only as a suitable parameter enumerating consecutive points of the one-dimensional collective path in a multidimensional configuration space.

The single-particle basis consisted of the lowest 1140 stretched states originating from the lowest 26 major oscillator shells. As discussed earlier [38], such a basis fully guarantees the stability of HFODD results. All canonical states obtained in HFB/HF+BCS were taken to compute the mass tensor, i.e., no further truncations were made.

The derivatives of the density matrices and the mean-field potentials have been obtained using the Lagrange formula (54), which requires the knowledge of self-consistent solutions in several neighboring deformation points. We have evaluated the density matrices for quadrupole deformations ranging from Q_{20}= 0 to 310 b in steps of 1 and 3 b. The derivatives were obtained by using the three-point Lagrange formula (55) and also the five-point Lagrange formula [19]. The results for collective mass obtained with three-point and five-point expressions differ only in the third significant place; hence, in the following, we shall stick to the three-point Lagrange formula.

It needs to be stressed that—to guarantee consistent labeling of canonical states—the underlying single-particle basis should be identical for all three or five points involved in the derivative evaluation. This was achieved by performing HF+BCS or HFB calculations using the same basis deformation for all neighboring points; that is, three or five paths have to be, in practice, determined. In order to guarantee the high accuracy of numerical derivatives, the constrained solutions were obtained on the Q_{20} mesh by using either quadratic constraints or by applying the augmented Lagrangian method (ALM) where both quadratic and linear constraints are employed. Our implementation of ALM [18] significantly improves the accuracy of computed derivatives and is well adapted to supercomputer applications. (For other implementations, see references cited in Ref. [18], in particular Refs. [39,40], where a similar method was adopted in the context of fission.)

V. RESULTS

This section contains examples of calculations illustrating various approximations to the collective quadrupole inertia $B(Q_{20}) = \mathcal{M}_{Q_{20}Q_{20}}$ along the static fission path of ^{256}Fm. The general properties of the fission pathway of this nucleus were studied in our previous work [32] using the SkM*-HF+BCS approach with the seniority pairing interaction. (For other self-consistent fission calculations in the Fm region, see Refs. [41–43].) It has been found that beyond the first barrier, at $Q_{20} \approx 130$ b, a reflection-asymmetric path corresponding to asymmetric elongated fragments branches away from the symmetric valley. Our HFB calculations displayed in Fig. 1 are consistent with this result. Except for the bifurcation point, the one-dimensional total-energy curve along the path to fission shown in Fig. 1(a) behaves fairly smoothly in spite of the single-particle configuration changes clearly seen in the particle-hole (HF) contribution to energy displayed in Fig. 1(c). Because of pairing correlations, these changes are adiabatic in character [14,44]. Indeed, as seen Fig. 1(b), the pairing energy does compensate for the mean-field variations by smoothing out single-particle crossings around the Fermi level that result from intersections of close-lying energy sheets.

For the self-consistent solutions determined along the fission pathway, we calculate the collective quadrupole mass parameter $B(Q_{20})$ using various approximations described in Sec. III. First, we discuss results obtained within the HFB formalism. Figure 2 compares the results of the nonperturbative cranking approach in the full quasiparticle basis

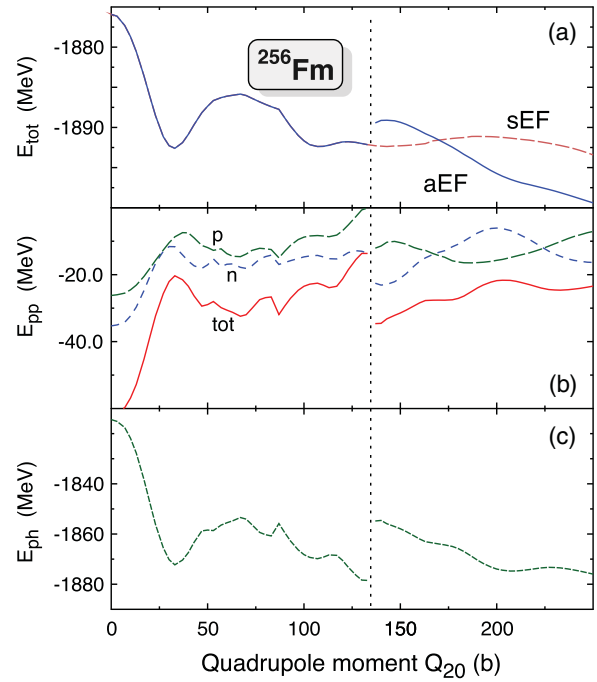

FIG. 1. (Color online) (a) Total SkM*+HFB energy. (b) Neutron (n), proton (p), and total (tot) pairing energies. (c) Particle-hole energy calculated along the static fission pathway for ^{256}Fm. At $Q_{20} \approx 130$ b, a reflection-asymmetric path (aEF) branches away from the symmetric pathway (sEF). The bifurcation point is marked by a vertical dashed line.

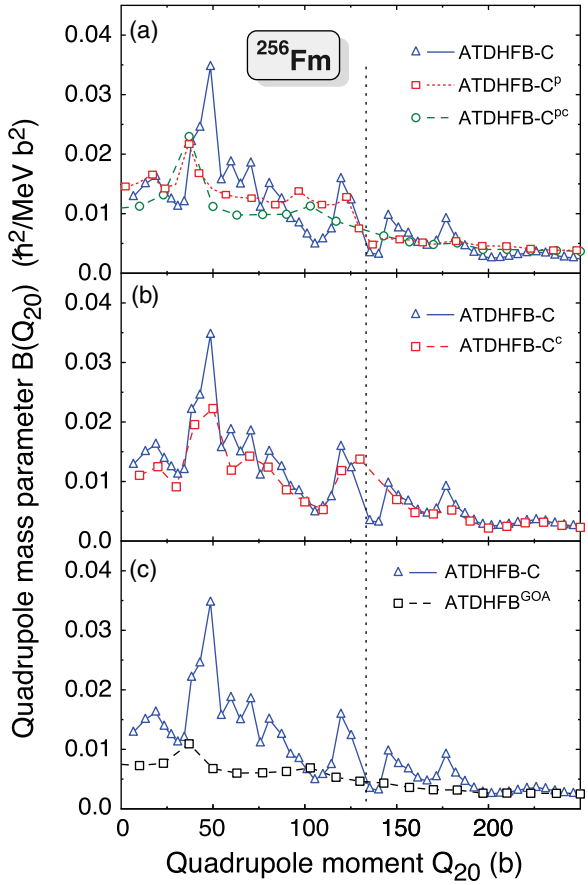

FIG. 2. (Color online) Quadrupole mass parameter $B(Q_{20})$ in ATDHFB-C (triangles) along the static fission pathway of ^{256}Fm calculated in SkM*+HFB as a function of the mass quadrupole moment. The ATDHFB-C values are compared with those obtained in the (a) perturbative cranking approximation ATDHFB-C^{p} and perturbative-canonical cranking approximation ATDHFB-C^{pc}, (b) canonical cranking approximation ATDHFB-C^{c}, and (c) Gaussian overlap approximation ATDHFB^{GOA}. The sEF-aEF bifurcation point is marked by a vertical dashed line. The diabatic jumps between various energy sheets around this point have been disregarded when computing the collective inertia.

(ATDHFB-C) with the perturbative cranking approximation (ATDHFB-C^{p}), the perturbative-canonical cranking approximation (ATDHFB-C^{pc}), the canonical cranking approximation (ATDHFB-C^{c}), and the Gaussian overlap approximation (ATDHFB^{GOA}).

As seen in Fig. 2, the total ATDHFB-C mass exhibits several maxima. The most pronounced peaks can be traced back to configuration changes along the fission pathway seen in Fig. 1(c) in the regions of large local variations in pairing and HF energies that are indicative of changes in the shell structure with elongation. The high-frequency fluctuations of collective ATDHFB-C mass can be traced back to the imperfect numerical convergence of HFB calculations. In the present work, we assumed the accuracy of 0.001 MeV for the total energy. If required, the precision of these calculations can be increased at the expense of an appreciably higher CPU time.

It is interesting to see that the collective mass in ATDHFB-C is very close to that obtained in ATDHFB-C^{c}. The peak-like structures are considerably suppressed in ATDHFB-C^{p}, ATDHFB-C^{pc}, and ATDHFB^{GOA} due to the very approximate treatment of density-matrix derivatives, i.e., the collective momentum. It can thus be concluded that the exact treatment of derivatives gives rise to less adiabatic behavior of the collective mass. We also note that ATDHFB-C^{p}, ATDHFB-C^{pc}, and ATDHFB^{GOA} results follow each other with the ATDHFB-C^{p} mass being systematically larger than that in ATDHFB-C^{pc} and the ATDHFB-C^{pc} mass being systematically larger than that in ATDHFB^{GOA}. Interestingly, the ATDHFB-C^{p} variant yields collective masses that differ from ATDHFB-C primarily around the ground-state minimum and the first barrier. At large elongations, beyond the bifurcation point, both approaches produce fairly similar collective inertias.

In Ref. [12], the quadrupole collective mass was evaluated in the canonical basis and exhibited a singular behavior at certain deformation points. The primary reason for this singularity was due to the pairing collapse at certain deformations that resulted in an unphysical phase transition and the presence of diabatic level crossings. In our work, the peak structures are present at nonzero pairing and—as discussed above—are related to the shell structure changes along the fission pathways.

In order to highlight the differences between HFB and HF+BCS treatments, Fig. 3 shows the quadrupole mass $B(Q_{20})$ obtained in these approaches in the region of the ground-state minimum and both the inner and outer fission

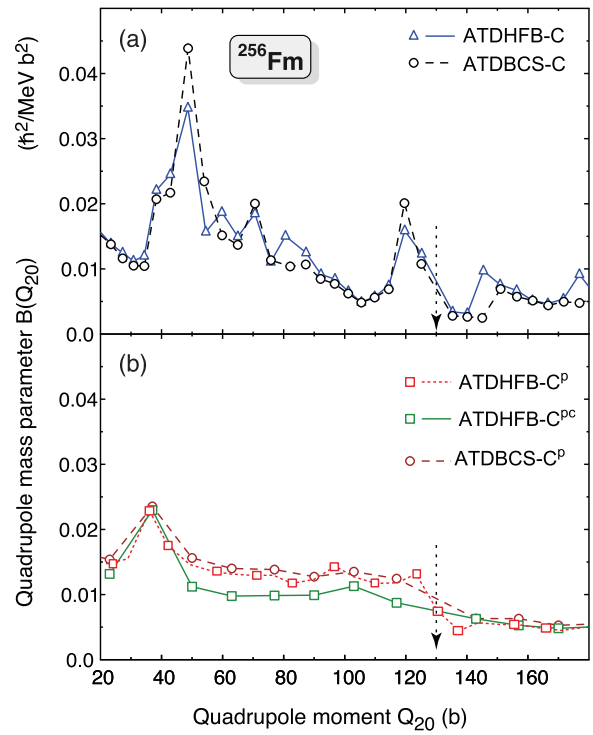

FIG. 3. (Color online) Comparison between HFB and HF+BCS variants of calculations: (a) ATDHFB-C and ATDBCS-C and (b) ATDHFB-C^{p}, ATDHFB-C^{pc}, and ATDBCS-C^{p}. The sEF-aEF bifurcation point is marked by vertical dashed lines and arrows.

barrier of ^{256}Fm $\{Q_{20} \in [20, 180]\}$. This region plays a crucial role in the evaluation of fission half-lives. It is evident that the nonperturbative cranking masses ATDHFB-C and ATDBCS-C have very similar behaviors. Also, the behavior of ATDBCS-C$^{\mathrm{p}}$, ATDHFB-C$^{\mathrm{pc}}$, and ATDHFB-C$^{\mathrm{p}}$ masses calculated in the perturbative approximation is fairly similar, with the BCS mass very close to that of HFB and the ATDHFB-C$^{\mathrm{pc}}$ mass slightly lower.

VI. SUMMARY

The primary motivation of the present work has been to assess various approximations to the collective mass for fission. The collective mass plays a crucial role in determining the adiabatic collective motion of the nucleus and strongly impacts predicted half-lives. In the majority of previous studies, perturbative cranking approximation to collective mass has been employed, in which the time-odd fields are ignored and the collective momenta (i.e., derivatives with respect to collective coordinates) needed in the evaluation of the ATDHFB mass are calculated using the perturbation theory.

In our study, we performed the full ATDHFB cranking treatment of quadrupole inertia. The numerical evaluation of the derivatives appearing in ATDHFB mass expression poses a serious computational challenge, as the accurate self-consistent HFB solutions need to be obtained at several neighboring points around every deformation along the fission pathway. By comparing three- and five-point approximations, we conclude that the three-point Lagrange formula provides a reasonable description of collective derivatives.

The main conclusions of this work can be summarized as follows.

(i) The collective masses obtained in nonperturbative treatment of derivatives show more variations due to shell structure changes along the fission path as compared to the perturbative approximation and GOA.

(ii) The collective mass in full ATDHFB-C is very close to that obtained in ATDHFB-C$^{\mathrm{c}}$ and ATDBCS-C. This means that the diagonal approximation (42) for the HFB energy matrix is a very reasonable one.

(iii) The perturbative ATDHFB-C$^{\mathrm{p}}$ variant yields collective masses that differ from the nonperturbative treatment primarily around the ground-state minimum. At large elongations, both approaches produce fairly similar collective inertias.

(iv) The ATDHFB-C$^{\mathrm{p}}$, ATDHFB-C$^{\mathrm{pc}}$, and ATDHFB$^{\mathrm{GOA}}$ inertias exhibit very similar patterns, with the perturbative cranking masses being systematically larger.

(v) The good agreement between HFB and BCS masses in the nonperturbative treatment extends to perturbative calculations: the collective masses calculated in ATDBCS-C$^{\mathrm{p}}$ are very close to those in ATDHFB-C$^{\mathrm{p}}$.

The present work deals with the cranking approximation to ATDHFB, in which only time-even mean fields have been kept when evaluating the collective inertia. The discussion of the full ATDHFB procedure, including the time-odd response that is expected to play a significant role in the description of collective dynamics [45], will be the subject of a forthcoming study.

ACKNOWLEDGMENTS

Computational resources were provided by the National Center for Computational Sciences at Oak Ridge National Laboratory and the National Energy Research Scientific Computing. This work was supported in part by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through the Department of Energy Grant No. DE-FG52-09NA29461; by the US Department of Energy under Contracts No. DE-FG02-96ER40963 (University of Tennessee) and No. DE-FC02-09ER41583 (Universal Nuclear Energy Density Functional Scientific Discovery Through Advanced Computing Collaboration); by the Nuclear Energy University Programs Grant No. DE-AC07-05ID14517 (Subaward No. 00091100); by the Polish Ministry of Science under Contracts No. N N202 328234 and No. N202 231137; and by the Academy of Finland and the University of Jyväskylä within the Finland Distinguished Professor Programme.

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