Microscopic and nonadiabatic Schrödinger equation derived from the generator coordinate method based on zero- and two-quasiparticle states

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(Received 16 May 2011; published 10 October 2011)

A new approach called the Schrödinger collective intrinsic model (SCIM) has been developed to achieve a microscopic description of the coupling between collective and intrinsic excitations. The derivation of the SCIM proceeds in two steps. The first step is based on a generalization of the symmetric moment expansion of the equations derived in the framework of the generator coordinate method (GCM), when both Hartree-Fock+BCS (HF+BCS) states and two-quasi-particle excitations are taken into account as basis states. The second step consists in reducing the generalized Hill and Wheeler equation to a simpler form to extract a Schrödinger-like equation. The validity of the approach is discussed by means of results obtained for the overlap kernel between HF+BCS states and two-quasiparticle excitations at different deformations.

DOI: 10.1103/PhysRevC.84.044308 PACS number(s): 21.10.Pc, 21.10.Re, 21.60.Jz, 24.75.+i

I. INTRODUCTION

The generator coordinate method (GCM) is a very useful approach to study large-amplitude collective modes. A review on the GCM and quantized collective motion is given in Ref. [1]. It is widely used for the study of ground-state properties and low-lying collective states in even-even nuclei. For instance, there is extensive work by the Tübingen group [2] based on the GCM using different types of projected solutions calculated with the VAMPIR approach (see, e.g., Ref. [2] and references therein). Also, in Ref. [3] the Hill-Wheeler equation is solved for the axial quadrupole collective coordinate, where the basis states are angular-momentum and particle-number projected Hartree-Fock-Bogoliubov states using the Skyrme energy density functional. In this reference, the comparison with experimental results is performed for the full calculation, but the effects due to angular momentum projection and those related to configuration mixing are discussed separately. The Madrid group has performed extensive configuration-mixing calculations based on the GCM using the effective D1S interaction and various types of projections (Ref. [4] and references therein) and, more recently, including variation after projection effects and projection of angular momentum and particle number [5]. Improvements have been made recently to generalize the GCM studies by taking into account the triaxial degree of freedom, with first results reported for ^{24}Mg using a Skyrme [6] or a finite-range [7] interaction. We mention also the recent work of Yao *et al.* [8] where the GCM is used to perform configuration mixing of three-dimensional angular-momentum projected relativistic mean-field wave functions.

When used with the Gaussian overlap approximation (GOA) and employed with the full quadrupole coordinate the GCM has been transformed using a few reasonable assumptions into a five dimensional collective Hamiltonian. This model has been extensively put to the test recently in Refs. [9,10], where predictions for yrast states up to 6^+, and nonyrast 0_2^+, 2_2^+, 2_3^+ states have been compared with experimental data. A time-dependent version of the GCM has also been used to study the fission process [11,12]. In these latter works, the collective dynamics is derived from a time-dependent quantum-mechanical formalism where the wave function of the system is of GCM form, and for which a reduction of the GCM equation to a Schrödinger equation has been made by means of the usual techniques based on the Gaussian overlap approximation.

While some of the aforementioned works include (multi-)quasiparticle excitations, the excited states are nevertheless constructed on top of adiabatic GCM calculations. Collective vibrations have been considered to be completely decoupled from intrinsic excitations. In the 1970s, a few pioneering works were published, in which the usual GCM was extended to include two-quasiparticle (qp) excitations (GCM+QP) [13,14]. In Ref. [14], the method was applied to $A \simeq 50$ nuclei, for which excitation spectra display both collective and noncollective features. In fact, calculations showed that vibrational degrees of freedom may be important to describe the 2^+ and 4^+ states, while 6^+ states may be dominated by 2-qp components. In these calculations, the whole pf shell was used as a basis assuming ^{40}Ca as an inert core, and a modified version of the Kuo matrix elements was considered for the residual interaction. In a more recent work [15], GCM+QP calculations, referred to as coupled-channels GCM calculations, have been performed in ^{186}Pb as a test case, where the 2-qp BCS states have been taken as pairwise excitation of the [514 $\frac{9}{2}$] time-reversed pair. In this reference, the mixing of diabatic configurations is discussed as function of the strength of the pairing. A GCM+QP approach is well suited for the study of many phenomena, for which the coupling between collective and intrinsic states may play a role: (i) shape coexistence where $K = 0$ individual states could be coupled to low-lying vibrational collective states, (ii) backbending phenomena in rotational bands, (iii) decay of superdeformed states to normally deformed states, and (iv) nonadiabatic effects during the fission process.

Where the fully microscopic treatment of the whole fission process from the initial stage of the fissioning system up to scission is concerned, GCM-based approaches are the best suited. They enable one to treat the fission dynamics as a time-dependent evolution in a collective space. Adiabatic calculations have shown that the dynamics is very important for fission fragment distributions [12]: It is responsible for the large widths of the distributions. These results have validated the adiabatic hypothesis made as a first approximation for the description of low-energy fission. In fact, nuclear superfluidity induced by pairing correlations, in addition to strongly influencing the magnitude of the collective inertia, is responsible for a strong rearrangement of the individual orbits with deformation. However, there are some experimental indications that pairs are broken during the fission process. For instance, manifestations of proton pair breaking are observed in ^{238}U and ^{239}U nuclei for an excitation energy of 2.3 MeV above the barrier: First, the proton odd-even effect observed in the fragment mass distributions decreases exponentially for an excitation energy slightly higher than 2.3 MeV [16] and then the total kinetic energy drops suddenly [17,18]. Some theoretical calculations have studied the dissipation during the fission process, most of them are based on a semiclassical formalism such as Focker-Plank equations [19–21], Hamiltonian equations with one-body dissipation and two-body viscosity [22,23], or Langevin equations [24,25]. Here we aim at developing a microscopic nonadiabatic Schrödinger equation, in order to obtain a microscopic description of the coupling between collective and intrinsic excitations. In particular, we tackle the difficult problem of the inversion of the overlap kernel, and outline a formalism that is independent of the choice of effective nucleon-nucleon interaction. We use in the following the abbreviation SCIM, which stands for Schrödinger collective intrinsic model. The newly developed SCIM formalism is presented in Sec. II. In Sec. III, the calculation of the N-dimensional overlap kernel between 0 and 2-qp HF+BCS states is shown, and the dependence of its moments on the deformation is analyzed in details. Section IV is then devoted to the derivation of the inverse of the overlap kernel. The Schrödinger equation is derived in Sec. V and conclusions are drawn in Sec. VI.

II. DESCRIPTION OF THE FORMALISM USED TO CONSTRUCT THE SCIM

Our derivation of the SCIM proceeds in two steps as described in the two following paragraphs. The first step is based on a straightforward generalization of the symmetric moment expansion of the equations derived in the framework of the GCM [26]. We refer to the extensive review of the GCM given in Ref. [27], where most of the material and references related to this subject are available. The second step consists in reducing the equation obtained in Sec. II A to a simpler form which will be the starting point to extract a Schrödinger-like equation.

A. Generalization of the symmetric moment expansion

In order to take into account the coupling between collective and intrinsic degrees of freedom we use the ansatz

$$|\Psi\rangle = \int dq f_0(q)|\Phi_0(q)\rangle + \sum_{i\neq 0}\int dq f_i(q)|\Phi_i(q)\rangle. \quad (1)$$

In the present study, $\Phi_0(q)$ is the ground state at the q value of the collective variable and $\Phi_i(q)$, with $i \neq 0$, are the associated 2-qp excitations whose precise definition and properties are given in Sec. III A. Following the usual procedure, the weight functions $f_i(q)$ are found by requiring that the total energy $\langle\Psi|\hat{H}|\Psi\rangle/\langle\Psi|\Psi\rangle$ calculated with the function defined in Eq. (1) be stationary with respect to arbitrary variation δf_i^*, which leads to the well-known Hill-Wheeler equation

$$\sum_j \int dq'[H_{ij}(q,q') - EN_{ij}(q,q')]f_j(q') = 0, \quad (2)$$

where the Hamiltonian and overlap kernels are defined in terms of matrix elements such as

$$H_{ij}(q,q') = \langle\Phi_i(q')|\hat{H}|\Phi_j(q)\rangle,$$
$$N_{ij}(q,q') = \langle\Phi_i(q')|\Phi_j(q)\rangle.$$

Equation (2) could be the starting point to derive a local expansion by means of a Taylor expansion of the $f_i(q')$ around q, as performed in Ref. [28]. However, we prefer here the symmetric expansion [26] which, in our point of view, provides a natural way to expand on the nonlocality. Its derivation is very simple if we express the variational principle after performing the change of the variables $\bar{q} = (q + q')/2$ and $s = q - q'$ in the expression of the total energy. We only give here the resulting Hill-Wheeler equation:

$$\int ds e^{isP/2}\left[H\left(\bar{q}+\frac{s}{2},\bar{q}-\frac{s}{2}\right) - EN\left(\bar{q}+\frac{s}{2},\bar{q}-\frac{s}{2}\right)\right]e^{isP/2}f(\bar{q}) = 0 \quad (3)$$

with

$$P = i\frac{\partial}{\partial q}. \quad (4)$$

Let us mention that in all the equations of this formalism, we set $\hbar = 1$. At this stage it is important to mention that Eq. (3) is obtained after performing successive integrations by parts and, consequently, the form given here supposes that the corresponding contributions of the integrated terms (surface terms) vanish at the boundary of the integration domain. Note that this is the case in all applications of the GCM in spectroscopy studies [9,10], as well as in nuclear fission studies [11,12]. In the following, we assume that we are in such a situation and pursue our derivation with Eq. (3) as given above. Now, the series expansion of the exponentials is inserted in Eq. (3) and terms of the same order in s are collected together. After integration with respect to s one is led to a symmetric moment expansion that includes the coupling between collective and intrinsic variables. Following the notations in Ref. [27], except for the imaginary number i, the moments of any operator A are defined as

$$A^{(n)}(\bar{q}) = i^n \int_{-\infty}^{+\infty} ds s^n A\left(\bar{q} + \frac{s}{2}, \bar{q} - \frac{s}{2}\right) \tag{5}$$

and symmetric ordered products of operators $A^{(n)}(\bar{q})$ and P as

$$[A^{(n)}(\bar{q})P]^{(n)} = \frac{1}{2^n}\sum_k C_n^k P^{n-k} A^{(n)}(\bar{q}) P^k. \tag{6}$$

With the procedure described above and the notations just given, Eq. (3) is transformed into

$$\sum_n \frac{1}{n!}\{[H^{(n)}(\bar{q})P]^{(n)} - E[N^{(n)}(\bar{q})P]^{(n)}\} f(\bar{q}) = 0. \tag{7}$$

Equation (7) is the compact form of a set of coupled equations for the different components $f_i(q)$. Note that the moments occurring in its definition are square matrices whose dimension depends on the number of excitations introduced in the description. It is worth pointing out here that another difference with the usual approach (no qp excitations) is that all moments, odd or even, must be included in the summation. In order to give more information about Eq. (7) we refer to Sec. III where we elaborate on the properties of the selected GCM collective excitations in the present work. There, it is shown that, with such a selection, the even moments and odd moments of Hermitian operators are represented by real symmetric matrices and imaginary antisymmetric matrices, respectively. As a consequence the operators in Eq. (7) are Hermitian. Finally, since the Hamiltonian is time-reversal invariant, it is easy to check that this operator is also invariant if collective and intrinsic coordinates are time reversed as well. We will comment later on the effect this result has on the Schrödinger equation we derive in Sec. V.

B. Reduction of the symmetric moment expansion to a Schrödinger-like equation

Equation (7) is an infinite series which is an exact expansion of the Hill-Wheeler equations in terms of local operators. It can be transformed into a local Schrödinger equation by inverting the expansion of the overlap kernel. The latter can be written formally as

$$\hat{N}(\bar{q}) = \sum_n \frac{1}{n!}[N^{(n)}(\bar{q})P]^{(n)} = [\hat{N}^{1/2}(\bar{q})]^+ \hat{N}^{1/2}(\bar{q}). \tag{8}$$

In the following we use the definitions

$$\begin{aligned} \hat{N}^{1/2}(\bar{q}) &= \hat{J}^{1/2}(\bar{q})\sqrt{N^{(0)}(\bar{q})} \\ [\hat{N}^{1/2}(\bar{q})]^+ &= \sqrt{N^{(0)}(\bar{q})}[\hat{J}^{1/2}(\bar{q})]^+, \end{aligned} \tag{9}$$

with

$$\begin{aligned} \hat{J}(\bar{q}) &= I + \hat{u}(\bar{q}) \\ \hat{u}(\bar{q}) &= \frac{1}{\sqrt{N^{(0)}(\bar{q})}} \sum_{n=1} \frac{1}{n!}[N^{(n)}(\bar{q})P]^{(n)} \frac{1}{\sqrt{N^{(0)}(\bar{q})}}. \end{aligned} \tag{10}$$

These notations require further explanation. We use the property that any Hermitian operator A can be written in the form $A = S^+ S$, with an operator S which is not necessarily Hermitian. Then, for the sake of simplicity, the notation $S = A^{1/2}$ is used although it is not, strictly speaking, the square root of A unless $S^+ = S$.

We proceed further by defining a new set of collective wave functions, $\{g_i(\bar{q})\}$, through the matrix relation,

$$f(\bar{q}) = \hat{N}^{-1/2}(\bar{q}) g(\bar{q}) = [N^{(0)}(\bar{q})]^{-1/2} \hat{J}^{-1/2}(\bar{q}) g(\bar{q}) \tag{11}$$

to arrive finally from Eq. (7) at the local Schrödinger equation

$$\begin{aligned} \Bigg\{[\hat{J}_{-1/2}(\bar{q})]^+ \left[\sum_n \frac{1}{n!}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}[H^{(n)}(\bar{q})P]^{(n)}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\right] \\ \times \hat{J}_{-1/2}(\bar{q}) - E\Bigg\} g(\bar{q}) = 0, \end{aligned} \tag{12}$$

where we have defined the operator

$$\hat{J}_{-1/2}(\bar{q}) \equiv \hat{J}^{-1/2}(\bar{q}). \tag{13}$$

Equation (12) is formally the same as the one given in Ref. [28] but differs from it in many respects. The definitions of the moments and the operator $\hat{u}(\bar{q})$ are not at all the same. Furthermore, the operators occurring in its definition are represented by matrices, including, as already mentioned, those corresponding to odd moments. Note that the normalization

$$\int d\bar{q}[g(\bar{q})]^+ g(\bar{q}) = 1 \tag{14}$$

guarantees the normalization of the wave function defined in Eq. (1). In this approach, the main difficulty is to determine the operator $\hat{J}_{-1/2}(\bar{q})$, which, according to the definitions given in Eq. (10), is the solution of the equation

$$[\hat{J}_{-1/2}(\bar{q})]^+[I + \hat{u}(\bar{q})]\hat{J}_{-1/2}(\bar{q}) = I. \tag{15}$$

In order to reduce its complexity, one is led to assume that the series expansion representing the overlap kernel converges rapidly and can be truncated after the second-order moment. That is to say, we approach Eq. (15) by use of the simpler one

$$\begin{aligned} [\hat{J}_{-1/2}(\bar{q})]^+ \Bigg[I + \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\Bigg\{[N^{(1)}(\bar{q})P]^{(1)} \\ + \frac{1}{2}[N^{(2)}(\bar{q})P]^{(2)}\Bigg\}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\Bigg]\hat{J}_{-1/2}(\bar{q}) = I. \end{aligned} \tag{16}$$

In Sec. IV we study Eq. (16) in some detail and explain how it can be solved with parametrizations of the form

$$\hat{J}_{-1/2}(\bar{q}) = \sum_{n=0}^{4}[j_{(n)}(\bar{q})P]^{(n)}. \tag{17}$$

The quantities $j_{(n)}(\bar{q})$ are unknown matrices which are determined by solving Eq. (16).

Once the inverse $\hat{J}_{-1/2}(\bar{q})$ is known it can be inserted in Eq. (12), and by means of the formulas given in the Appendix A, there is no difficulty in finding a general expansion in terms of symmetric ordered products of operators. In other words one can express Eq. (12) in the form

$$\sum_n \{[S^{(n)}(\bar{q})P]^{(n)} - E\}g(\bar{q}) = 0. \tag{18}$$

Then a second-order differential Schrödinger equation is derived by limiting the summation to $n = 2$. However, for obvious practical reasons, one does not extract the $S^{(n)}(\bar{q})$ with the full expansion of the Hamiltonian kernel but with a truncation similar to the one introduced in the case of the overlap kernel. Thus, in all that follows, our derivation of a Schrödinger equation relies on the approximated expression

$$\left([\hat{J}_{-1/2}(\bar{q})]^{+}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\left\{H^{(0)}(\bar{q}) + [H^{(1)}(\bar{q})P]^{(1)} + \frac{1}{2}[H^{(2)}(\bar{q})P]^{(2)}\right\}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\hat{J}_{-1/2}(\bar{q}) - E\right)g(\bar{q}) = 0, \tag{19}$$

with $\hat{J}_{-1/2}(\bar{q})$ satisfying Eq. (16).

Such an approach assumes that the series expansions of the overlap and Hamiltonian kernels converge rapidly. If the moments were independent of $\bar{q}$ or if we could neglect their variations, Eq. (7) would simply be a power expansion in the collective momentum P. One then could conclude naturally that this approach is limited to the study of collective motions with momenta that are not too large, or, equivalently, at moderate energies. Note, that if we approximate the kernels with a Gaussian [27] of width $\sigma(\bar{q})$ the expansion [Eq. (7)] becomes a series with terms $[\sigma^n(\bar{q})P]^{(n)}$. In that form it appears that a rapid convergence of Eq. (7) requires that the collective wave functions, as well as the moments, are slowly varying functions in a range given by the width of the Gaussian. These arguments are only qualitative in the sense that they do not give precise information regarding the energies up to which one can expect the approximation to be reasonable. In relation to this discussion we refer to the work by Bonche *et al.* [29] which contains a detailed comparison between two calculations of large amplitude quadrupole dynamics in ^{194}Hg. One is based on a direct resolution of the Hill-Wheeler equation (HWE) as extracted with the GCM, while the other uses a collective Schrödinger equation (CSE) resulting from a local expansion of the HWE into a second-order differential equation. Although their approach to the CSE approximation is not rigorously identical to the one described here, we think that one can extract general deductions from their work. We will only quote some of their conclusions here. The GCM and the CSE reproduced the energies of most collective states fairly well. However, one observes significant differences in the collective wave functions at excitation energies around 6 MeV and above. More precisely the corresponding HWE collective wave functions display more and more irregular structures and rapid variations that a CSE approach is not able to reproduce. We do not deny the fact that it is important to have a fair description of the collective wave functions, but we do make the observation that for excitations above 4 or 5 MeV one also has to worry about their possible coupling with qp excitations, which is the main motivation of this work.

At this stage one needs some more information on the kernel overlap to proceed further in the reduction of the equations given above. It is the purpose of the next section to present a numerical study of this kernel in a wide range of deformations that would be encountered in a microscopic description of the symmetric fission of ^{236}U.

III. THE N-DIMENSIONAL OVERLAP KERNEL

A. Selection of the 2-qp generating wave function

In this paragraph, a set of generating wave functions is constructed by means of the constrained HF+BCS method with the finite-range effective force D1S [30,31] as described in Refs. [11,12]. We limit this study to the case of one generator coordinate q associated to the total quadrupole deformation of the even-even nucleus ^{236}U. Furthermore, the calculations are restricted to axial symmetry. As a consequence the qp are characterized by their projection K of the total angular momentum on the symmetry axis. We denote the ground state (or Bogoliubov vacuum) at deformation q by $|\Phi_0(q)\rangle$ and recall here its definition in terms of the qp destruction operators $\eta_i(q)$ and their time-reversal conjugate $\eta_{\bar{i}}(q) = \hat{T}^{+}\eta_i(q)\hat{T}$, where $\hat{T}$ is the time-reversal operator:

$$|\Phi_0(q)\rangle = \prod_{i>0}\eta_i(q)\eta_{\bar{i}}(q)|0\rangle. \tag{20}$$

Furthermore, we restrict our calculations by introducing another symmetry which is associated with the invariance of the Bogoliubov fields when performing a reflexion with respect to the x-y plane. In that case the parity π is an additional quantum number and the qp operators are then characterized by $k \equiv \{n_k, \pi_k, K_k\}$ where n_k is an index which distinguishes single qp states inside the same block $\{\pi_k, K_k\}$. At each deformation we can then define a set of 2-qp excitations

$$\eta_{i_1}^{+}(q)\eta_{i_2}^{+}(q)|\Phi_0(q)\rangle. \tag{21}$$

This study is limited to the description of the coupling of the ground state with 2-qp excitations. Consequently, since the Hill-Wheeler equation conserves the total projection of the angular momentum on the symmetry axis (z) and since the ground state is a state $K = 0$, it is clear that the quantum number of 2-qp excited states must satisfy $K_{i_1} + K_{i_2} = 0$. In addition, by using similar arguments with the time-reversal transformation, we arrive at the conclusion that the qp excitations must be symmetric under time reversal. Thus, the N selected configurations at deformation q are written in the form:

$$\begin{cases} |\Phi_0(q)\rangle \\ |\Phi_i(q)\rangle = \frac{1}{\sqrt{2}}\left[1 + \delta_{i_1 i_2}\left(\frac{1}{\sqrt{2}} - 1\right)\right]\left[\eta_{i_1}^{+}(q)\eta_{i_2}^{+}(q) \right. \\ \qquad \left. + \eta_{i_2}^{+}(q)\eta_{\bar{i}_1}^{+}(q)\right]|\Phi_0(q)\rangle, \quad i = 1, N-1. \end{cases} \tag{22}$$

Note that for the 2-qp states, the index i denotes the couple (i_1, i_2). For simplicity of notation we have not added another index to indicate whether the excited configurations are built with two neutrons or two protons qp. Finally, for sake of convenience and since the 2-qps i_1, i_2 are in the same block $\{\pi_i, K_i\} \equiv \{\pi_{i_{1(2)}}, K_{i_{1(2)}}\}$, we also use in the following the notation $i = \{K_i^{\pi_i}, (a_i)\}$ where the letter a_i which distinguishes the couple (n_{i_1}, n_{i_2}) in the same block $\{\pi_i, K_i\}$ is used if necessary. These wave functions which are not eigenfunctions of the proton and neutron number operators $\hat{N}_p$, $\hat{N}_n$ should, in principle, be projected on the subspace of states with good particle numbers. The expression of the overlap kernel is readily expressed with the usual techniques to calculate the overlap between two Bogoliubov vacuum [32]. The difficulty in projecting is essentially numerical, since the projection method requires repeating the calculation of the overlap at different angles in order to calculate an integral with a discretization method [33]. Such calculation, if feasible in the study proposed here, would represent a considerable amount of computational work and numerical studies. At this stage it is worth pointing out that a description of the fission process from the first barrier to scission involves a wide range of deformations typically in the interval [50 b, 550 b]. Furthermore, an accurate calculation of the potential energy surface, in particular, close to the scission point, necessitates the use of a very large dimensional space of harmonic oscillator basis states. As an example, we indicate that in a one-center basis the size of the $K = 1/2$ block is $[150 \times 150]$. In view of these remarks, we find some justification in presenting this formalism with unprojected wave functions. We stress that until now our formalism does not depend on the particular model used to calculate the kernels. Finally, let us conclude this section with a different issue which is still related to this question of particle number. It concerns the restoration of the correct average values of the number of protons and neutrons of the Hill-Wheeler solutions. This problem is studied in details in Ref. [29] where the authors introduce in the Hill-Wheeler equation the kernels calculated with the two operators $\hat{N}_p$, $\hat{N}_n$ and their associated Lagrange parameters. The implementation of this method in our formalism is straightforward.

B. Calculation of the overlap kernel

1. Generality

Calculations presented in this paper correspond to different excitations along the symmetric fission barrier in ^{236}U. The HF+BCS equations are solved by expanding the single-particle states onto an axial harmonic oscillator (HO) basis. A one-center basis with $N = 14$ major shells has been used. The calculations are performed with the Hartree-Fock+BCS method and a constraint on the quadrupole operator. They have been restricted to axial and left-right symmetries. The full Bogoliubov approach has not been considered here for reasons of computational time only. In the present microscopic and self-consistent BCS approximation of the HF+BCS formalism, the diagonalization of the full HFB generalized matrix H has been replaced by the diagonalization of the mean-field matrix, and the block matrix associated with the pairing field has been taken as diagonal in this representation. Because of the symmetries imposed in this calculation, the Bogoliubov or (HF+BCS) transformation can be chosen to be real. As a result, all quantities occurring in the formalism are

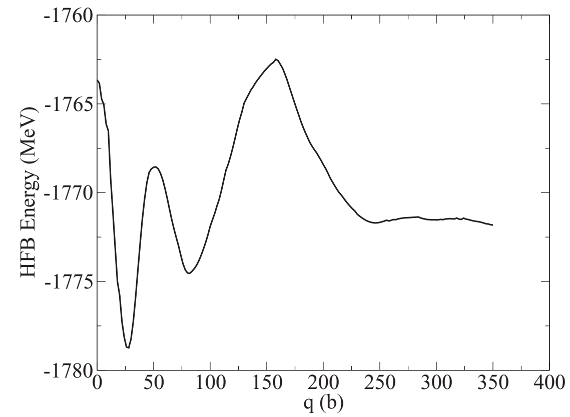

FIG. 1. HF+BCS potential energy along the symmetric fission barrier in ^{236}U.

real. This is the case, in particular, of the overlap matrix which is denoted by

$$N_{ij}(q, q') = \langle \Phi_i(q) | \Phi_j(q') \rangle. \tag{23}$$

Calculations of this matrix have been performed at different elongations along the symmetric barrier. The formalism used to extract these matrix elements is given in detail in Appendix B. In the following, the results are presented in the variables $\bar{q}$ and s defined in the first paragraph of Sec. II. More precisely at each $\bar{q}$ given in barns, we plot the matrix elements $N_{ij}(\bar{q} + s/2, q - s/2)$ as function of s running in intervals wide enough that the overlaps $N_{ij}(\bar{q} + s/2, q - s/2)$ drop to zero. The $\{\bar{q}\}$ have been chosen in the range [20 b, 350 b] with a step of 10 b up to $\bar{q} = 100$ b and a step of 25 b beyond. Let us mention that deformations close to 160 b, namely $\bar{q} = 150$ b and $\bar{q} = 175$ b, are not discussed here, since they correspond to a junction between two valleys having different hexadecapole deformations. Such a study requires treating explicitly the hexadecapole degree of freedom [34,35].

The symmetric barrier is plotted in Fig. 1. The ground state is located near 30 b, the first barrier at 50 b, the second well at 80 b, and the second saddle point at 160 b. The intrinsic levels chosen to construct the 2-qp excitations are the lowest-energy proton $K^\pi = 1/2^-, 1/2^+, 3/2^-, 3/2^+, \ldots,$ qp levels. Among them, the selected intrinsic excitations are those which minimize the deviation from the average proton and neutron numbers. Results are presented in the present work only for proton excitations and similar results and conclusions are expected for neutron excitations.

Some comments are in order concerning phase problems that we encountered in the construction of these 2-qp excitations. In fact, the qp states or operators η_i which result from the diagonalization of the Bogoliubov Hamiltonian are defined up to an arbitrary phase which in the present case is real, i.e., ± 1. The phases of two conjugate qps $\eta_{\bar{i}}$, η_i are then the same by construction and, consequently, the Bogoliubov vacuum defined above does not depend on these phases. The same conclusion applies to the case of two conjugate qp excitations $|\Phi_i(q)\rangle = \eta_{i_1}^+ \eta_{\bar{i}_1}^+ |\Phi(q)\rangle$ but it is not the case for all other 2qp excitations. It is worth stressing that if we were using the qp as they come out of the diagonalization of the Bogoliubov

Hamiltonian, the corresponding nondiagonal matrix elements of the kernels can become discontinuous at random as function of the deformation, which would prevent the extension of the GCM with those excitations. In order to solve this problem, the single-qp excitations used in the construction of the 2-qp excitations have been followed continuously as a function of deformation. This is achieved with the following simple procedure. Any single-qp state $|i, q + \delta q\rangle$ at deformation $q + \delta q$ is associated with $|i, q\rangle$ by maximizing the single-particle overlap $|\langle i, q|k, q + \delta q\rangle|$ among all k in the 1-qp spectrum at deformation $q + \delta q$. This overlap is nothing but the anticommutator $\{\eta_i^+(q), \eta_k(q + \delta q)\}$. Denoting by k the qp which achieves this maximization, we set $|i, q + \delta q\rangle \equiv \varphi_i(q)|k, q + \delta q\rangle$ where a phase given by

$$\varphi_i(q) = \frac{\langle i, q|k, q + \delta q\rangle}{|\langle i, q|k, q + \delta q\rangle|} \tag{24}$$

has been introduced. It is clear that with such a procedure the matrix elements of the overlap kernel become continuous functions of the deformation. Let us mention that the problem of the sign of the overlap has been recently addressed by L. Robledo in Ref. [36] for general HF+BCS wave functions that have no spatial symmetry (triaxial) and also breaking of the time-reversal symmetry.

The evolution of the energy of 2-qp excitations is plotted in Fig. 2 as a function of the deformation around $\bar{q} = 70$ b. It shows that the lowest excitation is located around 3 MeV. No significant difference is observed between proton and neutron excitations. Let us mention that we need not limit ourselves to excitations that conserve the average number of particles, but as a result the number of excitations increases rapidly when we allow the mean particle numbers $\bar{N}_i$ and $\bar{Z}_i$ to vary by 1 particle around their average value. For instance, for an energy below only 5 MeV and with a mean particle number in the range $92 - 1 \leqslant \bar{Z}_i \leqslant 92 + 1$, $144 - 1 \leqslant \bar{N}_i \leqslant 144 + 1$, we already find 6.5 proton 2-qp excitations and 11.5 neutrons per deformation.

As we follow the single-quasiparticle states by continuity as a function of deformation, levels with the same K and π quantum numbers can occasionally cross or be pushed back

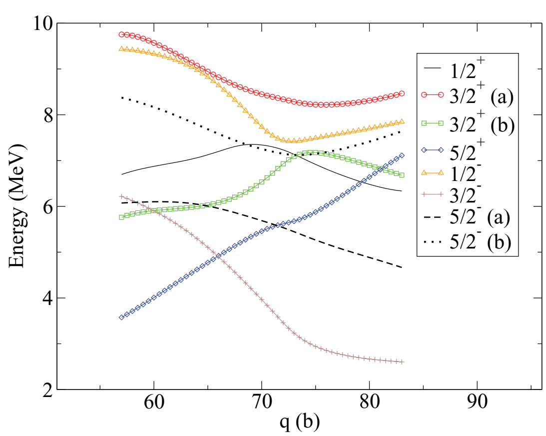

FIG. 2. (Color online) Energy of the selected 2-qp excitations around $q = 70$ b as a function of deformation. Letters are used to differentiate excitations with same K^π.

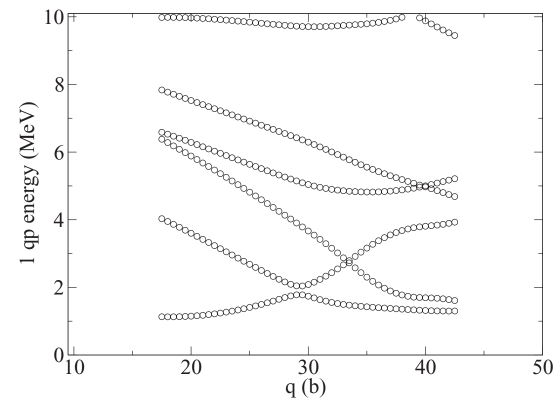

FIG. 3. Energy of the single-quasiparticle excitations around $q = 30$ b for $K^\pi = 1/2^+$.

from each other. Such features are common and can occur anywhere along the deformation. Such cases are illustrated in Fig. 3 around $q = 30$ b for $K^\pi = 1/2^+$. The figure shows that a repulsion occurs between the two first levels at a deformation $q_r = 29.5$ b, defined as the deformation where the difference in energy between the two levels is minimal, whereas crossings are observed at $q = 34$ b and $q = 40$ b. Note that, unlike crossings, repulsions correspond to a mixing of the two incoming levels.

C. Numerical results for the matrices $N_{ij}(\bar{q} + s/2, \bar{q} - s/2)$ of the overlap kernel

As already mentioned in Ref. [29], an accurate calculation of the complex behavior of the overlap kernel requires a careful determination of the HF+BCS states. The overlap kernels are the determinants of the matrices built from the overlaps of all pairs of individual orbits: They are very sensitive to the details of those orbits. For this reason, one must achieve a very accurate convergence of the HF+BCS wave functions if one wants to get reliable values of the overlap kernels. As a consequence, all the HF+BCS states here have been obtained with a very high degree of accuracy. More precisely, a convergence of 10^{-6} fm^{-3} has been achieved on the generalized density matrix. Let us note that the parameters of the harmonic oscillators used to develop the HF+BCS states have been optimized in each region at the deformation $\bar{q}$ (i.e., $q = q'$) and kept constant for the neighboring deformations. For reference we think it interesting to show the plot of these matrices as function of s for different values of $\bar{q}$ even though the quantities which count in this formalism are their moments. The latter are presented in Sec. III C3.

1. Calculation of the diagonal matrices $N_{ii}(\bar{q} + s/2, \bar{q} - s/2)$

In Fig. 4 the overlaps $N_{00}(\bar{q} + s/2, \bar{q} - s/2)$ between HF+BCS solutions at different deformations are plotted as functions of s for different values of $\bar{q}$. At first glance, all the overlaps shown in Fig. 4 suggest that they are close to a Gaussian shape, independently of the mean quadrupole deformation $\bar{q}$. Although the SCIM formalism derived in this

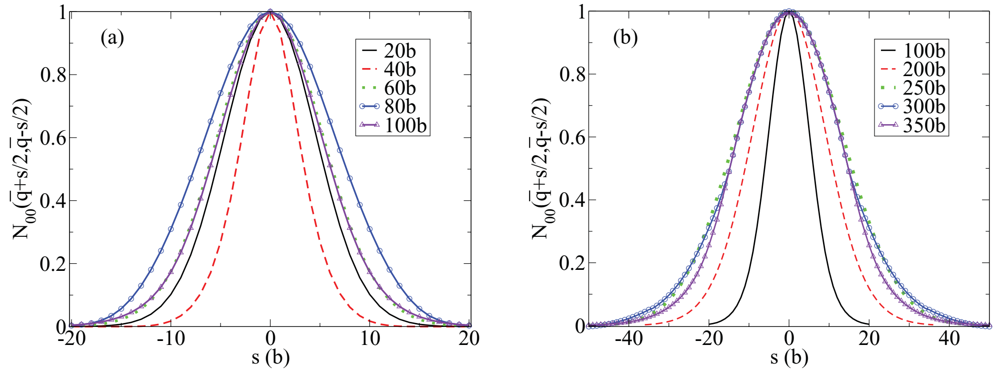

FIG. 4. (Color online) Comparison between the overlaps $N_{00}(\bar{q}+s/2, \bar{q}-s/2)$ calculated for different $\bar{q}$ as functions of s for $20\,\mathrm{b} \leqslant \bar{q} \leqslant 100\,\mathrm{b}$ (a) and $100\,\mathrm{b} \leqslant \bar{q} \leqslant 350\,\mathrm{b}$ (b).

paper does not require that the overlaps be Gaussian, it is instructive to check the validity of this assumption as a further motivation for the more general moment-based approach we use. The width of the overlap is found to strongly depend on the deformation. In general, the width increases with the deformation, with local minima all along the barrier. The extent to which the Gaussian shape is a good approximation can be investigated by comparing different ways to associate a width to these overlaps. In fact, assuming that they can be represented by a Gaussian

$$I(q,q') = e^{-(q-q')^2/2\sigma^2}, \tag{25}$$

their moments of even order should verify the relations

$$\begin{aligned} N^{(0)}(\bar{q}) &= \sqrt{2\pi}\,\sigma(\bar{q}),\\ N^{(2n)}(\bar{q}) &= (-1)^n \frac{(2n)!}{2^n n!}\sigma^{2n}(\bar{q})N^{(0)}(\bar{q}), \end{aligned} \tag{26}$$

which provide different ways to extract the width $\sigma(\bar{q})$. The same procedure can be applied *a priori* to all the diagonal terms of $N(\bar{q}+s/2, \bar{q}-s/2)$. In Fig. 5(a) a few diagonal elements of the overlap matrix are plotted at $\bar{q} = 50\,\mathrm{b}$ where a comparison is made between overlaps of HF+BCS vacuum and 2-qp states. The different overlaps are very close together, but we notice some difference in the tails. As we will see, these small deviations in the tails have a significant influence on the value of the second-order moments. Furthermore, we find that level crossings do not generate any sizable change in $N_{ii}^{(n)}(\bar{q})$, whereas repulsions are responsible for a quite rapid but continuous change in the overlap. Three different cases are plotted in Fig. 5(b). First, we observe that the overlap (plotted as dashed line) of the excitation built with two $K_i^\pi = 3/2^+$ qp, one of them being involved in a repulsion at $q_r = 57$ b, is not sizably disturbed by the repulsion. Conversely, for the same configuration, one single excitation involved in a repulsion at $q_r = 57$ b, the overlap built with $K_i^\pi = 1/2^+$ qp is sharper (smaller width) than the previous one. The most pathological case is found for the overlap built this time with two $5/2^+$ excitations involved in a mutual repulsion at $q_r = 47.5$ b, close to $\bar{q} = 50$ b. This overlap even becomes negative in the region close to the level repulsion. The comparison with a Gaussian overlap is, therefore, clearly unjustified here. Let us note that these numerical results are in agreement with the analysis of the repulsions we made in Sec. III B1.

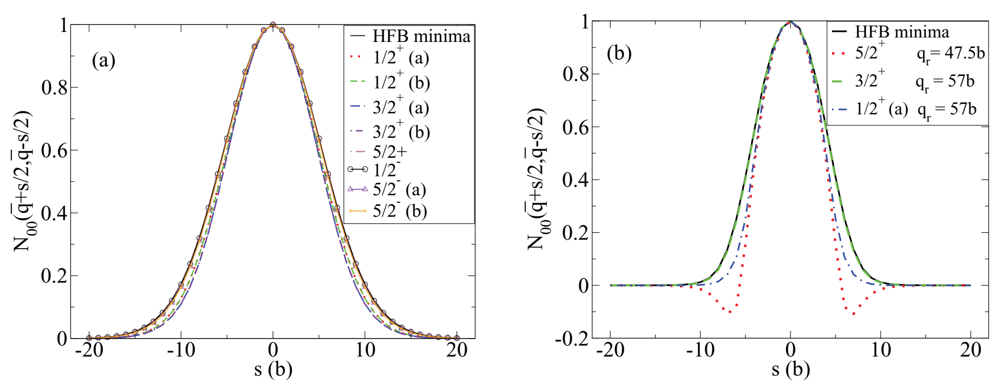

FIG. 5. (Color online) Overlap kernel $N_{ii}(\bar{q}+s/2, \bar{q}-s/2)$ for HF+BCS solutions and different 2-qp excitations not involved in repulsions [labeled $K^\pi(i)$] at $\bar{q} = 60$ b, plotted as functions of s (a). Overlap kernel $N_{ii}(\bar{q}+s/2, \bar{q}-s/2)$ for HF+BCS solutions and different 2-qp excitations involved in repulsions [labeled by $K^\pi(i)$, and q_r the deformation where the repulsion occurs] at $\bar{q} = 50$ b, plotted as functions of s (b). Letters are used to differentiate the same K^π excitations in both figures.

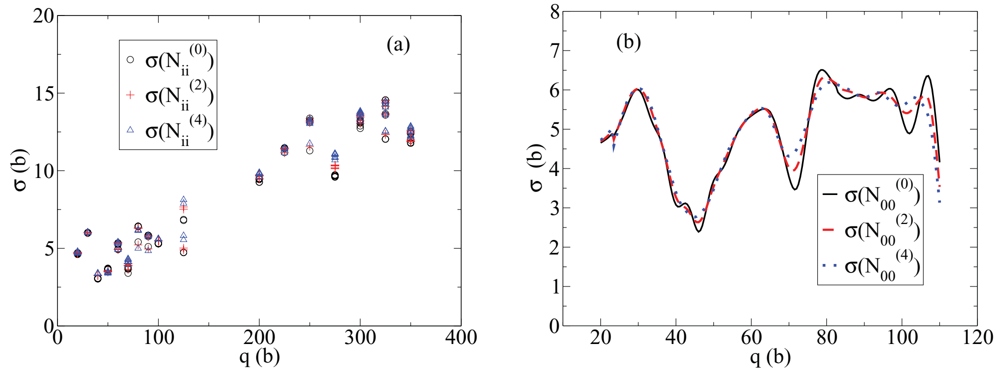

FIG. 6. (Color online) Widths of the overlap extracted from the moments of zero, second, and fourth orders, as functions of the elongation, shown with the black circle, red cross, and blue triangle, respectively. Full lines correspond to the widths from $N_{00}^{(n)}$ terms and circles to diagonal terms $N_{ii}^{(n)}$, $i \neq 0$. (a) Results for a large range of deformation [0, 350 b]. (b) Widths from $N_{00}^{(n)}$ in the region [0, 110 b].

The widths, obtained from Eq. (26) using the moments of zero, second, and fourth orders, are plotted in Fig. 6 as functions of the deformation for the overlaps $N_{00}(\bar{q}+s/2, \bar{q}-s/2)$ and $N_{ii}(\bar{q}+s/2, \bar{q}-s/2)$. Particular attention has been paid to the widths extracted from the $N_{00}^{(n)}(q)$ overlaps: Calculations of the widths have been performed in the range [20 b, 110 b] with a step of 0.5 b. In Fig. 6(b) we observe that the three widths for $N_{00}^{(n)}(q)$ do not differ too much in most cases, which corroborates the fact that the overlaps are reasonably close to those from a Gaussian shape. For the lowest deformations, the largest differences occur when the width is minimum, at 46, 72, and 102 b with a maximal deviation of 22% at 72 b, between the widths extracted from the moments of zero and fourth orders.

Widths of the overlaps $N_{ii}(\bar{q})$, with $i \neq 0$ are also plotted up to 350 b in Fig. 6(a). Since the excitations involved in repulsions do not lead to Gaussian shapes, as illustrated in Fig. 5(b), they are not taken into account in this analysis. The maximal deviation between the widths obtained from $N^{(0)}(\bar{q})$, $N^{(2)}(\bar{q})$, and $N^{(4)}(\bar{q})$ for a given excitation is found to be about 19%. The average of this maximal deviation over all the different excitations and over all the deformations is about 5%. However, we emphasize that these deviations will pose no problem in our approach since we do not rely on a Gaussian-overlap assumption at all.

2. *Calculation of the nondiagonal terms* $N_{ij}(\bar{q}+s/2, \bar{q}-s/2)$

Nondiagonal overlaps $N_{ij}(\bar{q}+s/2, \bar{q}-s/2)$ $(i \neq j)$ are plotted in Fig. 7. $N_{0i}(\bar{q}+s/2, \bar{q}-s/2)$ are displayed in Fig. 6(a), and $N_{ij}(\bar{q}+s/2, \bar{q}-s/2)$ in Fig. 6(b). For the sake of visibility, only a few overlaps are drawn.

At this point, let us emphasize that nondiagonal overlaps have no *a priori* reason to be even or odd functions of s. However, they must be zero for $s=0$, since, at the same deformation, 2-qp excitations are orthogonal to the ground state and any other 2-qp excitation. We observe on this plot that, in fact, they are odd or even functions of s near the origin, depending on the indices i, j of the excitations. Note that the amplitudes of these nondiagonal overlaps are much smaller than the diagonal ones. Furthermore, the overlaps between two excited states are also small in comparison to those between the ground state and excited states. The exceptions are found for qp states having the same quantum numbers $K^\pi(i) = K^\pi(j)$, as shown by the blue curve with open circles in Fig. 7(b). This result is not surprising since, using the generalized Wick theorem when $K^\pi(i) \neq K^\pi(j)$, the following relation is found:

$$\begin{aligned} N_{ij}(\bar{q}+s/2, \bar{q}-s/2) &= \frac{1}{N_{00}(\bar{q}+s/2, \bar{q}-s/2)} N_{0i}(\bar{q}-s/2, \bar{q}+s/2) \\ &\quad \times N_{0j}(\bar{q}+s/2, \bar{q}-s/2). \end{aligned} \tag{27}$$

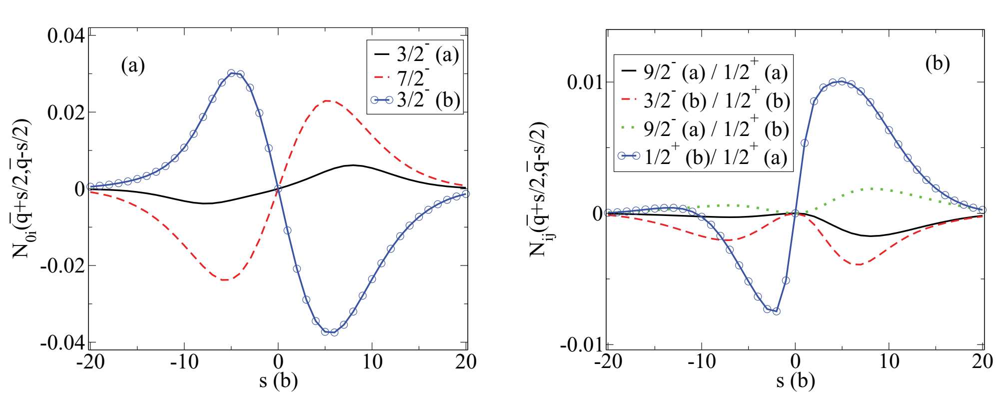

FIG. 7. (Color online) Overlaps $N_{0i}(\bar{q}+s/2, \bar{q}-s/2)$ (a) and $N_{ij}(\bar{q}+s/2, \bar{q}-s/2)$ (b) at $\bar{q} = 30$ b for different excitations labeled by K^π as a function of s. Letters are used to differentiate same K^π excitations.

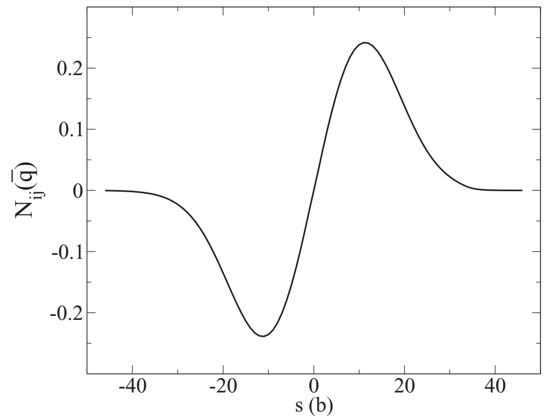

FIG. 8. Nondiagonal term $N_{ij}(\bar{q})$ built with excitations involved in a repulsion at $q_r = 218$ b.

We also mention here that the overlap matrix is not block-diagonal in isospin, since

$$\mathcal{N}_{ij}^{\tau_i\tau_j}(q,q') = \langle \Phi(q)|\eta_{i_2}^{\tau_i}\eta_{i_1}^{\tau_i}\eta_{j_1}^{\tau_j+}\eta_{j_2}^{\tau_j+}|\Phi(q')\rangle$$

is nonzero for $\tau_i \neq \tau_j$.

Conclusions obtained for the diagonal terms of $N^{(0)}(\bar{q})$ about repulsions and crossings still apply here: nondiagonal overlaps are not disturbed by crossing levels but can vary rapidly when a repulsion occurs. In Fig. 8 the overlap N_{ij} for a couple of 2-qp excitations $i = (i_1, i_2)$ and $j = (j_1, j_2)$ with $K^{\pi}_{i(j)} = 1/2^-$ is depicted. In this case, i_1 and i_2 are both involved in a mutual repulsion at $q_r = 218$ b and $i_2 = j_2$. The amplitude of this overlap is much larger than that of the standard (without repulsion) nondiagonal overlap. Let us mention that this kind of configuration is encountered several times along the deformation and corroborates our observation in Sec. III A that the qp states i_1 and j_1 are mixed in the repulsion area.

3. *Numerical study of the moments $N_{ij}^{(n)}(\bar{q})$, $n = 0, 1, 2$*

According to our approximation [see Eq. (16)], the overlap kernel has to be analyzed through its moments up to the second order. At this point it is useful to introduce some important properties of the moments defined in Sec. II A. Their demonstration being straightforward, we only list them here:

(i) All moments of a Hermitian operator are Hermitian:

$$\hat{A}^+ = \hat{A} \Rightarrow A^{(p)+} = A^{(p)}.$$

By applying this property to the overlap kernel, whose matrix elements are real for reasons given at the beginning of this section, the matrices associated with even-order moments are found to be real symmetric while those associated with odd-order moments are imaginary antisymmetric.

(ii) Finally, let us indicate that the even moments of an operator have the same parity with respect to the time-reversal symmetry ($\hat{T}$) as the operator considered, while the opposite is true for odd moments

$$\hat{T}^+\hat{A}\hat{T} = \epsilon\hat{A} \Rightarrow \hat{T}^+A^{(p)}\hat{T} = (-1)^p\epsilon A^{(p)},$$

where $\epsilon = \pm 1$.

With these properties established, we can now analyze numerical calculations of each of the three moments $N_{ij}^{(n)}(\bar{q})$ for $n = 0, 1, 2$.

The zero-order moment matrix $N^{(0)}(\bar{q})$. This matrix plays an essential role in the formalism as observed in Eqs. (16) and (19). In fact, it is the inverse of its square root which occurs in these expressions and whose determination requires, in principle, the diagonalization of $N^{(0)}(\bar{q})$ with a matrix $U(\bar{q})$ which itself depends on the deformation $\bar{q}$. As a consequence, the transformation of the symmetric operators in Eqs. (16) and (19) to the new representation necessitates the calculation of the first and second derivatives of $U(\bar{q})$, thereby including a number of terms which significantly increase the size of the expressions (16) and (19). In light of the numerical calculations presented above, we propose instead a set of reasonable approximations to avoid these unnecessary complications.

First, in Fig. 9, the moment $N_{00}^{(0)}(\bar{q})$, as well as its first and second derivatives, all of which intervene in various quantities, are shown at different deformations.

The moment generally increases between 8 b and 37 b as a function of the quadrupole deformation. Its first two derivatives, $N_{00}^{(0)'}(\bar{q})$ and $N_{00}^{(0)''}(\bar{q})$, are found to be much smaller by at least one order of magnitude. Their values vary rapidly in the interval $[-0.9, 0.5]$ for $N_{00}^{(0)'}(\bar{q})$ and $[-0.4\,\mathrm{b}^{-1}, 0.6\,\mathrm{b}^{-1}]$ for $N_{00}^{(0)''}(\bar{q})$.

In Table I we give the matrix elements of $N^{(0)}(\bar{q})$ for different excitations at $\bar{q} = 60$ b. At this deformation, we

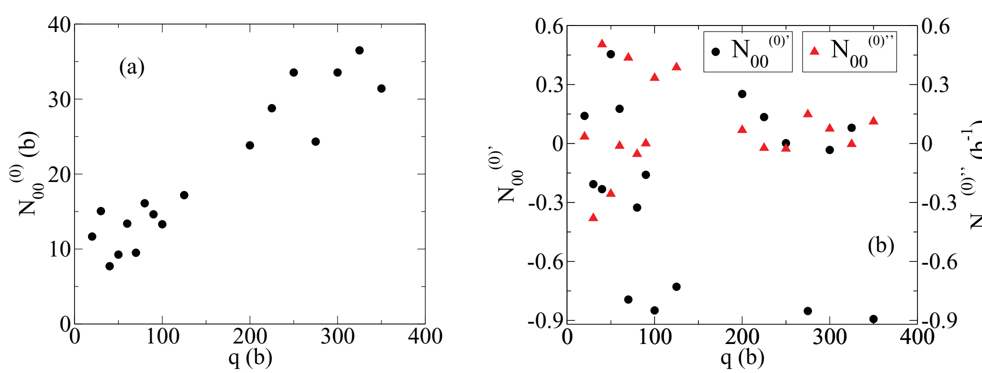

FIG. 9. (Color online) $N_{00}^{(0)}(\bar{q})$ (a) and its first and second derivatives (b) as functions of the deformation.

TABLE I. Matrix elements of $N^{(0)}(\bar{q})$ at $\bar{q} = 60$ b. Centers of repulsion q_r are mentioned if needed. Letters are used to differentiate the same K^π excitations.

K^π	0	$5/2^-$(a)	$5/2^-$(b)	$1/2^-$	$1/2^+$(a)	$1/2^+$(b)	$3/2^+$(a) $q_r = 57$ b	$3/2^+$(b) $q_r = 57b$	$5/2^+$
0	13								
$5/2^-$(a)	2.1×10^{-2}	13							
$5/2^-$(b)	-1.7×10^{-2}	-6.0×10^{-3}	13						
$1/2^-$	-1.2×10^{-2}	4.3×10^{-3}	5.4×10^{-3}	13					
$1/2^+$(a)	6.8×10^{-2}	-2.1×10^{-3}	-3.3×10^{-3}	3.5×10^{-3}	12				
$1/2^+$(b)	-7.4×10^{-2}	8.1×10^{-3}	1.1×10^{-2}	-1.3×10^{-2}	-2.2×10^{-3}	12			
$3/2^+$(a), $q_r = 57$ b	-4.5×10^{-2}	6.3×10^{-3}	8.4×10^{-3}	-1.0×10^{-2}	4.5×10^{-3}	-2.0×10^{-2}	12		
$3/2^+$(b), $q_r = 57$ b	-1.3×10^{-1}	-3.1×10^{-3}	-2.6×10^{-3}	4.2×10^{-3}	-4.0×10^{-3}	9.2×10^{-3}	5.2×10^{-3}	12	
$5/2^+$	8.9×10^{-3}	5.4×10^{-3}	6.6×10^{-3}	-8.3×10^{-3}	4.6×10^{-3}	-1.7×10^{-2}	-1.3×10^{-2}	4.5×10^{-3}	13

observe that the diagonal elements do not depend too much on the 0- or 2-qp states under consideration: they are found to be between 12.0 b and 13.4 b. Such a feature is also observed for most of the deformations. However, let us mention that in a few cases, repulsions between single-particle states induce larger variations of the diagonal elements $N_{ii}^{(0)}(\bar{q})$. This observation suggests we should introduce the diagonal terms $N_{AV}^{(0)}(\bar{q})$ defined as

$$N_{AV}^{(0)}(\bar{q}) = \frac{1}{N}\mathrm{Tr}[N^{(0)}(\bar{q})],$$

with N the dimension of the matrix $N^{(0)}(\bar{q})$. With such a definition, the matrix $N^{(0)}(\bar{q})$ can then be written in the form

$$N^{(0)}(\bar{q}) = N_{AV}^{(0)}(\bar{q})[I + \Delta(\bar{q})], \quad \Delta(\bar{q}) = \frac{N^{(0)}(\bar{q}) - N_{AV}^{(0)}(\bar{q})I}{N_{AV}^{(0)}(\bar{q})}.$$

The diagonal and off-diagonal matrix elements of Δ are all found to be small for all deformations, and, therefore, the inverse of $N^{(0)}(\bar{q})$ can be calculated by means of the series expansion of $[I + \Delta(q)]^{-1/2}$. As a result of this study, it appears that considering this inverse square root as diagonal is a reasonable approximation.

At this point, we introduce normalized moments for non-zero-order moments of the overlap kernel since they are the quantities of interest in the formalism developed in Secs. IV and V,

$$\bar{N}^{(p)}(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}} N^{(p)}(\bar{q}) \frac{1}{\sqrt{N^{(0)}(\bar{q})}}, \quad p \geqslant 1. \quad (28)$$

Taking advantage of our previous discussion, these moments are calculated in the approximation that the inverse square root of $N^{(0)}(\bar{q})$ is diagonal. Their properties are discussed in the next paragraph.

(b) First-order matrix moment $\bar{N}^{(1)}(\bar{q})$. The matrix elements of normalized first-order moment $\bar{N}^{(1)}(\bar{q})$ are given in Table II for different excitations at $\bar{q} = 60$ b. Since $\bar{N}^{(1)}(\bar{q})$ is antisymmetric, the diagonal terms are zero. From Eq. (28), it is clear that the value of $\bar{N}_{ij}^{(1)}(\bar{q})$ depends on the amplitude of the overlap $N_{ij}^{(1)}(\bar{q})$. As shown in Table II, the absolute value of $\bar{N}_{ij}^{(1)}(\bar{q})$ is generally small although some specific excitations associated with level repulsions lead to non-negligible values.

Over the whole range of deformation, the most singular case concerns two excitations involved in a mutual repulsion for which $|N_{ij}^{(1)}(\bar{q})| = 6.9$ b. All along the deformation, only 27 matrix elements $|N_{ij}^{(1)}(\bar{q})|$ (of 612) are higher than 1 b.

(c) Second-order moment $\bar{N}^{(2)}(\bar{q})$. As we will see in Sec. IV, the derivation of the inverse of $\hat{J}_{1/2}(\bar{q}) = [I + \hat{u}(\bar{q})]^{1/2}$ requires the determination of not only the second-order moments but also its first and second derivatives. For the sake of brevity, we display only in Figs. 10(a) and 10(b) those

TABLE II. Matrix elements of normalized first-order moment $\bar{N}^{(1)}(\bar{q})$ for different excitations at $\bar{q} = 60$ b. All the values are divided by i in order to be real. Centers of repulsion q_r are mentioned if needed. Letters are used to differentiate the same K^π excitations.

K^π	0	$5/2^-$(a)	$5/2^-$(b)	$1/2^-$	$1/2^+$(a)	$1/2^+$ (b)	$3/2^+$(a) $q_r = 57$ b	$3/2^+(b)$ $q_r = 57b$	$5/2^+$
0	0.0								
$5/2^-$(a)	-7.9×10^{-2}	0.0							
$5/2^-$(b)	-9.8×10^{-2}	-9.9×10^{-1}	0.0						
$1/2^-$	1.2×10^{-1}	3.7×10^{-4}	-8.1×10^{-4}	0.0					
$1/2^+$(a)	-6.9×10^{-2}	1.1×10^{-3}	2.0×10^{-3}	-1.8×10^{-3}	0.0				
$1/2^+$(b)	2.5×10^{-1}	-5.9×10^{-4}	-2.5×10^{-3}	1.5×10^{-3}	7.3×10^{-2}	0.0			
$3/2^+$(a), $q_r = 57$ b	1.9×10^{-1}	-3.1×10^{-4}	-1.9×10^{-3}	-1.2×10^{-3}	-1.8×10^{-3}	4.0×10^{-4}	0.0		
$3/2^+$(b), $q_r = 57$ b	-7.3×10^{-2}	-2.6×10^{-3}	-2.2×10^{-3}	-3.7×10^{-3}	3.7×10^{-3}	-7.6×10^{-3}	$2.5 \times 10^{+0}$	0.0	
$5/2^+$	1.5×10^{-1}	-8.4×10^{-4}	-4.5×10^{-4}	6.1×10^{-4}	-2.5×10^{-3}	2.8×10^{-3}	2.0×10^{-3}	3.6×10^{-3}	0.0

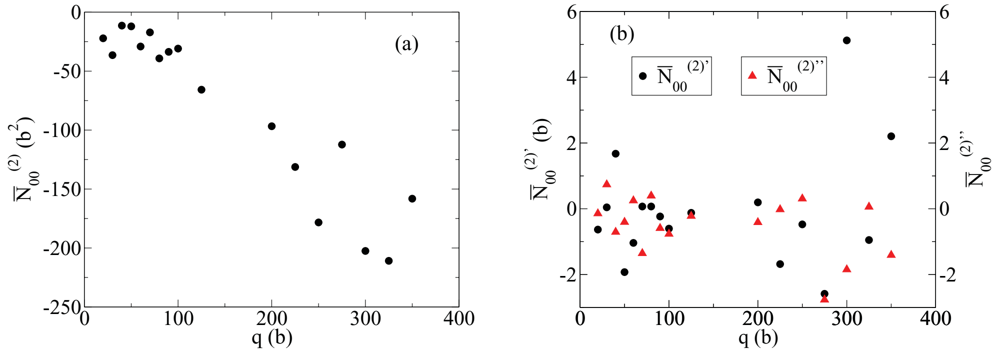

FIG. 10. (Color online) The normalized second-order moment $\bar{N}^{(2)}(\bar{q})$ (a) and its first (black solid circles) and second (red solid triangles) derivatives (b) of the nonexcited overlap along the deformation.

quantities in the case of the diagonal element in the ground state.

In Fig. 10(a) we note that all these quantities not only vary rapidly with the deformation but also undergo oscillations of very large amplitude. The moment itself varies between -5 b^2 and -211 b^2 in a range of deformations [20 b, 350 b]. As for the first and second derivatives, they are contained in the range [-3 b, 6 b] and [-2.1, 1], respectively [Fig. 10(b)].

In Table III, diagonal and nondiagonal normalized second-order moments are given for the HF+BCS minimum and the selected excitations at $\bar{q} = 80$ b. Diagonal terms are negative due to our definition of the second-order moment. As expected from our discussion on nondiagonal matrix element of the overlap, most of the nondiagonal terms are at least two orders of magnitude smaller than the diagonal ones. It is also seen that they strongly depend on the excitations. Very similar features are observed for all deformations up to $\bar{q} = 350$ b. However, the maximum value of a nondiagonal term is found to be sup$i \neq j, \bar{q}|\bar{N}_{ij}^{(2)}(\bar{q})| = 78.4$ b^2 at $\bar{q} = 250$ b, which corresponds to 44% of $\bar{N}_{00}^{(2)}(\bar{q})$ in this region. This case corresponds to $i = (i_1, i_2)$ and $j = (j_1, j_2)$ excitations for which repulsion occurs between i_1 and j_1 at $q_r = 242$ b and between i_2 and j_2 at $q_r = 265$ b.

It is worth stressing that perturbations in the overlap matrix due to repulsions, such as the change in amplitude of a nondiagonal term as depicted in Fig. 8 or the reduction of the diagonal terms [see Fig. 5(b)], disturbs the values of the moments, which are the quantities of interest in the present formalism, in a brutal but still continuous way.

IV. STUDY AND DETERMINATION OF $\hat{J}_{\pm 1/2}(\bar{q})$

In the previous section we have seen that the moments and their derivatives vary rapidly as function of the deformation. As we will see in the following these quantities occur everywhere in the calculation of $\hat{\tilde{J}}_{\pm 1/2}(\bar{q})$ [with $\hat{J}_{\pm 1/2}(\bar{q}) = \hat{J}^{\pm 1/2}(\bar{q})$], which seriously complicates the derivation of the inverse of the overlap kernel. This question of the dependence of the moments on the deformation has been studied in detail in the GOA [1] and in the symmetric-moment expansion for the one-dimensional case of no intrinsic excitations [37] (although, even in the one-dimensional case, our solution below is more complete), but in the context of the present study we have found no information on this subject in the open literature. In the discussion that follows, we will call $[.P]^{(n)}$ a symmetric operator of order n despite the fact that, strictly speaking, an order cannot be attributed to such an operator since it contains all orders up to n.

TABLE III. Matrix elements of normalized second-order moment $\bar{N}_{ij}^{(2)}(\bar{q})$ for different excitations at $\bar{q} = 80$ b. Centers of repulsion q_r are mentioned if needed. Letters are used to differentiate the same K^π excitations.

K^π	0	$3/2^-$(a)	$3/2^-$(b) $q_r = 82.5$ b	$1/2^-$	$1/2^+$(a) $q_r = 85$ b	$1/2^+$(b) $q_r = 85$ b	$1/2^+$(c) $q_r = 85$ b $q'_r = 86$ b	$5/2^+$	$9/2^+$
0	-39								
$3/2^-$(a)	$1.1 \times 10^{+0}$	-26							
$3/2^-$(b)	-1.9×10^{-1}	$1.2 \times 10^{+0}$	-30						
$1/2^-$	2.4×10^{-2}	4.3×10^{-1}	3.2×10^{-2}	-39					
$1/2^+$(a), $q_r = 85$ b	-3.7×10^{-1}	1.1×10^{-1}	2.7×10^{-3}	6.3×10^{-3}	-32				
$1/2^+$(b), $q_r = 85$ b	-8.7×10^{-2}	-2.7×10^{-1}	-2.1×10^{-2}	-1.9×10^{-2}	-2.2×10^{-2}	-32			
$1/2^+$(c), $q_r = 85$ b, $q'_r = 86$ b	1.1×10^{-1}	-2.4×10^{-1}	-1.6×10^{-2}	-1.9×10^{-2}	2.4×10^{0}	2.3×10^{-1}	-29		
$5/2^+$	2.3×10^{-1}	8.6×10^{-1}	6.6×10^{-2}	7.1×10^{-2}	1.5×10^{-2}	-4.5×10^{-2}	-3.8×10^{-2}	-39	
$9/2^+$	2.3×10^{-1}	2.9×10^{-1}	2.1×10^{-1}	2.5×10^{-2}	8.5×10^{-3}	-1.5×10^{-2}	-1.4×10^{-2}	5.7×10^{-2}	-39

A. Discussion and generalities about the inversion of the one-dimensional overlap kernel

The difficulty mentioned above already occurs in the standard (one-dimensional) approach and, consequently, the discussion is first restricted to this simple case. Let us recall here that when the moments are independent of the deformation, the derivation of the operators in question is straightforward. They are given by [27]

$$\hat{J}_{\pm 1/2}(\bar{q}) = [1+\hat{u}(\bar{q})]^{\pm 1/2} \simeq 1 \pm \tfrac{1}{2}\hat{u}(\bar{q})$$

with

$$\hat{u}(\bar{q}) = \frac{N^{(2)}(\bar{q})}{2N^{(0)}(\bar{q})}P^2.$$

This form is consistent with an expansion of the kernel overlap up to second order in the collective momentum P. Besides, we are justified in stopping the expansion of $\hat{J}_{-1/2}(\bar{q})$ at the second order in P since, in the usual derivation of a Schrödinger equation, one neglects the derivatives of the Hamiltonian kernel of order greater than 2. The situation is quite different here since symmetric operators of order four give contributions to the expansion of the Hamiltonian kernel involving derivatives less then or equal to 2. In order to go beyond this approximation, successive transformations have been performed which allow $\hat{J}(\bar{q})$ to be expressed in a suitable form for our purposes. First, the normalized moment $\bar{N}^{(2)}(\bar{q})$ defined above (Sec. III) is introduced in the definition of $\hat{u}(\bar{q})$ which leads to

$$\begin{aligned}\hat{u}(\bar{q}) &= \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\frac{1}{2}[N^{(2)}(\bar{q})P]^{(2)}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\\ &= -\frac{1}{2}C^{(2)}(N^{(2)},N^{(0)}) + \frac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}.\end{aligned}$$

The derivation of this expression is given in Appendix C. The coefficient $C^{(2)}$ is a function of the first and second derivatives of the moment of zero order. If the latter were constant, then $C^{(2)}$ would vanish. After inserting this expression in the definition of $\hat{J}(\bar{q})$ given in equation (10) we obtain

$$\hat{J}(\bar{q}) = 1 + \alpha_{(0)}(\bar{q}) + \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}$$

with

$$\alpha_{(0)}(\bar{q}) = -\tfrac{1}{2}C^{(2)}(N^{(2)},N^{(0)}).$$

According to Fig. 11, $\alpha_{(0)}(\bar{q})$ is not negligible since it can reach 10% at several deformations. It is possible, however, to rewrite $\hat{J}(\bar{q})$ in the following form:

$$\hat{J}(\bar{q}) = \sqrt{A_{(0)}(\bar{q})}\left\{1+\alpha_{(1)}(\bar{q}) + \frac{1}{2}\left[\bar{N}_R^{(2)}(\bar{q})P\right]^{(2)}\right\}\sqrt{A_{(0)}(\bar{q})}$$

with

$$\begin{cases}\alpha_{(1)}(\bar{q}) = -\frac{1}{2}C^{(2)}(N^{(2)},A_{(0)})\\ \sqrt{A_{(0)}(\bar{q})} = \sqrt{1+\alpha_{(0)}(\bar{q})}\\ \bar{N}_R^{(2)}(\bar{q}) = \frac{1}{\sqrt{A_{(0)}(\bar{q})}}\bar{N}^{(2)}\frac{1}{\sqrt{A_{(0)}(\bar{q})}}\end{cases}. \tag{29}$$

Coming back to Fig. 11 we observe that $\alpha_{(1)}(\bar{q})$ is at most 4% (at $q = 30$ b) in the whole range of deformation. At this stage it seems reasonable to neglect this term but it is clear that, if a better approximation is needed, one can iterate this procedure starting with $\alpha_{(1)}$ which gives the quantity $A_{(1)}$ and so on. If one refers to Eqs. (16) and (19), one concludes in the light of this study that the entire formalism remains unchanged with a $\hat{J}(\bar{q})$ still given by

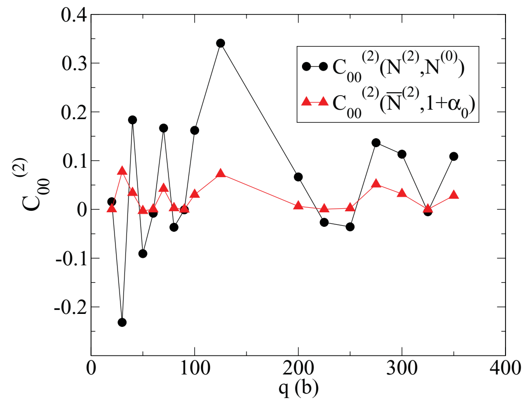

FIG. 11. (Color online) Comparison between $C^{(2)}(N^{(2)}, N^{(0)})$ and first iterated $C^{(2)}(\bar{N}^{(2)}, 1+\alpha)$ values as a function of the deformation.

$$\hat{J}(\bar{q}) = 1 + \hat{u}(\bar{q}) = 1 + \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}, \tag{30}$$

provided we substitute in all expressions a renormalized zero moment $N_R^{(0)}(\bar{q}) = \prod_{i=0}^{p-1} A_{(i)}N^{(0)}(\bar{q})$ instead of the usual moment $N^{(0)}(\bar{q})$. An index i is used to take into account the number of times the procedure described above has been iterated. From now on the notation is kept unchanged, with the understanding that, in fact, a renormalized zero moment is used.

Thus, we are led to determine $\hat{J}_{\pm 1/2}(\bar{q})$ with $\hat{J}(\bar{q})$ given in Eq. (10). In fact, we are mainly interested in the determination of $\hat{J}_{-1/2}(\bar{q})$, since it is this operator we need to express the contribution of the Hamiltonian kernel in Eq. (19). In the one-dimensional case it must be solution of the equation:

$$\hat{J}_{-1/2}(\bar{q})\left\{1+\tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}\right\}\hat{J}_{-1/2}(\bar{q}) = 1. \tag{31}$$

As suggested in Ref. [27], we attempt to solve Eq. (31) with an ansatz of the form

$$\hat{J}_{-1/2}(\bar{q}) = A_{-1/2}(\bar{q}) + [B_{-1/2}(\bar{q})P]^{(2)} + [C_{-1/2}(\bar{q})P]^{(4)}. \tag{32}$$

After inserting this ansatz in Eq. (31) we are led to a complicated coupled set of nonlinear equations among $A_{-1/2}(\bar{q})$, $B_{-1/2}(\bar{q})$, and $C_{-1/2}(\bar{q})$ and their derivatives up to high orders. Solving these equations, including the second derivative of $N^{(2)}(\bar{q})$ is not a trivial problem and it would be a considerable amount of work. This is an extensive study in its own right that goes far beyond the scope of the present paper. In the following we take advantage of the fact that the size of the problem is reduced considerably if we neglect these second derivatives and, consequently, we limit ourselves to finding solutions including only the first derivative of $N^{(2)}(\bar{q})$. Even in this simple case it is important to find approximated solutions as a starting point in order to overcome some difficulties in solving Eq. (31). A natural choice for these approximated solutions is to approach $\hat{J}_{\pm 1/2}(\bar{q})$ by the first terms of their series expansion. For instance, we will define a $\hat{J}_{A,1/2}(\bar{q})$ as:

$$\hat{J}_{A,1/2}(\bar{q}) \equiv 1 + \tfrac{1}{2}\hat{u}(\bar{q}) - \tfrac{1}{8}\hat{u}^2(\bar{q}) \approx [1+\hat{u}(\bar{q})]^{1/2},$$

where the operator $\hat{u}(\bar{q})$ is defined by Eq. (30). By inserting the definition of $u(\bar{q})$ in $\hat{J}_{A,1/2}(\bar{q})$ we readily obtain this operator in the form:

$$\hat{J}_{A,1/2}(\bar{q}) = A_{1/2}(\bar{q}) + [B_{1/2}(\bar{q})P]^{(2)} + [C_{1/2}(\bar{q})P]^{(4)}.$$

For the sake of brevity, the derivation of this expression and the coefficients are given in Appendix C 2. At this stage we have thought it interesting to study qualitatively the influence of the derivatives of $\bar{N}^{(2)}(\bar{q})$ in this formalism. For this we check the accuracy the approximation used by calculating $\hat{J}_{A,1/2}(\bar{q})\hat{J}_{A,1/2}(\bar{q})$ which we write in the form:

$$\hat{J}_{A,1/2}(\bar{q})\hat{J}_{A,1/2}(\bar{q}) = 1 + \hat{u}(\bar{q}) + R(\bar{q}).$$

The remainder $R(\bar{q})$, whose calculation is given in details in Appendix C 3, is in fact an operator

$$R(\bar{q}) \simeq A[\bar{N}^{(2)''}(\bar{q})] + \tfrac{1}{2}[C(\bar{N}^{(2)}, \bar{N}^{(2)'}, \bar{N}^{(2)''})\bar{N}^{(2)}(\bar{q})P]^{(2)}. \tag{33}$$

The symbol $\simeq$ is used to indicate that symmetric operators $[.P]^{(n)}, n > 2$ are neglected in the expression of $R(\bar{q})$. This operator, which should be zero if the moments were constant, provides some quantitative information on the accuracy of our approximation as function of the first and second derivatives of $\bar{N}^{(2)}(\bar{q})$. In Fig. 12 we give a plot of the coefficients A and C over a wide range of deformations between 30 b and 350 b. It is seen that $\sup_{\bar{q}}|A| = 1.9\times10^{-2}$ and $\sup_{\bar{q}}|C| = 9.8\times10^{-2}$ over the whole range of deformations considered here, which suggests that this ansatz is a reasonable zeroth-order approximation, despite the large variations in the moments $\bar{N}^{(2)}$. On the other hand, the expressions for the coefficients A and C given in Appendix C tell us that A and C vanish independently if one can neglect the second derivative of $\bar{N}^{(2)}(\bar{q})$. In that case, $\hat{J}_{A,1/2}(\bar{q})$ becomes an "exact" solution consistent with the truncation we made in the expansion of the kernel overlap. Note also that such an approximation takes into account all the derivatives of $N^{(0)}(\bar{q})$ up to second order and still includes the first derivative of $\bar{N}^{(2)}(\bar{q})$.

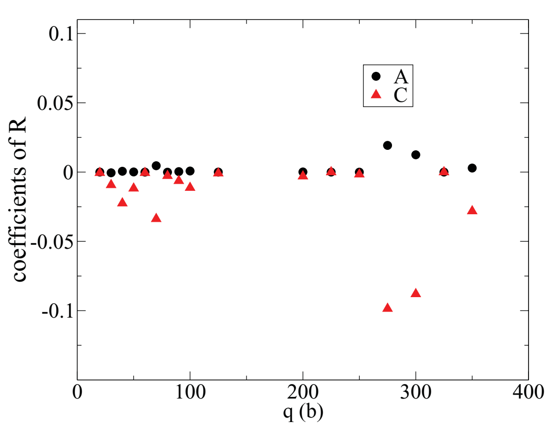

FIG. 12. (Color online) A and C coefficients in Eq. (33) as function of the deformation.

The same discussion applies to the operator $\hat{J}_{A,-1/2}(\bar{q})$ which is written in the form

$$\hat{J}_{A,-1/2}(\bar{q}) = A_{-1/2}(\bar{q}) + [B_{-1/2}(\bar{q})P]^{(2)} + [C_{-1/2}(\bar{q})P]^{(4)},$$

with the coefficients $A_{-1/2}(\bar{q})$, $B_{-1/2}(\bar{q})$, and $C_{-1/2}(\bar{q})$ being given in Appendix C 2. In particular, if we neglect $\bar{N}^{(2)''}(\bar{q})$ this operator satisfies $\hat{J}_{A,-1/2}(\bar{q})\hat{J}_{A,+1/2}(\bar{q}) \simeq 1$ and, more importantly, it is also solution of Eq. (31) up to second order. Inspection of the equations reveals that the coefficient $C_{-1/2}(\bar{q})$ is not completely defined at this order. A complete determination of this coefficient is achieved by canceling the contribution of fourth order in Eq. (31). Its value is then given by

$$C_{-1/2}(\bar{q}) = \tfrac{3}{32}[\bar{N}^{(2)}(\bar{q})]^2\left[1 - \tfrac{15}{8}\xi(\bar{q}) + \tfrac{105}{64}\xi^2(\bar{q})\right]$$

with $\xi(\bar{q}) = [\bar{N}^{(2)'}(\bar{q})]^2/\bar{N}^{(2)}(\bar{q})$.

To obtain this expression, the third and fourth derivatives of $C_{-1/2}(\bar{q})$ are set to zero. It turns out that these conditions are satisfied by the solution given above since we set to zero the derivatives $[\bar{N}^{(2)}(\bar{q})]^{(p)}$, $p \geqslant 2$. Thus, we conclude that it is a solution in the whole range of deformations consistent with our assumptions on the derivatives of $\bar{N}^{(2)}(\bar{q})$. To summarize, the operator

$$\hat{J}_{-1/2}(\bar{q}) = 1 - \tfrac{1}{4}\left[\bar{N}^{(2)}(\bar{q})\left[1 - \tfrac{3}{8}\xi(\bar{q})\right]P\right]^{(2)} + \tfrac{3}{32}\left[[\bar{N}^{(2)}(\bar{q})]^2\left[1 - \tfrac{15}{8}\xi(\bar{q}) + \tfrac{105}{64}\xi^2(\bar{q})\right]P\right]^{(4)}$$

is solution of Eq. (31) up to fourth order in the symmetric operator $[.P]^{(n)}$. This expansion takes into account not only the derivatives of $\bar{N}^{(0)}(\bar{q})$ up to second order but also the first derivative of $\bar{N}^{(2)}(\bar{q})$. Even though it is not complete, since we do not include the second derivative of $\bar{N}^{(2)}(\bar{q})$, this operator represents a significant improvement over what was generally used in previous works. We now proceed to the N-dimensional case by following step by step the procedure described in this section. Consequently, we will also neglect the contribution of the second derivatives of $\bar{N}^{(2)}(\bar{q})$ in the expression of the inverse overlap kernel. One finds a justification for this approximation in the fact that the general structure of the Schrödinger equation we derive does not depend on the precise determination of the coefficients entering in the definition of our ansatz for the inverse.

B. Determination of the inverse in the N-dimensional case

A similar analysis to the one-dimensional case can be performed here by considering instead the operator

$$\hat{u}(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}}\left\{[N^{(1)}(\bar{q})P]^{(1)} + \frac{1}{2}[N^{(2)}(\bar{q})P]^{(2)}\right\}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}.$$

First, it is written in terms of normalized moments according to the expression

$$\hat{u}(\bar{q}) = [W_N(\bar{q})P]^{(1)} + \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)} + \alpha_{(0)}(\bar{q}),$$

where we have introduced the quantities:

$$W_N(\bar{q}) = \bar{N}^{(1)}(\bar{q}) + iC^{(1)}(N^{(2)}, N^{(0)})$$
$$\alpha_{(0)}(\bar{q}) = \tfrac{i}{2}C^{(1)}(N^{(1)}, N^{(0)}) - \tfrac{1}{2}C^{(2)}(N^{(2)}, N^{(0)}).$$

The expression of $C^{(1)}(N^{(1)}, N^{(0)})$ is given in Appendix C 1. According to the definition of $\hat{J}(\bar{q})$ [Eq. (10)] this operator becomes

$$\hat{J}(\bar{q}) = I + \alpha_{(0)}(\bar{q}) + [W_N(\bar{q})P]^{(1)} + \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}.$$

The difference with the one-dimensional case is the occurrence of an additional first-order symmetric operator and the fact that all operators are matrices. At this stage we proceed as we did in the one-dimensional case by introducing renormalized zero-order moments and using an iterative procedure. Let us mention here that our numerical result tell us that the matrix elements of $\alpha_{(0)}(\bar{q})$ never exceed 2×10^{-1}. Consequently, a series expansion with few terms gives the operator $[I + \alpha_{(0)}(\bar{q})]^{-1/2}$ with excellent accuracy. We recall that we keep the same notation $N^{(0)}(\bar{q})$ to denote this renormalized moment. With these renormalizations we are finally led to solve Eq. (31) which can be written as

$$\begin{aligned} &\hat{J}_{-1/2}(\bar{q})[I + \hat{u}(\bar{q})]\hat{J}_{-1/2}(\bar{q}) = I \\ &\hat{u}(\bar{q}) = [W_N(\bar{q})P]^{(1)} + \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}. \end{aligned} \tag{34}$$

One could attempt to solve this equation with an appropriate ansatz which, in the N-dimensional case, should also include odd-order symmetric operators with an ansatz of the form

$$\begin{aligned} \hat{J}_{-1/2}(\bar{q}) = {} & A_{-1/2}(\bar{q}) + [D_{-1/2}(\bar{q})P]^{(1)} + [B_{-1/2}(\bar{q})P]^{(2)} \\ & + [E_{-1/2}(\bar{q})P]^{(3)} + [C_{-1/2}(\bar{q})P]^{(4)}. \end{aligned} \tag{35}$$

This expression should be inserted in Eq. (34) but for reasons given in the one-dimensional case, it is advantageous to start with an approximation to $\hat{J}_{A,-1/2}(\bar{q})$ chosen as the series expansion of $[I + \hat{u}(\bar{q})]^{-1/2}$ up to second order in $\hat{u}(\bar{q})$, i.e., we set

$$\hat{J}_{A,-1/2}(\bar{q}) = I - \tfrac{1}{2}\hat{u}(\bar{q}) + \tfrac{3}{8}\hat{u}^2(\bar{q}),$$

with the operator $\hat{u}(\bar{q})$ defined this time by Eq. (34). It is straightforward to express $\hat{J}_{-1/2}(\bar{q})$ in a form similar to Eq. (35) and to rewrite Eq. (35) as:

$$\begin{aligned} \hat{J}_{-1/2}(\bar{q}) = {} & I - \frac{1}{2}[W_N(\bar{q})P]^{(1)} - \frac{1}{2}\Bigg[\Bigg\{\frac{\bar{N}^{(2)}(\bar{q})}{2} - \frac{3}{16}[\bar{N}^{(2)'}(\bar{q})]^2 \\ & - \frac{3}{4}[W_N(\bar{q})]^2 - \frac{3i}{16}[W_N(\bar{q})\bar{N}^{(2)'}(\bar{q})]_-\Bigg\}P\Bigg]^{(2)} \\ & + [E_{-1/2}(\bar{q})P]^{(3)} + [C_{-1/2}(\bar{q})P]^{(4)} \end{aligned}$$

with the notation

$$(X, Y)_{\pm} = XY \pm YX.$$

The first derivative of $W_N(\bar{q})$ has been neglected since it is generally very small. The operator defined by the first three lines of this expression is solution to Eq. (34) up to second order. The coefficients $E_{-1/2}(\bar{q})$ and $C_{-1/2}(\bar{q})$ can then be determined by canceling the third- and fourth-order contribution in Eq. (34). For practical reasons we neglect their contributions and derive in the next section a Schrödinger equation with the inverse defined by

$$\begin{aligned} \hat{J}_{-1/2}(\bar{q}) = {} & I - \frac{1}{2}[W_N(\bar{q})P]^{(1)} - \frac{1}{2}\Bigg[\Bigg\{\frac{\bar{N}^{(2)}(\bar{q})}{2} - \frac{3}{16}[\bar{N}^{(2)'}(\bar{q})]^2 \\ & - \frac{3}{4}[W_N(\bar{q})]^2 - \frac{3i}{16}[W_N(\bar{q})\bar{N}^{(2)'}(\bar{q})]_-\Bigg\}P\Bigg]^{(2)}. \end{aligned} \tag{36}$$

Otherwise the expression would have contained an exceedingly large number of terms. Again, we justify this approximation by the fact that it does not affect the general structure of the Schrödinger equation that we propose.

V. DERIVATION OF A SCHRÖDINGER-LIKE EQUATION

According to Eq. (19) and taking into account the fact that the inverse operator $\hat{J}_{-1/2}(\bar{q})$ given by Eq. (36) is Hermitian, the contribution of the Hamiltonian kernel to the Hill-Wheeler equation reduces to the form

$$\begin{aligned} &\hat{J}_{-1/2}(\bar{q})\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\Big\{H^{(0)}(\bar{q}) + [H^{(1)}(\bar{q})P]^{(1)} \\ &\quad + \frac{1}{2}[H^{(2)}(\bar{q})P]^{(2)}\Big\}\frac{1}{\sqrt{N^{(0)}(\bar{q})}}\hat{J}_{-1/2}(\bar{q}). \end{aligned}$$

Now, we proceed as we did in the case of the overlap kernel by introducing this time normalized moments of the Hamiltonian defined by

$$\bar{H}^{(n)}(\bar{q}) = \frac{1}{\sqrt{N^{(0)}(\bar{q})}}H^{(n)}(\bar{q})\frac{1}{\sqrt{N^{(0)}(\bar{q})}}$$

and rewrite the equation given above as function of these moments

$$\begin{aligned} &\hat{J}_{-1/2}(\bar{q})\big[\bar{H}^{(0)}(\bar{q}) + \tfrac{i}{2}C^{(1)}(\bar{H}^{(1)}, \bar{N}^{(0)}) - \tfrac{1}{2}C^{(2)}(\bar{H}^{(1)}, \bar{N}^{(0)}) \\ &\quad + \big[\big[\bar{H}^{(1)}(\bar{q}) + \tfrac{i}{2}C^{(1)}(\bar{H}^{(2)}, \bar{N}^{(0)})\big]P\big]^{(1)} \\ &\quad + \tfrac{1}{2}[\bar{H}^{(2)}(\bar{q})P]^{(2)}\big]\hat{J}_{-1/2}(\bar{q}). \end{aligned} \tag{37}$$

The next step is to extract a Schrödinger-like equation following the procedure described in [27]. To this end we insert the definition from Eq. (36) in Eq. (37) and make an expansion in terms of symmetric ordered product that we truncate at order two. We illustrate in the following how we achieve this goal by rewriting Eq. (37) in condensed notation

$$\hat{J}_{-1/2}(\bar{q})\mathcal{H}(\bar{q})\hat{J}_{-1/2}(\bar{q}),$$

with

$$\begin{cases} \mathcal{H}(\bar{q}) = \sum_{i=0}^{2}[h_{(i)}(\bar{q})P]^{(i)} \\ \hat{J}_{-1/2}(\bar{q}) = \sum_{i=0}^{2}[j_{(i)}(\bar{q})P]^{(i)} \end{cases}, \tag{38}$$

where the quantities $j_{(i)}(\bar{q})$, $h_{(i)}(\bar{q})$ are obtained by identification of these operators with those defined in Eqs. (36) and (37), respectively. With these notations we can rewrite Eq. (37) in the convenient form

$$\sum_{p,q,r=0}^{2}[j_{(p)}(\bar{q})P]^{(p)}[h_{(q)}(\bar{q})P]^{(q)}[j_{(r)}(\bar{q})P]^{(r)},$$

which has the advantage of showing the typical terms occurring in this formalism. The expansion we are looking for is then derived very simply by means of general formulas that are given in Appendix A [Eqs. (A3) and (A4)]. This derivation is straightforward, but requires nevertheless quite cumbersome manipulations that we do not describe here. Thus, we limit ourselves to giving the final expression of a Schrödinger equation which takes into account the coupling between collective and intrinsic excitations. This equation is written as

$$[H(\bar{q}) - E]g(\bar{q}) = 0,$$
$$H(\bar{q}) = S(\bar{q}) + [T(\bar{q})P]^{(1)} + [U(\bar{q})P]^{(2)}, \quad (39)$$

where the quantities S, T, and U are matrices whose expression is

$$\begin{aligned}
S &= h_{(0)} + \tfrac{1}{8}\big(h^{(2)}_{(0)} j_{(2)}\big)_+ + \tfrac{1}{16} j^{(1)}_{(2)} h^{(2)}_{(0)} j^{(1)}_{(2)} - \tfrac{1}{4}\big(h^{(1)}_{(0)} j_{(1)}\big)_- \\
&\quad - \tfrac{1}{16} j_{(1)} h^{(2)}_{(0)} j_{(1)} + \tfrac{1}{32}\big(j_{(1)} h^{(2)}_{(0)} j^{(1)}_{(2)}\big)_A \\
T &= h_{(1)} + \tfrac{1}{2}\big(h_{(0)} j_{(1)}\big)_+ - \tfrac{1}{2}\big(h^{(1)}_{(0)} j_{(2)}\big)_- - \tfrac{1}{16}\big(j_{(1)} h^{(2)}_{(0)} j_{(2)}\big)_S \\
&\quad - \tfrac{1}{8}\big(j_{(1)} h^{(1)}_{(0)} j^{(1)}_{(1)}\big)_S - \tfrac{1}{16}\big(j_{(2)} h^{(2)}_{(0)} j^{(1)}_{(2)}\big)_A \\
U &= h_{(2)} + \tfrac{1}{2}\big(h_{(0)} j_{(2)}\big)_+ - \tfrac{1}{2}\big(h^{(1)}_{(2)} j^{(1)}_{(2)}\big)_+ - \tfrac{1}{4} j^{(1)}_{(2)} h_{(0)} j^{(1)}_{(2)} \\
&\quad - \tfrac{1}{8} j_{(2)} h^{(2)}_{(0)} j_{(2)} - \tfrac{1}{8}\big(j^{(1)}_{(2)} h^{(1)}_{(0)} j_{(2)}\big)_S + \tfrac{1}{2}\big(h_{(1)} j_{(1)}\big)_+ \\
&\quad + \tfrac{1}{4}\big(h_{(1)} j^{(1)}_{(2)}\big)_- - \tfrac{1}{4}\big(h^{(1)}_{(2)} j_{(1)}\big)_- + \tfrac{1}{4} j_{(1)} h_{(0)} j_{(1)} \\
&\quad + \tfrac{1}{8}\big(j_{(2)} h^{(1)}_{(0)} j_{(1)}\big)_A - \tfrac{1}{8}\big(j^{(1)}_{(2)} h_{(0)} j_{(1)}\big)_A \qquad (40)
\end{aligned}$$

For the sake of convenience, the dependence in $\bar{q}$ has been removed in all the quantities in this formula where we use the compact notation

$$(XYZ)_S = XYZ + ZYX$$
$$(XYZ)_A = XYZ - ZYX.$$

Furthermore, the expression for the matrix elements of the moments of $H(\bar{q})$ suggest that we make the same assumptions as for the derivatives of the overlap moments. Thus in the derivation of the formulas proposed here it has been assumed that:

$$\begin{cases} h^{(p)}_{(0)}(\bar{q}) = 0 & \text{for} \quad p \geqslant 3 \\ h^{(p)}_{(1)}(\bar{q}) = 0 & \text{for} \quad p \geqslant 1 \\ h^{(p)}_{(2)}(\bar{q}) = 0 & \text{for} \quad p \geqslant 2. \end{cases} \qquad (41)$$

These assumptions serve to reduce significantly the number of terms in the expressions of the different contributions $S(\bar{q})$, $T(\bar{q})$, and $U(\bar{q})$.

We discuss now some aspects related to the properties and the general structure of the Schrödinger equation defined by Eqs. (39) and (40) which contains all the necessary ingredients to build it. First, we note that this Hamiltonian is Hermitian and time-reversal invariant. This is easily demonstrated using the properties of the matrix elements of the moments listed in Sec. III C3. As a consequence, if we treat collective and intrinsic excitations on the same footing, there is no dissipation but only a reversible exchange of energy between these two kinds of excitation. Note, in particular, that a linear term as it occurs in Eq. (39) does not induce a dissipative force as introduced in studies of fission using a macroscopic-microscopic approach [23]. However, it may be that for practical reasons we need to treat explicitly a reduced set of intrinsic excitations and take into account the remainder implicitly because they are too numerous and their spectrum too dense. In that case we may be led to introduce a dissipation mechanism. We do not consider for the moment applications at high excitation energies where such situations would occur [38]. Concerning the general structure of the Schrödinger Eq. (39), we analyze separately the three different terms which are present in its definition. In Eq. (40) we have arranged the terms in such a way that even moments come first and odd ones at the end in $S(\bar{q})$ and $U(\bar{q})$. We recall that odd moments occur only in the multidimensional case. Accordingly, in evaluating $S(\bar{q})$ and $U(\bar{q})$ in the one-dimensional case, we must consider only the first three terms in $S(\bar{q})$ and the first six in $U(\bar{q})$. Their expressions are readily obtained with the formulas given previously but they are very long and, for the sake of brevity, we do not give them here. Note that if we neglect the derivatives of the overlap moments we recover, as we should, the simple Hamiltonian given in Ref. [27]. In the multidimensional case all the terms in Eq. (40) must be retained. They involve products of matrices of the moments of the overlap and Hamiltonian kernels and their derivatives. Each of them can be interpreted as effective vertices inducing transitions between excitations. At this point it is important to note that these vertices, by the definition of the moments, are the result of an average over a wide range of deformations around $\bar{q}$ and, consequently, the coupling between collective and intrinsic degrees of freedom is very nonlocal in the present work. This contrasts with the other approach [39] which couples the nuclear collective dynamics to internal excitations defined at every deformation along the adiabatic fission path. To conclude this analysis, it is appropriate to recast our Hamiltonian Eq. (39) in a familiar form. With more conventional notations, first, we express its diagonal matrix elements which leads to the expression

$$H_{ii}(\bar{q}) = \frac{1}{2}\left[\left[\frac{1}{M(\bar{q})}\right]_{ii} P\right]^{(2)} + V_{ii}(\bar{q}).$$

We have taken into account the fact that the matrix T is zero along the diagonal and identified a collective potential as $V(\bar{q}) = S(\bar{q})$. We also have defined the mass as $M^{-1}(\bar{q}) = 2U(\bar{q})$. We recognize standard Hamiltonians which describe separately the collective dynamics on each potential energy surfaces built with the various 2-qp excitations considered. In the same manner we introduce the coupling between 2-qp surfaces by considering the nondiagonal matrix elements of Eq. (39). They are written in the form

$$H_{ij}(\bar{q}) = \frac{1}{2}\left[\left[\frac{1}{M(\bar{q})}\right]_{ij} P\right]^{(2)} + [T_{ij}(\bar{q})P]^{(1)} + V_{ij}(\bar{q}),$$

with the definition of a nondiagonal mass as $[\frac{1}{M(\bar{q})}]_{ij} = 2U_{ij}(\bar{q})$.

This form of the interaction term is interesting because it separates the coupling between collective and intrinsic degrees of freedoms into terms of different nature. The first two, which depend on the collective momentum, can be interpreted as a dynamical coupling while the last contribution is a potential coupling. In appearance the Hamiltonian derived here has a general structure very similar to the classical Hamiltonian given by the authors in Ref. [39]. However, their derivation and ours rely on very different approaches. In particular the one presented here is based on a quantum description from the start, while the classical Hamiltonian in Ref. [39] needs to be quantized after the fact.

For completeness, we could have included in our discussion the explicit calculation of the moments associated with neutron- and proton-number operators, in order to use the method [29] which incorporates the conservation of the average particle number in the GCM formalism. Similarly, we could have included the moments of the operator associated with the subtraction of the center-of-mass energy of the nucleus. These contributions are straightforward to calculate but are omitted here in order to avoid further complicating the expression for the Hamiltonian above.

VI. CONCLUSION

In this paper we have presented a theoretical framework, the SCIM, which allows in a microscopic way, the simultaneous coupling of single-particle and collective degrees of freedom. Such an approach is based on a generalized GCM, where the general GCM ansatz of the nuclear wave function is extended by a few excited configurations. In fact, one considers as generating wave functions not only HF+BCS ground-state configurations with different values for the collective generator coordinate but also 2-qp excited states. Such an approach has the advantage of describing in a completely quantum-mechanical fashion, and without phenomenological parameters, the coupling of quasiparticle degrees of freedom to the collective motion of the nucleons. Our derivation of the SCIM proceeds in two steps. The first step is based on the generalization of the symmetric moment expansion of the equations derived in the framework of the GCM, including the coupling between collective and intrinsic variables. The moments occurring in the equations are matrices whose dimensions depend on the number of excitations introduced in the description. Contrary to the usual case—without qp excitations—all moments, odd and even, must be included in the summation. Such an exact expansion in terms of local operators of the generalized Hill-Wheeler equation is then transformed into a local Schrödinger equation by inverting the expansion of the overlap kernel. A second-order differential Schrödinger equation then is derived by limiting the summation to second-order terms under the assumption that the series expansion of the overlap and Hamiltonian kernels converge rapidly. The derivation of the inverse of the overlap has been seriously complicated by the fact that the moments and their derivatives vary rapidly as function of the deformation, as observed in the numerical study of the overlap kernel in a wide range of deformations in ^{236}U. A quantitative information on the accuracy of our approximation as function of the first and second derivatives of second-order moment of the overlap has been given in the present paper for the scalar case. The Schrödinger equation is finally written in a convenient form that has the advantage of exhibiting typical terms occurring in the formalism such as the potential coupling and the dynamical coupling between intrinsic and collective excitations. There are a number of avenues that could be pursued now with this new formalism. Among them, the study of the fission dynamics and the coupling between intrinsic and collective excitations in the descent from saddle to scission represents one of the most challenging problems in many-body theory. Also, a particularly interesting use for this new approach is in those nuclei which exhibit excitation spectra showing collective as well as noncollective effects. This would surely improve the energies of the 0_2^+ states, which is one of the problems of collective models today. In all these studies, the microscopic nuclear wave function will be analyzed to determine the influence of the different degrees of freedom on nuclear properties. This would, of course, add to the computational burden, but the ingredients to perform the calculation are ready for the most part. We conclude this article by commenting briefly about the generality and potential of our model and applications we plan to explore in the future. We recall, first, that Eq. (40) gives the definition of our Schrödinger equation (SCIM) in terms of quantities that can be calculated with any choice of interaction under the condition that all matrix elements occurring in these quantities are well defined. One also can imagine using moments calculated with more sophisticated states than those considered in our study. For instance, one could use states generated with different projectors (projection on states with good particle number, projection of states with good parity, etc.). Another option would be to use the quasiparticle random-phase approximation (QRPA) correlated ground state in place of the Bogoliubov vacuum and to consider QRPA excitations instead of the simple free two-qp excitations. Of course, the direct use of Eq. (40) supposes that the approximations we made to invert the overlap kernel are still valid in those cases. Concerning future applications, in spectroscopy or fission studies, we will use the D1S density-dependent interaction [30,31], which we recall has the required properties of treating on the same footing the mean and pairing fields. In passing we note that this is an important feature since, as shown in Refs. [33,40], it avoids divergences in the evaluation of the Hamiltonian kernel with solutions projected on good particle number. Finally, since D1S is density dependent we are going to be confronted with the delicate problem of choosing a prescription to extend its definition and calculate matrix elements between two HFB solutions that are not only at different deformations but also between two different excitations as they occur in the present formalism. While prescriptions for the overlap between HFB states at different deformations with density-dependent interactions have been largely discussed in the literature (see, for instance, Refs. [41,42]), the added complexity of quasiparticle excitations in those states has not, and we will explore this question in a future publication. A more detailed discussion of the difficulties just mentioned is far beyond the scope of present paper, which is mainly concerned with deriving, in the framework of the GCM approach, a general form of a Schrödinger equation accounting for the coupling between collective and intrinsic degrees of freedom.

ACKNOWLEDGMENTS

The authors warmly thank J. F. Berger and N. Dubray for enlightening discussions and for very useful advice for the computational part. This work was performed in part under the auspices of the US Department of Energy by the Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Funding for this work was provided in part by the United States Department of Energy Office of Science, Nuclear Physics Program pursuant to Contract DE-AC52-07NA27344 Clause B-9999, Clause H-9999 and the American Recovery and Reinvestment Act, Pub. L. 111-5.

APPENDIX A: SYMMETRIC ORDERED PRODUCT OF OPERATORS

The symmetric ordered product of operators (SOPO) is defined by [27] (p. 421):

$$[A(q+s/2,q-s/2)P]^{(n)} = \frac{1}{2^n}\sum_{q=0}^{n} C_n^q P^{n-q} A(q+s/2,q-s/2)P^q, \quad \text{(A1)}$$

where A is any operator and P is the derivative operator $P = i\frac{\partial}{\partial \bar{q}}$. For instance, the first three SOPO are:

$$[AP]^{(0)} = A,$$
$$[AP]^{(1)} = \tfrac{1}{2}(AP + PA),$$
$$[AP]^{(2)} = \tfrac{1}{4}(AP^2 + 2PAP + P^2A),$$

where the action of PA on a vector $g(q)$ is

$$PAg(q) = A^{(1)}g(q) + APg(q), \quad \text{(A2)}$$

with $A^{(n)}$ defined as $A^{(n)} = (P^nA) = (i)^n\frac{\partial^n A}{\partial q^n}$. Let us note that for a Hermitian operator A, $A^{(n)}$ is Hermitian or anti-Hermitian according to the parity of n:

$$(A^{(n)})^+ = (-1)^n A^{(n)}.$$

For any operators A, B, and C, which depend on the collective variable q, we have the following properties:

(i) The symmetric ordered product is linear:

$$[AP]^{(n)} + [BP]^{(n)} = [(A+B)P]^{(n)}$$

(ii) The symmetric ordered product preserves the hermiticity:

$$A^+ = A \Rightarrow ([AP]^{(n)})^+ = [AP]^{(n)}$$
$$\begin{cases} A^+ = A \\ B^+ = B \end{cases} \Rightarrow ([AP]^{(n)}[BP]^{(q)})^+ = [BP]^{(q)}[AP]^{(n)}$$

(iii) More generally, the product of two and three SOPO can be expanded as a linear combination of symmetric ordered product. This property is used throughout the paper in the derivation of various expressions.

We give these expansions in a form convenient for retrieving the contribution of a SOPO of a given order

$$[AP]^{(n)}[BP]^{(q)} = \sum_{i=0}^{n+q}\frac{1}{2^i}\sum_{s=\max(0,i-q)}^{\min(n,i)} C_n^s C_q^{i-s}(-1)^{i-s}[A^{(i-s)}B^{(s)}P]^{(n+q-i)} \quad \text{(A3)}$$

$$[AP]^{(n)}[BP]^{(q)}[CP]^{(r)} = \sum_{p=0}^{n+q+r}\frac{(-1)^p}{2^p}\sum_{i=0}^{\min(p,q+r)}\sum_{t=\max(0,p-q-r)}^{\min(p-i,n)} C_n^t C_{q+r-i}^{p-i-t}(-1)^t \times [A^{(p-i-t)}F(B,C,r,i,t)P]^{(n+q+r-p)} \quad \text{(A4)}$$

with

$$F(B,C,r,i,t) = \sum_{s=\max(0,i-r)}^{\min(i,q)} (-1)^s C_q^s C_r^{i-s}(B^{(i-s)}C^{(s)})^{(t)}.$$

In particular, using (A4) with $n=0$, $q=1,2$, $r=0$ we find:

$$A[BP]^{(1)}C = [ABCP]^{(1)} + \tfrac{1}{2}(ABC^{(1)} - A^{(1)}BC)$$
$$A[BP]^{(2)}C = [ABCP]^{(2)} + [(ABC^{(1)} - A^{(1)}BC)P]^{(1)} + \tfrac{1}{4}(A^{(2)}BC - 2A^{(1)}BC^{(1)} + ABC^{(2)}). \quad \text{(A5)}$$

Formulas (A5) and (A4) are the formulas used to develop the formalism in terms of normalized moments. In fact, after setting

$$A = C = \frac{1}{\sqrt{N^{(0)}}}$$

we obtain

$$\frac{1}{\sqrt{N^{(0)}}}[BP]^{(1)}\frac{1}{\sqrt{N^{(0)}}} = [\bar{B}P]^{(1)} + \frac{i}{2}C^{(1)}(B,N^{(0)})$$
$$\frac{1}{\sqrt{N^{(0)}}}[BP]^{(2)}\frac{1}{\sqrt{N^{(0)}}} = [\bar{B}P]^{(2)} + iC^{(1)}(B,N^{(0)}) - C^{(2)}(B,N^{(0)}) \quad \text{(A6)}$$

with the definitions

$$C^{(1)}(A,N^{(0)}) = \frac{1}{\sqrt{N^{(0)}}}A\left(\frac{1}{\sqrt{N^{(0)}}}\right)' - \left(\frac{1}{\sqrt{N^{(0)}}}\right)'A\frac{1}{\sqrt{N^{(0)}}},$$
$$C^{(2)}(A,N^{(0)}) = \frac{1}{4}\left[\left(\frac{1}{\sqrt{N^{(0)}}}\right)''A\frac{1}{\sqrt{N^{(0)}}} + 2\left(\frac{1}{\sqrt{N^{(0)}}}\right)' \times A\left(\frac{1}{\sqrt{N^{(0)}}}\right)' + \frac{1}{\sqrt{N^{(0)}}}A\left(\frac{1}{\sqrt{N^{(0)}}}\right)''\right].$$

APPENDIX B: OVERLAP KERNEL

The matrix elements of the overlap kernel are expressed as $N_{ij}(q,q') = \langle\Phi_i(q)|\Phi_j(q')\rangle$, where $|\Phi_i(q)\rangle$ is defined by Eq. (22). More explicitly, their calculation involves quantities of the form

$$\langle\Phi(q)|\eta_{\bar{l}}^q\eta_k^q\eta_i^{+q'}\eta_{\bar{j}}^{+q'}|\Phi(q')\rangle. \quad \text{(B1)}$$

The calculation of the overlap kernel between two HF+BCS states at different deformations is detailed in Refs. [32,44]. We use the formalism in Refs. [32,44] because we are most familiar with it, but, of course, other derivations can be found elsewhere in the literature (e.g., Refs. [13,27,29,43] and references therein). For example, in Ref. [43] the generalized Wick's theorem for multiquasiparticle overlaps has been obtained out of the corresponding statistical version. In this latter reference, the contractions are given by compact expressions that can accommodate many quasiparticle excitations. It is worth stressing that the formalism given in Refs. [32,44] was developed especially for applications in fission, where we encounter configurations with very different shapes which require the use of single-particle bases with different basis parameters that are function of the deformation and possibly with different dimensions. These references provide a nontrivial extension of Wick's theorem and overlap formulas in this circumstance. We comment on this aspect briefly at the end of this Appendix.

Let us introduce the quantities "S, T, and Y" of Refs. [32,44]

$$\begin{aligned} S_{ij} &= \frac{\langle\Phi(q)|a_j^{+q'}a_i^{q'}|\Phi(q')\rangle}{\langle\Phi(q)|\Phi(q')\rangle},\\ T_{ij} &= \frac{\langle\Phi(q)|a_i^{+q'}a_j^{+q'}|\Phi(q')\rangle}{\langle\Phi(q)|\Phi(q')\rangle},\\ Y_{ij} &= \frac{\langle\Phi(q)|a_i^{q'}a_j^{q'}|\Phi(q')\rangle}{\langle\Phi(q)|\Phi(q')\rangle}, \end{aligned} \tag{B2}$$

where the particle operators $\{a_i^q, a_i^{+q}\}$ are related to the qp operators $\{\eta_i^q, \eta_i^{+q}\}$ through the BCS transformation:

$$\begin{cases} \eta_i^q = u_i^q a_i^q - v_i^q a_{\bar{i}}^{+q} \\ \eta_{\bar{i}}^{+q} = u_i^q a_{\bar{i}}^{+q} + v_i^q a_i^q \end{cases}. \tag{B3}$$

By means of Wick's theorem, Eq. (B1) is expressed in terms of

$$\begin{aligned} \langle\Phi(q)|\eta_i^{+q'}\eta_{\bar{j}}^{+q'}|\Phi(q')\rangle &= \langle\Phi(q)|\Phi(q')\rangle\big[u_i^{q'}u_j^{q'}T_{i\bar{j}} + u_i^{q'}v_j^{q'}S_{ji}\\ &\quad - v_i^{q'}u_j^{q'}(\delta_{ij} - S_{ij}) + v_i^{q'}v_j^{q'}Y_{j\bar{i}})\big],\\ \langle\Phi(q)|\eta_l^q\eta_k^q|\Phi(q')\rangle &= \langle\Phi(q)|\Phi(q')\rangle\sum_{pp'}\tau_{lp}^{qq'}\tau_{kp'}^{qq'}\big[u_l^q u_k^q Y_{\bar{p}p'}\\ &\quad - u_l^q v_k^q(\delta_{pp'} - S_{pp'}) + v_l^q u_k^q S_{p'p}\\ &\quad - v_l^q v_k^q T_{p\bar{p}'}\big], \end{aligned} \tag{B4}$$

where the transformation $\tau_{ij}^{qq'}$ is defined through the relation

$$a_j^{+q'} = \sum_{i=1}^{n}\tau_{ij}^{qq'}a_i^{+q}, \tag{B5}$$

where n is the dimension of the basis at deformation q. The different quantities in Eq. (B4) can be expressed as [32,44]:

$$\begin{aligned} \langle\Phi(q)|\Phi(q')\rangle &= \det(\tau^{qq'})\det(Z)\\ \delta_{ij} - S_{ij} &= (\tau^{qq'-1}u^q Z'^{-1}u^{q'})_{ij}\\ T_{i\bar{j}} &= (u^{q'}Z^{-1}v^q\tau^{qq'})_{ji}\\ Y_{i\bar{j}} &= -(\tau^{qq'-1}u^q Z'^{-1}v^{q'})_{ij}, \end{aligned} \tag{B6}$$

with $Z = u^q(\tau^+)^{-1}u^{q'} + v^q\tau v^{q'}$ and $Z' = u^{q'}(\tau)^{-1}u^q + v^{q'}\tau^+v^q$.

Note that Eq. (B5) is nothing more than the expansion of the single-particle basis at q' on the states of the basis at q. Since we do not use a complete basis in Eq. (B5), the matrix $\tau_{ij}^{qq'}$ is not a unitary transformation. As a consequence, note that it is the matrix inverse $\tau^{qq'-1}$ that appears in Eq. (B6) rather than its adjoint. It may also happen that the dimensions of the bases at q and q' are not the same. In that case, one can proceed as explained in Ref. [32], p. 1003.

APPENDIX C: CALCULATION OF $I + \hat{u}(q)$ AND RELATED QUANTITIES IN TERMS OF NORMALIZED MOMENTS

1. Calculation of $I + \hat{u}(q)$

According to Eq. (16), the operator $I + \hat{u}(q)$ is

$$\begin{aligned} I + \hat{u}(q) = I + \frac{1}{\sqrt{N^{(0)}(q)}}\bigg\{&[N^{(1)}(q)P]^{(1)}\\ &+ \frac{1}{2}[N^{(2)}(q)P]^{(2)}\bigg\}\frac{1}{\sqrt{N^{(0)}(q)}}. \end{aligned} \tag{C1}$$

By use of Eqs. (A5) and (A6), $\hat{u}(q)$ can be expressed, after straightforward calculations, as

$$\hat{u}(q) = C_N^+(q) + [W_N(q)P]^{(1)} + \tfrac{1}{2}[\bar{N}^{(2)}(q)P]^{(2)} \tag{C2}$$

with

$$\begin{aligned} W_N(q) &= \bar{N}^{(1)}(q) + iC^{(1)}(N^{(2)}, N^{(0)})\\ C_N^+(q) &= \tfrac{i}{2}C^{(1)}(N^{(1)}, N^{(0)}) - \tfrac{1}{2}C^{(2)}(N^{(2)}, N^{(0)}) \end{aligned}$$

and

$$\begin{aligned} C^{(1)}(A, N^{(0)}) &= \frac{1}{\sqrt{N^{(0)}(q)}}A\left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]'\\ &\quad - \left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]'A\frac{1}{\sqrt{N^{(0)}(q)}}\\ C^{(2)}(A, N^{(0)}) &= \frac{1}{4}\Bigg\{\left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]''A\frac{1}{\sqrt{N^{(0)}(q)}}\\ &\quad + 2\left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]'A\left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]'\\ &\quad + \frac{1}{\sqrt{N^{(0)}(q)}}A\left[\frac{1}{\sqrt{N^{(0)}(q)}}\right]''\Bigg\}. \end{aligned}$$

It is worth noticing that in the scalar case, the coefficient $C^{(1)}(A, N^{(0)})$ and $\bar{N}^{(1)}(q)$ are zero so that the operator u reduces to

$$\hat{u}(q) = -\tfrac{1}{2}C^{(2)}(N^{(2)}, N^{(0)}) + \tfrac{1}{2}[\bar{N}^{(2)}(q)P]^{(2)}.$$

2. Calculation of the operators $[I + \hat{u}(\bar{q})]^{1/2}$ and $[I + \hat{u}(\bar{q})]^{-1/2}$

For sake of simplicity, we restrict our discussion to the standard (one-dimensional) case. $\hat{J}_{1/2}(\bar{q})$ the square root of the operator $1 + \hat{u}(\bar{q})$ is approximated by the first terms of the series expansion up to the order $\hat{u}^2(\bar{q})$:

$$\hat{J}_{1/2}(\bar{q}) = [I + \hat{u}(\bar{q})]^{1/2} = 1 + \tfrac{1}{2}\hat{u}(\bar{q}) - \tfrac{1}{8}\hat{u}^2(\bar{q}) \quad \text{(C3)}$$

with

$$\hat{u}(\bar{q}) = \tfrac{1}{2}[\bar{N}^{(2)}(\bar{q})P]^{(2)}.$$

Using the property (A3), $[\hat{u}(\bar{q})]^2$ is

$$\hat{u}^2(\bar{q}) = \tfrac{1}{4}\big(\tfrac{1}{16}[\bar{N}^{(2)''}(\bar{q})]^2 + \tfrac{1}{2}[\{\bar{N}^{(2)''}(\bar{q})\bar{N}^{(2)}(\bar{q}) - 2[\bar{N}^{(2)'}(\bar{q})]^2\}P]^{(2)} + [[\bar{N}^{(2)}(\bar{q})]^2P]^{(4)}\big)$$

and the operator $\hat{J}_{1/2}(\bar{q})$ can be expressed in terms of SOPO as

$$\hat{J}_{1/2}(\bar{q}) = A_{1/2}(\bar{q}) + [B_{1/2}(\bar{q})P]^{(2)} + [C_{1/2}(\bar{q})P]^{(4)} \quad \text{(C4)}$$

with

$$\begin{cases} A_{1/2}(\bar{q}) = 1 - \frac{1}{2^9}[\bar{N}^{(2)''}(\bar{q})]^2 \\ B_{1/2}(\bar{q}) = \frac{1}{4}\big\{1 + \frac{1}{16}\bar{N}^{(2)''}(\bar{q}) - \frac{1}{8}\frac{[\bar{N}^{(2)'}(\bar{q})]^2}{\bar{N}^{(2)}(\bar{q})}\big\}\bar{N}^{(2)}(\bar{q}). \\ C_{1/2}(\bar{q}) = -\frac{1}{32}[\bar{N}^{(2)}(\bar{q})]^2 \end{cases} \quad \text{(C5)}$$

The same derivation applies for $\hat{J}_{-1/2}(\bar{q})$, the inverse of the root square of $1 + \hat{u}(\bar{q})$, which can be expressed as:

$$\begin{aligned}\hat{J}_{-1/2}(\bar{q}) &\equiv 1 - \tfrac{1}{2}\hat{u}(\bar{q}) + \tfrac{3}{8}\hat{u}^2(\bar{q}) \approx [I + \hat{u}(\bar{q})]^{-1/2} \\ &= A_{-1/2}(\bar{q}) + [B_{-1/2}(\bar{q})P]^{(2)} + [C_{-1/2}(\bar{q})P]^{(4)}\end{aligned}$$

with

$$\begin{cases} A_{-1/2}(\bar{q}) = 1 - \frac{3}{2^9}[\bar{N}^{(2)''}(\bar{q})]^2 \\ B_{-1/2}(\bar{q}) = -\frac{1}{4}\big\{1 + \frac{1}{16}\bar{N}^{(2)''}(\bar{q}) - \frac{3}{8}\frac{[\bar{N}^{(2)'}(\bar{q})]^2}{\bar{N}^{(2)}(\bar{q})}\big\}\bar{N}^{(2)}(\bar{q}). \\ C_{-1/2}(\bar{q}) = \frac{3}{32}[\bar{N}^{(2)}(\bar{q})]^2 \end{cases} \quad \text{(C6)}$$

3. Validity of the approximation used to calculate the operator $[I + \hat{u}(\bar{q})]^{1/2}$

The validity of the truncation made on the expansion of the square root of the overlap kernel $\hat{J}_{1/2}(\bar{q})$, Eq. (C3), is checked here, by estimating the extent to which the relation $[I + \hat{u}(\bar{q})]^{1/2}[I + \hat{u}(\bar{q})]^{1/2} = [I + \hat{u}(\bar{q})]$ is satisfied. In other words, using the expression of $[I + \hat{u}(\bar{q})]^{1/2}$ given in Eq. (C3), the residual $R(\bar{q})$ is defined by the relation

$$[I + \hat{u}(\bar{q})]^{1/2}[I + \hat{u}(\bar{q})]^{1/2} = [I + \hat{u}(\bar{q})] + R(\bar{q})$$

with

$$R(\bar{q}) = -\tfrac{1}{8}[\hat{u}(\bar{q})]^3 + \tfrac{1}{64}[\hat{u}(\bar{q})]^4.$$

Consistently with the truncations made in Sec. II, the residual $R(\bar{q})$ is restricted to its lower orders in its development in symmetric ordered products. Thus $R(\bar{q})$ is

$$R(\bar{q}) = A(\bar{q}) + \tfrac{1}{2}[C(\bar{q})\bar{N}^{(2)}(\bar{q})P]^{(2)}.$$

Neglecting the derivatives $[\bar{N}^{(2)}(\bar{q})]^{(p)}$ for $p > 2$, after tedious but straightforward calculations using Eqs. (A3) and (A4), the coefficients $A(\bar{q})$ and $C(\bar{q})$ are

$$\begin{aligned} A(\bar{q}) &= \frac{-3}{2^{11}}[\bar{N}^{(2)''}(\bar{q})]^3 + \frac{73}{2^{18}}[\bar{N}^{(2)''}(\bar{q})]^4, \\ C(\bar{q}) &= \frac{-1}{2^9}\left\{9[\bar{N}^{(2)''}(\bar{q})]^2 + 32\frac{\bar{N}^{(2)''}(\bar{q})[\bar{N}^{(2)'}(\bar{q})]^2}{\bar{N}^{(2)}(\bar{q})}\right\} \\ &\quad + \frac{5}{2^{13}}\left\{34\frac{[\bar{N}^{(2)''}(\bar{q})]^2[\bar{N}^{(2)'}(\bar{q})]^2}{\bar{N}^{(2)}(\bar{q})} + [\bar{N}^{(2)''}(\bar{q})]^3\right\}. \end{aligned}$$

The smaller the residual $R(\bar{q})$, and, by extension, $A(\bar{q})$ and $C(\bar{q})$, the best the approximation. In particular, we find $A(\bar{q}) = C(\bar{q}) = 0$ for $\bar{N}^{(2)''}(\bar{q}) = 0$. Similar conclusions are found for $\hat{J}_{-1/2}(\bar{q})$.

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