Anharmonicities of nuclear vibrations from periodic mean-field orbits

A. Abada and D. Vautherin
Division de Physique Théorique, Institut de Physique Nucléaire, F-91406, Orsay CEDEX, France
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A new method for constructing periodic orbits of the time-dependent Hartree-Fock equations is proposed. It is based on a perturbative expansion in the amplitude of the collective vibration. We present applications to the case of octupole vibrations in ^{16}O and ^{40}Ca. From calculations performed up to second order we determine the splitting of the two-phonon states. We discuss the problems which, for the quadrupole mode, arise from a resonant coupling of the vibration with states of the continuum.

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I. INTRODUCTION

The experimental discovery of high-energy structures in heavy-ion grazing collisions and their interpretation in terms of multiphonon excitations of giant quadrupole resonances [1] has renewed interest in the descriptions of collective motions with more general scope than the usual random-phase approximation (RPA). In the past, the problem of large-amplitude collective vibrations has been approached along different lines. Among the most popular, one can mention the adiabatic time-dependent Hartree-Fock method [2,3], the generator coordinate method [4], and the boson expansion method [4,5]. A basic tool of the first two approaches is the so-called collective path, which specifies the nature of the collective motion. Although it can in principle be determined self-consistently [2], it is often generated by a constrained Hartree-Fock calculation using a constraining operator chosen *a priori*. In the boson-expansion method the lowest order is generated by solving the RPA equations, which yield a set of noninteracting RPA bosons in this order. Subsequent corrections lead to anharmonic and interaction terms between the bosons.

In the present article we present a method based on an explicit construction of finite-amplitude periodic orbits of the time-dependent Hartree-Fock (TDHF) equations. The question of the existence of these solutions has raised much interest, because of the analogy with classical mechanics [6]. Their importance has been recognized in various contexts, especially in studies of nuclear collective motion [7–9] (our purpose), in the requantization problem [10–12], and in the determination of corrections to TDHF by means of time-dependent Feynman diagrams [13]. Their central role was already emphasized by Poincaré who noted that [14,15] "What renders these periodic solutions so precious to us is that they are, so to speak, the only breach through which we might try to penetrate into a stronghold, hitherto reputed inaccessible."

The construction of periodic TDHF orbits is a difficult task [7], which has been carried out only in simple cases such as monopole oscillations [8]. The method presented here is more general and can be applied to collective oscillations of any given multipolarity. It relies on an expansion in the amplitude of the collective vibration. Since in lowest order it reduces to the RPA approximation, it bears some similarity with the boson-expansion approach mentioned above. The higher-order terms provide anharmonic corrections to the RPA. It is also analogous to the expansion methods which, in celestial mechanics, are used to construct periodic trajectories as power series in the amplitude of the motion [14]. Although in this paper we restrict ourselves to the study of the TDHF equations, we believe our method to be applicable to any time-dependent self-consistent equation displaying periodic solutions. As an example, periodic orbits of the breathing mode in the Skyrme model [16] are under investigation and will be the subject of a forthcoming publication [17].

The present article is organized as follows. In Sec. II we review the main properties of the TDHF equations and of their periodic orbits. Section III explains how one can build periodic orbits by means of a Taylor expansion in their amplitudes. Explicit expressions are presented up to third order. In Sec. IV, we specialize the equations to the case of the Skyrme interaction, for which more explicit formulas are provided. Section V deals with the problem of performing an angular momentum reduction of the corresponding equations, which is especially important in numerical applications. We show that the usual angular reduction of the RPA matrix can still be used to simplify calculations of higher orders. In Sec. VI, using a semiclassical quantization of these periodic orbits we calculate actual nuclear collective spectra. In the same section we indicate how this procedure can be used to evaluate the splitting of two-phonon states. Section VII presents our results concerning octupole modes in ^{16}O and ^{40}Ca. In Sec. VIII we describe a method suitable to handle the problems arising when a resonant coupling occurs between the vibration and states of the continuum. Results are given in the case of quadrupole modes in ^{40}Ca. Section IX contains our main conclusions.

II. PERIODIC ORBITS OF THE MEAN-FIELD EQUATIONS

Within the time-dependent Hartree-Fock (TDHF) approximation the many-body wave function $\Psi(t)$ is taken as a Slater determinant for all times. The associated

one-body density matrix $\rho(t)$, which is Hermitian, satisfies the conditions

$$\mathrm{Tr}\rho(t)=A \ , \tag{2.1a}$$

$$\rho^2(t)=\rho(t) \ , \tag{2.1b}$$

where A is the number of particles. Its time evolution is given by

$$i\hbar\dot{\rho}(t)=[W(t),\rho(t)] \ , \tag{2.2}$$

where $W(t)$ is the mean-field Hamiltonian, $W(t)=\delta E/\delta\rho$, E being the Hartree-Fock energy $E=\langle\Psi|H|\Psi\rangle$.

In what follows we construct solutions of Eq. (2.2) such that $\rho(t)=\rho(t+T)$, where T is the period. The single-particle states $|h(t)\rangle$, which are solutions of the time-dependent mean-field equations,

$$i\hbar\frac{\partial}{\partial t}|h(t)\rangle=W(t)|h(t)\rangle \ , \tag{2.3}$$

are not periodic, but quasiperiodic:

$$|h(t+T)\rangle=e^{-i\theta_h}|h(t)\rangle \ , \tag{2.4}$$

where θ_h is the so-called Floquet-Lyapounov phase. In the following it will be convenient to use the periodic part $|h^P(t)\rangle$ of $|h(t)\rangle$ which we define as

$$|h^P(t)\rangle=\exp\left[i\frac{e_h t}{\hbar}\right]|h(t)\rangle \ , \tag{2.5}$$

where $e_h=\theta_h\hbar/T$. The states $|h^P(t)\rangle$ satisfy a modified evolution equation, namely,

$$i\hbar\frac{\partial}{\partial t}|h^P(t)\rangle=[W(t)-e_h]|h^P(t)\rangle \ . \tag{2.6}$$

Of course phases disappear in the expression of the one-body density matrix,

$$\rho(t)=\sum_h|h(t)\rangle\langle h(t)|=\sum_h|h^P(t)\rangle\langle h^P(t)| \ , \tag{2.7}$$

where the sum is over the occupied states.

III. PERTURBATIVE CONSTRUCTION OF PERIODIC ORBITS

We look for solutions of the time-dependent mean-field equation [Eq. (2.2)] in the form

$$\rho(t)=\rho_0+\epsilon\rho_1\left[\frac{\omega}{\omega_0}t\right]+\epsilon^2\rho_2\left[\frac{\omega}{\omega_0}t\right]+\epsilon^3\rho_3\left[\frac{\omega}{\omega_0}t\right]+\cdots \ . \tag{3.1}$$

In the expansion (3.1) we use $\omega t/\omega_0$ as the argument of the functions $\rho_1,\rho_2,\rho_3,\ldots$. This is a standard technique introduced in the theory of nonlinear oscillations [19] to take into account the dependence of the frequency ω on the amplitude ϵ of the periodic orbit:

$$\omega=\omega_0+\epsilon\omega_1+\epsilon^2\omega_2+\cdots \ . \tag{3.2}$$

Similarly we expand the mean-field Hamiltonian $W(\rho)$ in the form

$$W(\rho)=W_0+\epsilon W_1+\epsilon^2W_2+\epsilon^3W_3+\cdots \ . \tag{3.3}$$

To zeroth order in ϵ we find that ρ_0 is the static Hartree-Fock solution satisfying

$$[W_0,\rho_0]=0 \ , \tag{3.4}$$

with the conditions $\rho_0^2=\rho_0$ and $\mathrm{Tr}\rho_0=A$.

To first order in ϵ we obtain for ρ_1 the following linearized mean field (or RPA) equation:

$$i\hbar\dot{\rho}_1=\mathcal{M}\rho_1 \ , \tag{3.5}$$

with

$$\mathcal{M}\rho_1\equiv[W_0,\rho_1(t)]+[W_1(t),\rho_0] \ . \tag{3.6}$$

This equation is solved via the usual ansatz [4]

$$\rho_1(t)=\eta e^{+i\omega_0 t}+\eta^+e^{-i\omega_0 t} \ , \tag{3.7}$$

where η is a time-independent operator which is a solution of the static RPA equations. We have adopted the standard normalization $\mathrm{Tr}\eta_n^+[\rho_0,\eta_m]=\delta_{nm}|\omega_{0n}|/\omega_{0n}$ [4].

Note that the condition $\rho^2=\rho$ [Eq. (2.1b)], to first order in ϵ, reads

$$\rho_0\rho_1+\rho_1\rho_0=\rho_1 \ . \tag{3.8}$$

If we denote $|p\rangle$ and $|h\rangle$ the particle and hole states relative to ρ_0 defined by

$$\rho_0|p\rangle=0,\rho_0|h\rangle=|h\rangle,W_0|h\rangle=e_h|h\rangle,W_0|p\rangle=e_p|p\rangle \ ,$$

then Eq. (3.8) implies that

$$\langle p|\rho_1|p'\rangle=\langle h|\rho_1|h'\rangle=0 \ .$$

Equation (3.8) also implies $\mathrm{Tr}\rho_1=0$ which ensures that particle number is unchanged in first order.

Let us now consider Eq. (2.2) in second order; it reads

$$i\hbar\dot{\rho}_2(t)=[W_0,\rho_2(t)]+[W_2(t),\rho_0]+[W_1(t),\rho_1(t)]-i\hbar\frac{\omega_1}{\omega_0}\dot{\rho}_1(t) \ . \tag{3.9}$$

Moreover, the physical solution of this evolution equation must preserve the condition $\rho^2=\rho$ in second order; i.e.,

$$\rho_2=\rho_0\rho_2+\rho_2\rho_0+\rho_1^2 \ .$$

The particle-hole matrix elements of this last equation are trivially satisfied, while the particle-particle and hole-hole matrix elements turn out to be completely determined by $\rho_1(t)$:

$$\langle p|\rho_2(t)|p'\rangle=\sum_h\langle p|\rho_1(t)|h\rangle\langle h|\rho_1(t)|p'\rangle \ , \tag{3.10a}$$

$$\langle h|\rho_2(t)|h'\rangle=-\sum_p\langle h|\rho_1(t)|p\rangle\langle p|\rho_1(t)|h'\rangle \ . \tag{3.10b}$$

These equations are consistent with the evolution equa-

tion (3.9). Indeed using the RPA equation (3.5) one can check that the particle-particle and hole-hole matrix elements of the right-hand side of (3.9) are identical to the time derivatives of Eqs. (3.10). Equation (3.10), which also implies that $\mathrm{Tr}\rho_2=0$, ensures particle number conservation in second order.

Therefore, the novel information contained in Eq. (3.9) concerns only the particle-hole and hole-particle matrix elements of ρ_2. We obtain their time-evolution by projecting Eq. (3.9) on this subspace with the result

$$(i\hbar\partial_t-\mathcal{M})\rho_2(t)=[W_1(t),\rho_1(t)]+[W_2'(t),\rho_0]-i\hbar\frac{\omega_1}{\omega_0}\dot{\rho}_1(t)\ . \tag{3.11}$$

In Eq. (3.11) $\mathcal{M}$ is the RPA matrix defined above. The operator W_2' is that part of W_2 which originates from the particle-particle and hole-hole matrix elements of ρ_2. For a density-independent interaction it is (the sum over repeated indices being implicit)

$$\langle p|W_2'|h\rangle=\frac{\delta^2E}{\delta\rho_{ph}\delta\rho_{p'p''}}\langle p'|\rho_2|p''\rangle+\frac{\delta^2E}{\delta\rho_{ph}\delta\rho_{h'h''}}\langle h'|\rho_2|h''\rangle\ . \tag{3.12}$$

Because of Eq. (3.10) W_2' is completely determined from the knowledge of ρ_1. In contrast, the remaining term in W_2, $[\delta^2E/(\delta\rho_{ph}\delta\rho_{p'h'})]\langle p'|\rho_2|h'\rangle$, involves the unknown matrix elements of ρ_2 and thus contributes to the matrix $\mathcal{M}$ on the left-hand side of Eq. (3.11).

The inhomogeneous linear equation (3.11) can be solved only when the right-hand side has no component on the zero modes of the operator $(i\hbar\partial_t-\mathcal{M})$. This is the case for the first two terms, whose time dependences are $e^{\pm 2i\omega_0 t}$ or 1 (see, however, Sec. VIII for an exception), but not for the last term since $i\dot{\rho}_1/\omega_0=\eta^+e^{-i\omega_0 t}-\eta e^{+i\omega_0 t}$ is just a sum of two zero modes. Thus the linear equation can only be solved if

$$\omega_1=0\ . \tag{3.13}$$

Therefore, the equation defining $\rho_2(t)$ reduces to

$$(i\hbar\partial_t-\mathcal{M})\rho_2(t)=[W_1(t),\rho_1(t)]+[W_2'(t),\rho_0]\ . \tag{3.14}$$

Let us now consider Eq. (2.2) in third order:

$$i\hbar\dot{\rho}_3(t)=[W_0,\rho_3(t)]+[W_3(t),\rho_0]+[W_1(t),\rho_2(t)]+[W_2(t),\rho_1(t)]-i\hbar\frac{\omega_2}{\omega_0}\dot{\rho}_1(t)\ . \tag{3.15}$$

In order to preserve the condition $\rho^2=\rho$ in third order we must have $\rho_3=\rho_0\rho_3+\rho_3\rho_0+\rho_1\rho_2+\rho_2\rho_1$. As above, it can be shown that this equation determines the particle-particle and hole-hole matrix elements of ρ_3 in terms of ρ_2 and ρ_1:

$$\langle p|\rho_3(t)|p'\rangle=\sum_h[\langle p|\rho_1(t)|h\rangle\langle h|\rho_2(t)|p'\rangle+\langle p|\rho_2(t)|h\rangle\langle h|\rho_1(t)|p'\rangle]\ , \tag{3.16a}$$

$$\langle h|\rho_3(t)|h'\rangle=-\sum_p[\langle h|\rho_1(t)|p\rangle\langle p|\rho_2(t)|h'\rangle+\langle h|\rho_2(t)|p\rangle\langle p|\rho_1(t)|h'\rangle]\ . \tag{3.16b}$$

Again one checks that Eqs. (3.16) are consistent with the evolution equation (3.15) and that $\mathrm{Tr}\rho_3=0$. The particle-hole matrix elements are solutions of the following equation:

$$(i\hbar\partial_t-\mathcal{M})\rho_3(t)=[W_1(t),\rho_2(t)]+[W_2(t),\rho_1(t)]+[W_3'(t),\rho_0]-i\hbar\frac{\omega_2}{\omega_0}\dot{\rho}_1(t)\ , \tag{3.17}$$

where W_3' is given (for a density-independent interaction) by

$$\langle p|W_3'|h\rangle=\frac{\delta^2E}{\delta\rho_{ph}\delta\rho_{p'p''}}\langle p'|\rho_3|p''\rangle+\frac{\delta^2E}{\delta\rho_{ph}\delta\rho_{h'h''}}\langle h'|\rho_3|h''\rangle\ . \tag{3.18}$$

By requiring the source term of Eq. (3.17) to be orthogonal to the vector $\eta e^{i\omega_0 t}(\eta^+e^{-i\omega_0 t})$ we determine the second-order correction to the frequency

$$\omega_2=\omega_0\frac{\int_0^T dt\,\mathrm{Tr}(([W_1,\rho_2]+[W_2,\rho_1]+[W_3',\rho_0])[\rho_0,\rho_1])}{\int_0^T dt\,\mathrm{Tr}(i\hbar\dot{\rho}_1[\rho_0,\rho_1])}\ . \tag{3.19}$$

Formulas for higher-order corrections to the frequency and the density can be derived along similar steps. Although straightforward the calculations already become rather cumbersome at fourth order. For this reason, applications presented in this work are restricted to studies in second order for ω and in third order for ρ.

IV. THE CASE OF A SIMPLIFIED SKYRME FORCE

For a symmetric, spin and isospin saturated nucleus, the energy density $H(r,t)$ calculated with a Skyrme interaction in the mean-field approximation reads

$$H(\mathbf{r},t)=\frac{\hbar^2}{2m}\tau+\frac{3}{8}t_0\rho^2+\frac{1}{16}t_3\rho^3+\frac{1}{16}(3t_1+5t_2)\rho\tau+\frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2-\frac{3}{4}w_0\rho\nabla\cdot J\ . \tag{4.1}$$

In Eq. (4.1) τ and J are respectively the kinetic-energy density and the spin density:

$$\tau(\mathbf{r},t)=\sum_{h,\sigma}|\nabla\langle\mathbf{r},\sigma|h(t)\rangle|^2\ , \tag{4.2a}$$

$$J(\mathbf{r},t)=-i\sum_{h,\sigma,\sigma'}\langle h(t)|\mathbf{r},\sigma\rangle[\nabla\langle\mathbf{r},\sigma'|h(t)\rangle\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle]\ . \tag{4.2b}$$

For simplicity we consider forces with $3t_1+5t_2=0$, i.e., such that the $\rho\tau$ does not appear in the energy density. In this case, the effective mass is equal to unity. Such forces are adequate for the purpose of our study. They are indeed simple and still general enough to allow a correct description of the collective vibrations we wish to investigate.

The mean-field potential reads [4,20,21] $W(\mathbf{r},t)=-(\hbar^2/2m)\Delta+U(\mathbf{r},t)$ with

$$U(\mathbf{r},t)=V(\mathbf{r},t)+u(\mathbf{r},t)\cdot(-i)(\nabla\times\sigma)\ , \tag{4.3}$$

where

$$V(\mathbf{r},t)=\frac{3}{4}t_0\rho+\frac{3}{16}t_3\rho^2-\frac{\hbar^2}{2m}\lambda\Delta\rho-\frac{3}{4}w_0\nabla\cdot J \tag{4.4a}$$

$$\mathbf{u}(\mathbf{r},t)=\frac{3}{4}w_0\nabla\rho+\frac{1}{16}(t_1-t_2)J\ . \tag{4.4b}$$

The quantity λ appearing in this equation is the combination

$$\lambda\equiv\frac{2m}{\hbar^2}\frac{1}{32}(9t_1-5t_2)\ . \tag{4.5}$$

The contribution to $\mathbf{u}$ arising from the last term in Eq. (4.4b) has been omitted in our calculations since it is known to produce negligible effects [20].

The explicit expressions of the potentials $W_i(\mathbf{r},t)$ appearing in Eq. (3.3) are

$$W_0(\mathbf{r})=\frac{-\hbar^2}{2m}\Delta+\left[\frac{3}{4}t_0+\frac{3}{16}t_3\rho_0(r)-\frac{\hbar^2}{2m}\lambda\Delta\right]\rho_0(\mathbf{r})+\frac{3}{4}w_0\nabla\rho_0\cdot(-i)(\nabla\times\sigma)\ , \tag{4.6}$$

$$W_1(\mathbf{r},t)=\left[\frac{3}{4}t_0+\frac{3}{8}t_3\rho_0(\mathbf{r})-\frac{\hbar^2}{2m}\lambda\Delta\right]\rho_1(\mathbf{r},t)\ , \tag{4.7a}$$

$$W_2(\mathbf{r},t)=\left[\frac{3}{4}t_0+\frac{3}{8}t_3\rho_0(\mathbf{r})-\frac{\hbar^2}{2m}\lambda\Delta\right]\rho_2(\mathbf{r},t)+\frac{3}{16}t_3\rho_1^2(\mathbf{r},t)\ , \tag{4.7b}$$

$$W_3(\mathbf{r},t)=\left[\frac{3}{4}t_0+\frac{3}{8}t_3\rho_0(\mathbf{r})-\frac{\hbar^2}{2m}\lambda\Delta\right]\rho_3(\mathbf{r},t)+\frac{3}{8}t_3\rho_1(\mathbf{r},t)\rho_2(\mathbf{r},t)\ . \tag{4.7c}$$

In these equations we have used the notation $\rho_i(\mathbf{r},t)=\langle\mathbf{r}|\rho_i(t)|\mathbf{r}\rangle$.

For Skyrme forces the source terms in the inhomogeneous equations defining the higher-order density matrices [cf. Eqs. (3.11), (3.17)] are more complicated because additional terms arise from the density dependence of the interaction. Explicitly one finds in second order

$$W_2'(\mathbf{r},t)=\left.\frac{dU}{d\rho}\right|_{\rho=\rho_0}\langle\mathbf{r}|(1-2\rho_0)\rho_1^2|\mathbf{r}\rangle+\frac{1}{2}\left.\frac{d^2U}{d\rho^2}\right|_{\rho=\rho_0}\rho_1^2(\mathbf{r},t)\ . \tag{4.8}$$

In third order the result is

$$W_3'(\mathbf{r},t)=\left.\frac{dU}{d\rho}\right|_{\rho=\rho_0}\langle\mathbf{r}|(1-2\rho_0)(\rho_1\rho_2+\rho_2\rho_1)|\mathbf{r}\rangle+\left.\frac{d^2U}{d\rho^2}\right|_{\rho=\rho_0}\rho_1(\mathbf{r},t)\rho_2(\mathbf{r},t)\ . \tag{4.9}$$

(See Appendix A for a derivation of these two formulas).

For more general Skyrme forces it is a straightforward, although a tedious task, to construct the potentials W_i. One complication is that, in this case, the potentials W_i include momentum operators.

V. REDUCTION OF THE ANGULAR VARIABLES

In the case of doubly-closed-shell nuclei one can simplify the evolution equations by introducing an angular decomposition. Let us begin with the static HF equations [see Eq. (3.4)]. We write the single-particle orbitals as

$$\langle\mathbf{r}|a\rangle=R_{\alpha_a}(r)\mathcal{Y}_{l_aj_am_a}(\hat{\mathbf{r}},\sigma)\chi_q(\tau)\ , \tag{5.1}$$

where $\mathcal{Y}$ is the usual angular wave function of particles with spin $\frac{1}{2}$ [see Eq. (2.15) of Ref. [4]] and where the index a stands for a particle (p) or hole (h) state index. We have also introduced the notation $\alpha_a\equiv(q_a,n_a,l_a,j_a)$, where q is the isospin, n the principal quantum number, l the orbital angular momentum, j the total angular momentum, and m_a the magnetic quantum number. The static density $\rho_0(\mathbf{r})$ depends on the radial coordinate r only:

$$\rho_0(r)=\frac{1}{4\pi}\sum_{\alpha_h}(2j_{\alpha_h}+1)R_{\alpha_h}^2(r)\ . \tag{5.2}$$

The same property holds for the average nuclear potential $W_0(\mathbf{r})$.

In first order the procedure is also standard. We first rewrite the RPA equation (3.5) in a form which exhibits its symplectic structure, namely,

$$i\hbar\partial_t\begin{bmatrix}Z\\Z^*\end{bmatrix}=\begin{bmatrix}A&B\\-B^*&-A^*\end{bmatrix}\begin{bmatrix}Z\\Z^*\end{bmatrix}\ , \tag{5.3}$$

where Z is the vector whose components are the particle-hole matrix elements of ρ_1, i.e., $Z_{ph}=\langle p|\rho_1|h\rangle$. To exploit rotational invariance we couple particle and hole states to a total angular momentum L, and use the following vectors:

$$Z^{LM}_{\alpha_p\alpha_h}=\sum_{m_pm_h}(-1)^{m_p-1/2}\begin{pmatrix}j_p&j_h&L\\-m_p&m_h&M\end{pmatrix}Z_{ph}\ . \tag{5.4}$$

In terms of these quantities $\rho_1(r,t)$ can be expressed as

$$\rho_1(\mathbf{r},t)=\frac{\hat{L}}{\sqrt{4\pi}}\sum_{\alpha_p\alpha_h}F^L_{\alpha_p\alpha_h}R_{\alpha_p}(r)R_{\alpha_h}(r)\times(Z^{LM}_{\alpha_p\alpha_h}Y_{LM}(\theta,\phi)+\text{c.c.})\ , \tag{5.5}$$

where $\hat{L}$ stands for $\sqrt{(2L+1)}$ and F is a combination of Clebsch-Gordan coefficients and 6-j symbol given by

$$F^{l}_{\alpha_p\alpha_h}=\hat{l}_p\hat{l}_h\hat{j}_p\hat{j}_h \begin{bmatrix} l_p & l_h & l \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} j_p & j_h & l \\ l_h & l_p & \frac{1}{2} \end{Bmatrix} .$$

The quantities $Z^{LM}_{\alpha_p\alpha_h}$ are solutions of RPA equations similar to (5.3) with matrices A and B replaced by $A^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}$ and $B^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}$ (see Appendix B) given by

$$B^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}=\frac{1}{4\pi}C_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}F^{L}_{\alpha_p\alpha_h}F^{L}_{\alpha_{p'}\alpha_{h'}} , \tag{5.6a}$$

$$A^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}=(e_{\alpha_p}-e_{\alpha_h})\delta_{\alpha_p\alpha_{p'}}\delta_{\alpha_h\alpha_{h'}}+B^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}} . \tag{5.6b}$$

The matrices being M independent, the solutions will be $(2L+1)$-fold degenerate. In these equations, e_{α_a} is the Hartree-Fock energy of the single-particle orbit a and C is the radial matrix element

$$C_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}} =\int_0^\infty R_{\alpha_p}(r)R_{\alpha_h}(r)\frac{dU}{d\rho}\bigg|_{\rho=\rho_0}R_{\alpha_{p'}}(r)R_{\alpha_{h'}}(r)r^2dr , \tag{5.7}$$

where $R_\alpha(r)$ is normalized to unity with the weight r^2dr. For the Skyrme force considered it is

$$C^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}=\int_0^\infty r^2dr\,R_{\alpha_p}(r)R_{\alpha_h}(r)\left[\frac{3}{4}t_0+\frac{3}{8}t_3\rho_0(r)-\frac{\hbar^2}{2m}\lambda\left[\frac{1}{r}\frac{d^2}{dr^2}r-\frac{l(l+1)}{r^2}\right]\right]R_{\alpha_{p'}}(r)R_{\alpha_{h'}}(r) . \tag{5.8}$$

If we now consider the second-order evolution equation we find that the angular components $\rho_2^{L'M'}$ of ρ_2, defined as in Eq. (5.4), satisfy

$$\left[i\hbar\partial_t-\begin{bmatrix} A^{L'} & B^{L'} \\ -B^{*L'} & -A^{*L'} \end{bmatrix}\right]\begin{bmatrix} \rho_2^{L'M'} \\ (-1)^{M'}\rho_2^{*L'-M'} \end{bmatrix}=\begin{bmatrix} S_2^{L'M'} \\ -(-1)^{M'}S_2^{*L'-M'} \end{bmatrix} . \tag{5.9}$$

Let us now investigate the angular momentum structure of the source term S_2. For this purpose we first note that the angular components of the product of two operators O_1,O_2 are given by the formula

$$(O_1O_2)^{L'M'}_{\alpha_p\alpha_h}=\sum_{\alpha_aL_1M_1L_2M_2}(-1)^{M'+j_{\alpha_p}+j_{\alpha_h}+j_{\alpha_a}}(2L_1+1)(2L_2+1)\begin{bmatrix} L_1 & L_2 & L' \\ M_1 & M_2 & -M' \end{bmatrix}\begin{Bmatrix} L_1 & L_2 & L' \\ j_{\alpha_h} & j_{\alpha_p} & j_{\alpha_a} \end{Bmatrix}O^{L_1M_1}_{1\alpha_p\alpha_a}O^{L_2M_2}_{2\alpha_a\alpha_h} . \tag{5.10}$$

Because W_1 has the angular components

$$W^{LM}_{1\alpha_p\alpha_h}=\sum_{\alpha_{p'}\alpha_{h'}}B^{L}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}[\rho^{LM}_{1\alpha_{p'}\alpha_{h'}}+(-1)^M\rho^{*L-M}_{1\alpha_{p'}\alpha_{h'}}] , \tag{5.11}$$

the source term $[W_1,\rho_1]$ in Eq. (3.9) contains even values L' of the angular momentum running from 0 to $2L$ for a collective mode of angular momentum L. By using Eq. (5.10) we obtain

$$[W_1,\rho_1]^{(LL)L'}_{\alpha_p\alpha_h}=\hat{L}^4\begin{bmatrix} L & L & L' \\ 0 & 0 & 0 \end{bmatrix}\left[\sum_{\alpha_{p'}\alpha_h\alpha_{p''}}(-1)^{j_p+j_h+j_{p''}+1/2}\begin{Bmatrix} L & L & L' \\ j_h & j_p & j_{p''} \end{Bmatrix}B^{L}_{\alpha_p\alpha_{p''}\alpha_{p'}\alpha_{h'}}(\rho^{L}_{1\alpha_{p'}\alpha_{h'}}+\text{c.c.})\rho^{L}_{1\alpha_{p''}\alpha_h}\right.$$
$$\left.-\sum_{\alpha_{p'}\alpha_h\alpha_{h''}}(-1)^{j_p+j_h+j_{h''}+1/2}\begin{Bmatrix} L & L & L' \\ j_p & j_h & j_{h''} \end{Bmatrix}B^{L}_{\alpha_{h''}\alpha_h\alpha_{p'}\alpha_{h'}}(\rho^{L}_{1\alpha_{p'}\alpha_{h'}}+\text{c.c.})\rho^{L}_{1\alpha_p\alpha_{h''}}\right] . \tag{5.12}$$

For the term $[W_2',\rho_0]$ we also have $L'=0,2,\ldots,2L$ with

$$W'^{L'M'}_{2\alpha_p\alpha_h}=\sum_{\alpha_{p'}\alpha_{p''}}B^{L'}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{p''}}(\rho_1^2)^{L'M'}_{\alpha_{p'}\alpha_{p''}}-\sum_{\alpha_{h'}\alpha_{h''}}B^{L'}_{\alpha_p\alpha_h\alpha_{h'}\alpha_{h''}}(\rho_1^2)^{L'M'}_{\alpha_{h'}\alpha_{h''}}$$
$$+\frac{1}{2}\sum_{m_pm_h}(-1)^{m_p-1/2}\begin{bmatrix} j_p & j_h & L' \\ -m_p & m_h & M' \end{bmatrix}\int d^3r\langle p|\mathbf{r}\rangle\langle\mathbf{r}|h\rangle\frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0}\rho_1^2(\mathbf{r},t) \tag{5.13}$$

where $\rho_1(\mathbf{r},t)$ is defined in (5.5). Consequently, ρ_2 contains also the same values of the angular momentum. Explicitly $\rho_2(r,t)$ can be written as

$$\rho_2(\mathbf{r},t)=\sum_{L'=0}^{2L}\sum_{M'=-L'}^{L'}\rho_2^{L'M'}(\mathbf{r},t) , \tag{5.14}$$

with

$$\rho_2^{L'M'}(r,t)=\frac{\hat{L}'}{\sqrt{4\pi}}Y_{L'M'}\left[\sum_{\alpha_p\alpha_h}F^{L'}_{\alpha_p\alpha_h}R_{\alpha_p}(r)R_{\alpha_h}(r)[\rho^{L'M'}_{2\alpha_p\alpha_h}+(-1)^{M'}\rho^{*L'-M'}_{2\alpha_p\alpha_h}]\right.$$
$$\left.+\sum_{\alpha_p\alpha_{p'}}F^{L'}_{\alpha_p\alpha_{p'}}R_{\alpha_p}(r)R_{\alpha_{p'}}(r)(\rho_1^2)^{L'M'}_{\alpha_p\alpha_{p'}}-\sum_{\alpha_h\alpha_{h'}}F^{L'}_{\alpha_h\alpha_{h'}}R_{\alpha_h}(r)R_{\alpha_{h'}}(r)(\rho_1^2)^{L'M'}_{\alpha_h\alpha_{h'}}\right] . \quad (5.15)$$

The fact that the source term and ρ_2 contain components of all the even angular momentum between 0 and $2L$ reflects the splitting of two-phonon states. This point will be further elaborated below.

VI. QUANTIZATION

How periodic orbits of the time-dependent Hartree-Fock equations can be used to construct the energies of many-body systems has been described by several authors. The standard procedure relies on the semiclassical quantization rule [6,10–12]. One looks for periodic solutions such that the mean-field action I along a periodic orbit $\rho(t)$,

$$I=\sum_h\int_0^T dt\left[\langle h(t)|i\hbar\frac{\partial}{\partial t}|h(t)\rangle-e_h\right] , \quad (6.1)$$

is equal to an integer multiple of the Planck constant: $I=nh$. In Eq. (6.1) the summation runs over the quasiperiodic single-particle occupied states h defined in Eq. (2.3). To second order in ϵ, the action I is given by

$$I=\epsilon^2\int_0^T\frac{dt}{2}i\hbar\,\mathrm{Tr}\rho_1(t)[\dot{\rho}_1(t),\rho_0] . \quad (6.2)$$

The integrand in Eq. (6.2) can be related to the second-order correction $\mathcal{E}_2$ to the total energy $E=E_{\mathrm{HF}}+\epsilon^2\mathcal{E}_2$ of the orbit $\rho(t)$

$$\mathcal{E}_2=\frac{i\hbar}{2}\mathrm{Tr}\rho_1(t)[\dot{\rho}_1(t),\rho_0] . \quad (6.3)$$

Since $\mathcal{E}_2$ (as E) is time independent one finds $I=\epsilon^2T\mathcal{E}_2$. The quantization rule $I=nh$ thus determines the amplitude ϵ_n of the n-quantum state according to the formula

$$\epsilon_n^2=\frac{n\hbar\omega_0}{\mathcal{E}_2-n\hbar\omega_2} . \quad (6.4)$$

The corresponding energies are given by

$$E_n^*\equiv E_n-E_{\mathrm{HF}}=n\hbar(\omega_0+\epsilon_n^2\omega_2) . \quad (6.5)$$

Equation (6.5) does not give the splitting of the two-phonon state according to the different values of the angular momentum. Using an analogy with angular momentum projection techniques, one can however make a reasonable guess for this splitting. The obvious prescription is to retain, in the semiclassical quantization, only that part $\rho_2^{L'}$ of ρ_2 which has a definite angular momentum $L'(L'=0,2,\ldots,2L)$, as defined by Eq. (5.9). Then the quantity ω_2 in Eqs. (6.4) and (6.5) is replaced by the contribution $\omega_2(L')$ of $\rho_2^{L'}$:

$$\epsilon^2(n,L')=\frac{n\hbar\omega_0}{\mathcal{E}_2-n\hbar\omega_2(L')} , \quad (6.6a)$$

$$E^*(n,L')=n\hbar[\omega_0+\epsilon^2(n,L')\omega_2(L')] . \quad (6.6b)$$

From this last formula one sees that the excitation energy of the nth state is still $n\hbar\omega$ but the frequency ω now includes the anharmonic corrections $\epsilon^2\omega_2$ with ϵ and ω_2 being adjusted on the desired value of the angular momentum.

VII. RESULTS FOR THE OCTUPOLE MODES

In this section, we present some results for octupole vibrations in ^{16}O and ^{40}Ca obtained with the semiclassical quantization rule. We have performed calculations up to third order in the elongation of the periodic orbits in order to discuss the two-phonon states. We have used a simplified Skyrme force. The single-particle wave functions have been obtained by static spherical Hartree-Fock calculations (3.4) in configuration space using a 50-point lattice with a 0.2-fm mesh size. As boundary conditions we have set wave functions to zero at the outer edge of the lattice. The single-particle basis used in RPA and second-order calculations includes all the single-particle eigenstates $\langle r|a\rangle$ of the discretized Hamiltonian W_0 with a principal quantum number $n_a\leq 8$. With such a basis, truncation effects are negligible. For instance the energy-weighted sum rules [4] (EWSR) obtained from RPA eigenstates agree within 0.2%, in both ^{16}O and ^{40}Ca, with the expectation value of the double commutator calculated in the HF ground state. Finally, using a 100-point mesh, we have checked that results are stable against an increase of the dimension of the lattice.

A. Octupole modes in ^{16}O

In a previous letter [7], we demonstrated the practicability of our method by calculating periodic orbits with a simplified interaction including no spin-orbit term. Numerical applications were made for octupole vibrations in ^{16}O and the splitting of two-phonon states was calculated. However these calculations were too schematic since the spin-orbit interaction is important to reproduce the position of the low-lying octupole state. This is remedied in the present calculation which uses a two-body force including a spin-orbit term. The Coulomb interaction is ignored, which is legitimate for light nuclei. For ^{16}O the parameters of the interaction are $t_0=-1048$ MeV fm^3, $t_3=19\,150$ MeV fm^6, $\lambda=0$, and $w_0=95$ MeV fm^5. The values of the parameters t_0 and t_3 were adjusted to obtain

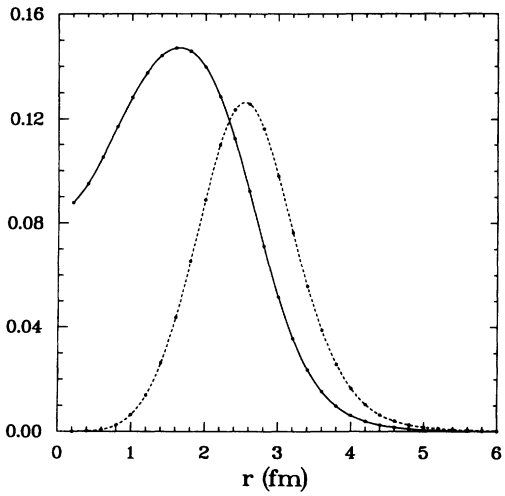

FIG. 1. Hartree-Fock density $\rho_0(r)$ (fm^{-3}) (full line), and transition density $\rho_1(r)$ (fm^{-3}) (dashed line) corresponding to the low-lying octupole state 3^- in the case of the ^{16}O.

a value of -7.95 MeV for the energy per nucleon and a value of 2.61 fm for the root-mean-square radius of ^{16}O. The value of the spin-orbit strength was adjusted to reproduce the observed energy of the low-lying octupole state [$\hbar\omega_0(3^-)=6.05$ MeV] in the random-phase approximation. The resulting value of the spin-orbit strength also provides a reasonable splitting (4.1 MeV) of the $1p$ levels in the Hartree-Fock approximation. We find that the low-lying 3^- RPA state exhausts 10.5% of the EWSR and 35% of the sum rule (SR) S_0. The radial part $\rho_1(r)$ of the transition density defined by

$$\rho_1(\mathbf{r},t)=\rho_1(r)Y_{30}(\hat{r})\cos(\omega_0 t) \tag{7.1}$$

is shown in Fig. 1. As expected, the low-lying octupole vibration is a surface mode and its form factor is similar to the derivative of the Hartree-Fock density $\rho_0(r)$ also shown in Fig. 1. The transition density vanishes rapidly at large distance. This behavior is characteristic of a bound RPA state.

To second order, we find $\hbar\omega_2=0.547$ MeV. The quantization rule (6.5) gives $E_1^*=6.66$ MeV and $E_2^*=14.78$ MeV. The corresponding anharmonicities, defined by

$$A_n=\frac{\epsilon_n^2\omega_2}{\omega} ,$$

are 9% for the first state and 18% for the second state. Therefore anharmonic terms are small for both states and comparable to, although smaller than, the values found in our earlier calculations (13% and 26%, respectively).

In order to calculate the splitting of the two-phonon states corresponding to different values of the angular momentum $L'=0,2,4,6$ we have solved Eqs. (6.6). The results are given in Table I, where we report, for each angular momentum L', the value of the second-order correction $\hbar\omega_2(L')$, the excitation energy $E_2^*(L')$ relative to the Hartree-Fock ground state, and the shift

$$\delta E_{L'}=E^*(2,L')-2\hbar\omega_0$$

with respect to the bare two-phonon energy. We find that the spreading of two-phonon states is 2 MeV, a value much smaller than that found in our previous calculation [7] which ignored the spin-orbit force (5 MeV). This illustrates the importance of the spin-orbit interaction.

Second-order corrections ρ_{2c} and ρ_{2f} to the transition density, defined by [see Eq. (5.15)]

$$\rho_2^{L'}(\mathbf{r},t)=[\rho_{2c}^{L'}(r)\cos(2\omega_0 t)+\rho_{2f}^{L'}(r)]Y_{L'0} , \tag{7.2}$$

where L' takes the values 0, 2, 4, and 6, are drawn respectively in Figs. 2(a) and 2(b). For $n=2$ the values of the elongation ϵ are 2.28, 2.19, 2, 1.96, for $L'=0,2,4,6$, respectively. Although these numbers do not look small, second-order corrections are in fact small since the relevant quantities to be looked at are the $\epsilon^2\rho_2$'s which are indeed small compared to $\epsilon\rho_1$. The largest corrections are obtained for small angular momenta.

It can be seen on Fig. 2 that the second-order densities $\rho_{2c}(r)$ and $\rho_{2f}(r)$ tend rapidly to zero at large distance. Indeed, although ρ_2 has nonzero particle-particle matrix elements for some single-particle states of the continuum, these matrix elements have a sufficiently smooth behavior as a function of energy.

B. Octupole modes in ^{40}Ca

The interaction parameters $t_0=-1018$ MeV fm^3, $t_3=15\,500$ MeV fm^6, $\lambda=5$ fm^3, and $w_0=100$ MeV fm^5 used for ^{40}Ca have been adjusted to give a root-mean-square radius of 3.38 fm, a binding energy of -8.41 MeV per nucleon and a value of 4.0 MeV for the excitation energy of the low-lying octupole. The low-lying 3^- state exhausts 7.5% of the energy-weighted sum rule and 29.2% of the nonweighted sum rule. In second order we find $\hbar\omega_2=0.547$, 4.63 MeV for the excitation energy of the one-phonon state and 11.0 MeV for the excitation en-

TABLE I. Two-octupole-phonon states in ^{16}O and ^{40}Ca. For each state are reported its spin and parity, $\hbar\omega_2$ (in keV), the excitation energy E^* (in MeV) and the shift δE (in MeV) with respect to the unperturbed energy $E_0^*=2\hbar\omega_0$.

	^{16}O				^{40}Ca		
J^π	$\hbar\omega_2$	E^*	δE	J^π	$\hbar\omega_2$	E^*	δE
0^+	369.4	13.793	1.683	0^+	421.2	10.134	2.134
2^+	260.7	13.251	1.141	2^+	121.2	8.516	.5161
4^+	-19.9	12.031	$-.079$	4^+	-16.1	7.936	$-.0639$
6^+	-63.5	11.861	$-.249$	6^+	20.9	8.085	.0845

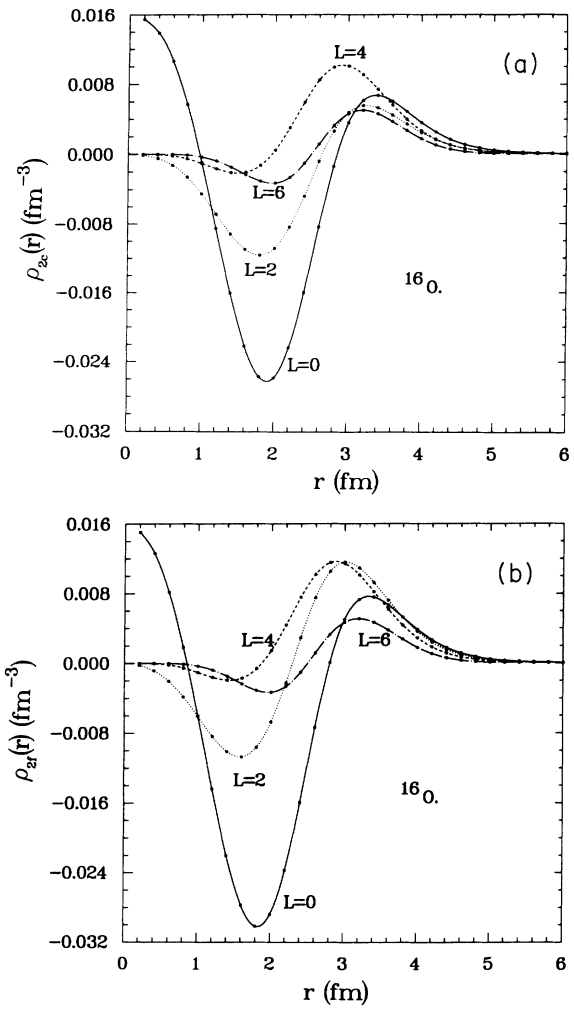

FIG. 2. Second-order corrections $\rho_{2c}^{L'}$ and $\rho_{2f}^{L'}$ (fm^{-3}) ($L'=0,2,4,6$) to the transition density in the case of the octupole mode in ^{16}O.

ergy of the two-phonon state. The corresponding anharmonicities are 14% and 27% respectively. These values are similar to those found in oxygen. The excitation energies of two-phonon states with angular momenta ranging from 0 to 6 are given in Table I. The root-mean-square deviation of these energies, weighted by the adequate degeneracy factors $(2L'+1)$, is 0.42 MeV. This is comparable to the value found in ^{16}O (0.59 MeV). It is similar to the deviation found by Catara, Chomaz, and Van Giai using boson expansion techniques. One difference, however, with these authors is that we find a larger shift of the 0^+ state. This may be due to the fact that our semiclassical angular momentum projection technique is accurate only for large momenta.

VIII. QUADRUPOLE MODES AND THE CONTINUUM PROBLEM

In this section we study quadrupole vibrations in ^{40}Ca which might be relevant for the understanding of the high-energy structures observed in [1]. For these modes we must use a modified perturbative construction procedure. Indeed the octupole mode is a bound RPA state whereas the giant quadrupole lies in the continuum. As a consequence, while the second-order source terms, proportional to $\exp(\pm 2i\omega_0 t)$, are nonresonant for octupoles, they are resonant for quadrupoles. In the latter case, the spectrum of the RPA matrix $\mathcal{M}$ contains an eigenstate whose energy is close to $2\hbar\omega_0$, so that the inhomogeneous linear equation defining the second-order density matrix is singular or nearly singular.

A. Treatment of resonant couplings with the continuum

To circumvent this difficulty, we use as first-order periodic orbit a superposition of the quadrupole mode and the resonant RPA mode with energy $2\hbar\omega_0$:

$$\rho_1(t)=\eta_Q e^{i\omega_0 t}+\eta_Q^+ e^{-i\omega_0 t}+\gamma\eta_R e^{2i\omega_0 t}+\gamma^*\eta_R^+ e^{-2i\omega_0 t} . \tag{8.1}$$

In second order the equation for ρ_2 reads

$$(i\hbar\partial_t-\mathcal{M})\rho_2(t)=S_2(t)-i\hbar\frac{\omega_1}{\omega_0}\dot{\rho}_1(t) , \tag{8.2}$$

where the source term S_2 is given as before by the formula

$$S_2(t)=[W_1(t),\rho_1(t)]+[W_2'(t),\rho_0] . \tag{8.3}$$

However S_2 is now a superposition of contributions arising from the quadrupole mode, from the resonant mode and from the cross term:

$$S_2=(S_{QQ}e^{2i\omega_0 t}+S_{Q\bar{Q}}+\gamma S_{\bar{Q}R}e^{i\omega_0 t}+\gamma S_{QR}e^{3i\omega_0 t} +\gamma^2 S_{RR}e^{4i\omega_0 t}+|\gamma|^2 S_{R\bar{R}})-\text{H.c.} \tag{8.4}$$

In Appendix C we give the explicit expression of the cross term $S_{\bar{Q}R}$ and $S_{Q\bar{R}}$ corresponding respectively to $e^{i\omega_0 t}$ and $e^{-i\omega_0 t}$.

The inhomogeneous linear equation defining ρ_2 can be solved only when there are no resonant terms in the right-hand side. This condition requires

$$\int_0^{T_0}\frac{dt}{T_0}\text{Tr}\left[\left[S_2(t)-i\hbar\frac{\omega_1}{\omega_0}\dot{\rho}_1(t)\right][\rho_0,\eta_Q e^{i\omega_0 t}]\right]=0 , \tag{8.5a}$$

$$\int_0^{T_0}\frac{dt}{T_0}\text{Tr}\left[\left[S_2(t)-i\hbar\frac{\omega_1}{\omega_0}\dot{\rho}_1(t)\right][\rho_0,\eta_R e^{2i\omega_0 t}]\right]=0 . \tag{8.5b}$$

These equations provide the value of the coupling strength γ and the first order correction ω_1 to the frequency:

$$\gamma^2=\text{Tr}(S_{QQ}[\rho_0,\eta_R^+])/2\text{Tr}(S_{\bar{Q}R}[\rho_0,\eta_Q^+]) , \tag{8.6a}$$

$$\hbar\omega_1=\gamma^*\text{Tr}(S_{\bar{Q}R}[\rho_0,\eta_Q^+]) . \tag{8.6b}$$

The presence of a coupling between two modes implies also a modification in the implementation of the semiclas-

sical quantization procedure described in Sec. V. Inserting the expression (8.1) into the quantization condition $I=nh$ where I is given by (6.2) we obtain the equation which gives the value of the elongation ϵ_n of the state with n quanta:

$$\epsilon_n^2(1+2|\gamma|^2)=n\left[1+\epsilon_n\frac{\omega_1}{\omega_0}\right]. \tag{8.7}$$

The excitation energy E_n^* corresponding to this state is

$$E_n^*=n\hbar\omega_0\left[1+\epsilon_n\frac{\omega_1}{\omega_0}\right]. \tag{8.8}$$

Since the source term S_2 also contains $e^{(\pm 3i\omega_0 t)}$ and $e^{(\pm 4i\omega_0 t)}$, one should in principle consider as well couplings to the resonant modes at $3\hbar\omega_0$, $4\hbar\omega_0$,.... We have found however that these states are nearly pure particle-hole configurations and that the corresponding couplings are small.

B. Results for quadrupole modes in ^{40}Ca

Let us now focus on the application of the above formulas to two-phonon quadrupole states ($n=2$) in ^{40}Ca. The first information we gain from our formulas is that, already in first order, there is a splitting of the two phonon states with angular momenta $L'=0,2,4$, since ω_1 is nonzero and angular momentum dependent. The next information is that, while in the case of uncoupled modes the excitation energy depends only on the square of the elongation, it now depends explicitly on the elongation itself. As a result, a splitting of the states n,L' will arise when the two roots of Eq. (8.7) are inserted into (8.8). The same phenomenon would arise in boson expansion methods. In this case, the degeneracy between the two-boson state and the single-boson states in the continuum would be lifted when including their coupling in perturbation theory.

In the ^{40}Ca case, the quadrupole mode is found at $\hbar\omega_0=15.54$ MeV in RPA calculations. We evaluated the source term with $L'=0,2,4$ and considered a resonant term in the channels $L_R=0,2,4$, respectively. The results obtained for the coupling strength γ^2, for the correction $\hbar\omega_1$ to the frequency, and for the excitation energies E^* of the two-phonon states are reported in Table II. Note that in the channel $L_R=4$ we find a negative value for γ^2 which implies purely imaginary values of γ and ω_1. This result is a signature of an instability of the corresponding orbit.

TABLE II. Two-quadrupole-phonon states in ^{40}Ca. For each state are reported its spin and parity, the square of the coupling constant γ, the first correction to the frequency $\hbar\omega_1$ (in MeV), and the excitation energy E^* (in MeV).

L_R^π	γ^2	$\hbar\omega_1$	E^*
0^+	0.22	0.31	31.82
			30.36
2^+	0.164	1.46×10^{-2}	31.12
			31.04
4^+	-0.11	$i1.94\times10^{-2}$	$31.1+i0.054$
			$31.1-i0.054$

In the two cases $L=2^+,4^+$, the value of $\hbar\omega_1$ is very small and compatible with zero. As compared to the Catara–Chomaz-Van Giai calculations, a similar root-mean-square deviation of the two-phonon states is found as was already the case for two-octupole phonon states.

IX. CONCLUSION

In this paper we have presented a perturbative construction method of the periodic orbits of the time-dependent Hartree-Fock equations. The solutions are found in the form of a power series in the amplitude of the collective motion. We have performed calculations using third-order expansions to determine the splitting of two-phonon states of the low-lying octupole vibration in ^{16}O and ^{40}Ca. In agreement with generator coordinate calculations [22] and with the boson expansion calculations of Catara, Chomaz, and Van Giai [18] we found small anharmonicities. We find root-mean-square deviations comparable to those of Ref. [18]. We have also investigated giant quadrupole vibrations. We had to generalize our method in order to account for the resonant coupling between the two-phonon state and one-phonon states in the continuum. This was done by introducing admixture of the resonant mode in the first-order expression of the periodic orbit. Calculations to second order have been performed. As in the nonresonant case we find small anharmonicities and root-mean-square deviations of the two-phonon energies comparable to Catara, Chomaz, and Van Giai.

Our results demonstrate that the method of quantization of periodic orbits of TDHF equation is a powerful tool to investigate the energy spectra of many-body systems. Although it sometimes involves large numerical summations, it only requires simple ingredients such as the RPA matrices and RPA amplitudes. Although it takes some computation it is easy to implement. In particular, it appears possible to extend the method to the construction of periodic orbits of the time-dependent Hartree-Fock-Bogoliubov equations. Such an extension would allow one to study the adiabaticity versus diabaticity of large-amplitude collective motion [23].

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APPENDIX A

The ith-order contribution to the mean-field, W_i can be decomposed into two parts:

$$W_i = W_i^{(ph)} + W_i' \ , \tag{A1}$$

where $W_i^{(ph)}$ involves only the particle-hole matrix elements of ρ_i. For a simplified Skyrme force we have

$$W_i^{(ph)}(\mathbf{r},t) = \frac{dU}{d\rho}\bigg|_{\rho=\rho_0} \langle \mathbf{r}|(1-\rho_0)\rho_i\rho_0 + \rho_0\rho_i(1-\rho_0)|\mathbf{r}\rangle \ . \tag{A2}$$

The term $W_i^{(ph)}$ contributes to the operator $i\hbar\partial_t - \mathcal{M}$ whereas W_i' generates the source term appearing in Eqs. (3.14) and (3.17).

In second order one finds

$$W_2'(\mathbf{r},t) = \frac{dU}{d\rho}\bigg|_{\rho=\rho_0} \langle \mathbf{r}|(1-\rho_0)\rho_i(1-\rho_0) + \rho_0\rho_i\rho_0|\mathbf{r}\rangle + \frac{1}{2}\frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0} \rho_1^2(\mathbf{r},t) \ . \tag{A3}$$

By using the identity $\rho_0\rho_2\rho_0 = -\rho_0\rho_1^2$ one obtains the following expression:

$$W_2'(\mathbf{r},t) = \frac{dU}{d\rho}\bigg|_{\rho=\rho_0} \langle \mathbf{r}|(1-2\rho_0)\rho_1^2|\mathbf{r}\rangle + \frac{1}{2}\frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0} \rho_1^2(\mathbf{r},t) \ . \tag{A4}$$

In third order the previous procedure yields

$$W_3'(\mathbf{r},t) = \frac{dU}{d\rho}\bigg|_{\rho=\rho_0} \langle \mathbf{r}|(1-\rho_0)\rho_3(1-\rho_0) + \rho_0\rho_3\rho_0|\mathbf{r}\rangle + \frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0} \rho_1(\mathbf{r},t)\rho_2(\mathbf{r},t) + \frac{1}{6}\frac{d^3U}{d\rho^3}\bigg|_{\rho=\rho_0} \rho_1^3(\mathbf{r},t) \ . \tag{A5}$$

In this case one uses the identity $\rho_0\rho_3\rho_0 = -\rho_0(\rho_1\rho_2 + \rho_2\rho_1)$. The previous expression thus reduces to

$$W_3'(\mathbf{r},t) = \frac{dU}{d\rho}\bigg|_{\rho=\rho_0} \langle \mathbf{r}|(1-2\rho_0)(\rho_1\rho_2 + \rho_2\rho_1)|\mathbf{r}\rangle + \frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0} \rho_1(\mathbf{r},t)\rho_2(\mathbf{r},t) + \frac{1}{6}\frac{d^3U}{d\rho^3}\bigg|_{\rho=\rho_0} \rho_1^3(\mathbf{r},t) \ . \tag{A6}$$

APPENDIX B

The particle-hole matrix element of ρ_1 satisfies the following equation [see Eq. (3.5)]:

$$i\hbar\frac{\partial}{\partial t}\langle p|\rho_1|h\rangle = \langle e_{\alpha_p} - e_{\alpha_h}\rangle\langle p|\rho_1|h\rangle + \langle p|W_1|h\rangle \ , \tag{B1}$$

which implies, by using the definition (5.4),

$$i\hbar\frac{\partial}{\partial t}\rho_{1\alpha_p\alpha_h}^{lm} = (e_{\alpha_p} - e_{\alpha_h})\rho_{1\alpha_p\alpha_h}^{lm} + \sum_{m_p m_h} (-1)^{m_p - 1/2} \begin{pmatrix} j_p & j_h & l \\ -m_p & m_h & m \end{pmatrix} \langle p|W_1|h\rangle \ , \tag{B2}$$

where

$$\langle p|W_1|h\rangle = \int d^3r \langle p|\mathbf{r}\rangle\langle \mathbf{r}|h\rangle \frac{dU}{d\rho}\bigg|_{\rho=\rho_0}(\mathbf{r})\rho_1(\mathbf{r},t) \ . \tag{B3}$$

By using the definition (5.1) for $\langle \mathbf{r}|p\rangle$ and $\langle \mathbf{r}|h\rangle$ one finds

$$\langle p|W_1|h\rangle = \frac{(2l+1)}{4\pi}(-1)^{m_p - 1/2} \begin{pmatrix} j_p & j_h & l \\ -m_p & m_h & m \end{pmatrix} \sum_{\alpha_{p'}\alpha_{h'}} C_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}^{l} F_{\alpha_p\alpha_h}^{l} F_{\alpha_{p'}\alpha_{h'}}^{l} (\rho_{1\alpha_p\alpha_h}^{lm} + (-1)^m \rho_{1\alpha_p\alpha_h}^{*\,l-m}) \ , \tag{B4}$$

where $C_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}^{l}$ is defined in Eq. (5.7), and where

$$F_{\alpha_p\alpha_h}^{l} = \hat{l}_p\hat{l}_h\hat{j}_p\hat{j}_h \begin{bmatrix} l_p & l_h & l \\ 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} j_p & j_h & l \\ l_h & l_p & \frac{1}{2} \end{Bmatrix} \ . \tag{B5}$$

In order to derive this relation we have used the well-known identity

$$\mathcal{Y}_{l_p j_p m_p}(\hat{r},\sigma)\mathcal{Y}_{l_h j_h m_h}^{*}(\hat{r},\sigma) = \sum_{lm} (-1)^{m_p - \frac{1}{2}} \begin{pmatrix} j_p & j_h & l \\ -m_p & m_h & m \end{pmatrix} \frac{\hat{l}}{\sqrt{4\pi}} F_{\alpha_p\alpha_h}^{l} Y_{lm}(\hat{r}) \ . \tag{B6}$$

Now we can rewrite (B2) as

$$i\hbar\frac{\partial}{\partial t}\rho^{lm}_{1\alpha_p\alpha_h}=\sum_{\alpha_{p'},\alpha_{h'}}[A^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}\rho^{lm}_{1\alpha_{p'}\alpha_{h'}} +B^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}(-1)^m\rho^{*l-m}_{1\alpha_{p'}\alpha_{h'}}] , \quad \text{(B7)}$$

where

$$B^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}\equiv\frac{1}{4\pi}C_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}F^{l}_{\alpha_p\alpha_h}F^{l}_{\alpha_{p'}\alpha_{h'}} , \quad \text{(B8a)}$$

$$A^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}}\equiv(e_{\alpha_p}-e_{\alpha_h})\delta_{\alpha_p\alpha_{p'}}\delta_{\alpha_h\alpha_{h'}}+B^{l}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{h'}} . \quad \text{(B8b)}$$

APPENDIX C

In this appendix we give the explicit expressions of the particle-hole matrix elements of the cross terms between the quadrupole mode and the resonant one $S_{\bar{Q}R}$ and $S_{Q\bar{R}}$, appearing in Eq. (8.4).

We use the notation $\rho_Q(r)$ and $\rho_R(r)$ for the radial part of the transition densities $\rho_{1Q}(\mathbf{r},t)$ and $\rho_{1R}(\mathbf{r},t)$ defined by

$$\rho_{1Q}(\mathbf{r},t)=\rho_Q(r)Y_{L_Q0}(\hat{r})\cos(\omega_0 t) , \quad \text{(C1a)}$$

$$\rho_{1R}(\mathbf{r},t)=\rho_R(r)Y_{L_R0}(\hat{r})\tfrac{1}{2}(\gamma e^{2i\omega_0 t}+\gamma^* e^{-2i\omega_0 t}) . \quad \text{(C1b)}$$

In terms of the angular components we have

$$\langle p|S_{\bar{Q}R}|h\rangle =(-1)^{m_p-1/2}\sum_{|L_Q-L_R|}^{L_Q+L_R}\hat{L}'^2\begin{bmatrix} j_p & j_h & L' \\ -m_p & m_h & 0\end{bmatrix}S^{L'}_{\bar{Q}R\alpha_p\alpha_h} \quad \text{(C2)}$$

where $S^{L'}_{\bar{Q}R\alpha_p\alpha_h}$ is given by

$$\begin{aligned}(S_{\bar{Q}R})^{L'}_{\alpha_p\alpha_h}=&\hat{L}_Q^2\hat{L}_R^2\begin{bmatrix}L_Q & L_R & L'\\ 0 & 0 & 0\end{bmatrix}\\
&\times\Bigg[\sum_{\alpha_{p'},\alpha_h,\alpha_{p''}}(-1)^{j_p+j_h+j_{p''}+1/2}\begin{Bmatrix}L_Q & L_R & L'\\ j_h & j_p & j_{p''}\end{Bmatrix}B^{L_Q}_{\alpha_p\alpha_{p''}\alpha_{p'}\alpha_{h'}}(\eta_{Q\alpha_{p'}\alpha_{h'}}+\eta^\dagger_{Q\alpha_{p'}\alpha_{h'}})\eta_{R\alpha_{p''}\alpha_h}\\
&+\sum_{\alpha_{p'},\alpha_h,\alpha_{p''}}(-1)^{j_p+j_h+j_{p''}+1/2}\begin{Bmatrix}L_R & L_Q & L'\\ j_h & j_p & j_{p''}\end{Bmatrix}B^{L_R}_{\alpha_p\alpha_{p''}\alpha_{p'}\alpha_{h'}}(\eta_{R\alpha_{p'}\alpha_{h'}}+\eta^\dagger_{R\alpha_{p'}\alpha_{h'}})\eta^\dagger_{Q\alpha_{p''}\alpha_h}\\
&-\sum_{\alpha_{p'},\alpha_h,\alpha_{h''}}(-1)^{j_p+j_h+j_{h''}+1/2}\begin{Bmatrix}L_Q & L_R & L'\\ j_p & j_h & j_{h''}\end{Bmatrix}B^{L_Q}_{\alpha_{h''}\alpha_h\alpha_{p'}\alpha_{h'}}(\eta_{Q\alpha_{p'}\alpha_{h'}}+\eta^\dagger_{Q\alpha_{p'}\alpha_{h'}})\eta_{R\alpha_p\alpha_{h''}}\\
&-\sum_{\alpha_{p'},\alpha_h,\alpha_{h''}}(-1)^{j_p+j_h+j_{h''}+1/2}\begin{Bmatrix}L_R & L_Q & L'\\ j_p & j_h & j_{h''}\end{Bmatrix}B^{L_R}_{\alpha_{h''}\alpha_h\alpha_{p'}\alpha_{h'}}(\eta_{R\alpha_{p'}\alpha_{h'}}+\eta^\dagger_{R\alpha_{p'}\alpha_{h'}})\eta^\dagger_{Q\alpha_p\alpha_{h''}}\\
&+\sum_{\alpha_{p'},\alpha_h,\alpha_{p''}}(-1)^{j_{p'}+j_{h'}+j_{p''}+1/2}\begin{Bmatrix}L_Q & L_R & L'\\ j_{p''} & j_{p'} & j_{h'}\end{Bmatrix}B^{L'}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{p''}}(\eta_{R\alpha_{p'}\alpha_{h'}}\eta_{Q\alpha_{p''}\alpha_{h'}}+\eta^\dagger_{Q\alpha_{p'}\alpha_{h'}}\eta^\dagger_{R\alpha_{p''}\alpha_{h'}})\\
&-\sum_{\alpha_{p'},\alpha_h,\alpha_{h''}}(-1)^{j_{p'}+j_{h'}+j_{h''}+1/2}\begin{Bmatrix}L_R & L_Q & L'\\ j_{h''} & j_{h'} & j_{p'}\end{Bmatrix}B^{L'}_{\alpha_p\alpha_h\alpha_{h'}\alpha_{h''}}(\eta_{Q\alpha_{p'}\alpha_{h'}}\eta_{R\alpha_{p'}\alpha_{h''}}+\eta^\dagger_{R\alpha_{p'}\alpha_{h'}}\eta^\dagger_{Q\alpha_{p'}\alpha_{h''}})\Bigg]\\
&+\frac{1}{2}\frac{\hat{L}_Q\hat{L}_R}{4\pi}\begin{bmatrix}L_Q & L_R & L'\\ 0 & 0 & 0\end{bmatrix}^2F^{L'}_{\alpha_p\alpha_h}\int_0^\infty dr\,r^2R_{\alpha_p}(r)R_{\alpha_h}(r)\frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0}2\frac{\rho_Q(r)}{2}\frac{\rho_R(r)}{2} .\end{aligned} \quad \text{(C3)}$$

Similarly the source term $S_{Q\bar{R}}$ reads

$$
\begin{aligned}
(S_{Q\bar{R}})^{L'}_{\alpha_p\alpha_h} = \hat{L}_Q^2 \hat{L}_R^2 \begin{bmatrix} L_Q & L_R & L' \\ 0 & 0 & 0 \end{bmatrix} \\
\times \Bigg[& \sum_{\alpha_{p'}\alpha_h\alpha_{p''}} (-1)^{j_p+j_h+j_{p''}+1/2} \begin{Bmatrix} L_Q & L_R & L' \\ j_h & j_p & j_{p''} \end{Bmatrix} B^{L_Q}_{\alpha_p\alpha_{p''}\alpha_{p'}\alpha_{h'}} (\eta_{Q\alpha_{p'}\alpha_{h'}} + \eta^{\dagger}_{Q\alpha_{p'}\alpha_{h'}}) \eta^{\dagger}_{R\alpha_{p''}\alpha_h} \\
& + \sum_{\alpha_{p'}\alpha_h\alpha_{p''}} (-1)^{j_p+j_h+j_{p''}+1/2} \begin{Bmatrix} L_R & L_Q & L' \\ j_h & j_p & j_{p''} \end{Bmatrix} B^{L_R}_{\alpha_p\alpha_{p''}\alpha_{p'}\alpha_{h'}} (\eta_{R\alpha_{p'}\alpha_{h'}} + \eta^{\dagger}_{R\alpha_{p'}\alpha_{h'}}) \eta_{Q\alpha_{p''}\alpha_h} \\
& - \sum_{\alpha_{p'}\alpha_h\alpha_{h''}} (-1)^{j_p+j_h+j_{h''}+1/2} \begin{Bmatrix} L_Q & L_R & L' \\ j_p & j_h & j_{h''} \end{Bmatrix} B^{L_Q}_{\alpha_{h''}\alpha_h\alpha_{p'}\alpha_{h'}} (\eta_{Q\alpha_{p'}\alpha_{h'}} + \eta^{\dagger}_{Q\alpha_{p'}\alpha_{h'}}) \eta^{\dagger}_{R\alpha_p\alpha_{h''}} \\
& - \sum_{\alpha_{p'}\alpha_h\alpha_{h''}} (-1)^{j_p+j_h+j_{h''}+1/2} \begin{Bmatrix} L_R & L_Q & L' \\ j_p & j_h & j_{h''} \end{Bmatrix} B^{L_R}_{\alpha_{h''}\alpha_h\alpha_{p'}\alpha_{h'}} (\eta_{R\alpha_{p'}\alpha_{h'}} + \eta^{\dagger}_{R\alpha_{p'}\alpha_{h'}}) \eta_{Q\alpha_p\alpha_{h''}} \\
& + \sum_{\alpha_{p'}\alpha_h\alpha_{p''}} (-1)^{j_{p'}+j_{h'}+j_{p''}+1/2} \begin{Bmatrix} L_Q & L_R & L' \\ j_{p''} & j_{p'} & j_{h'} \end{Bmatrix} B^{L'}_{\alpha_p\alpha_h\alpha_{p'}\alpha_{p''}} (\eta_{Q\alpha_{p'}\alpha_{h'}} \eta_{R\alpha_{p''}\alpha_{h'}} + \eta^{\dagger}_{R\alpha_{p'}\alpha_{h'}} \eta^{\dagger}_{R\alpha_{p''}\alpha_{h'}}) \\
& - \sum_{\alpha_{p'}\alpha_h\alpha_{h''}} (-1)^{j_{p'}+j_{h'}+j_{h''}+1/2} \begin{Bmatrix} L_R & L_Q & L' \\ j_{h''} & j_{h'} & j_{p'} \end{Bmatrix} B^{L'}_{\alpha_p\alpha_h\alpha_{h'}\alpha_{h''}} (\eta_{R\alpha_{p'}\alpha_{h'}} \eta_{Q\alpha_{p'}\alpha_{h''}} + \eta^{\dagger}_{Q\alpha_{p'}\alpha_{h'}} \eta^{\dagger}_{R\alpha_{p'}\alpha_{h''}}) \Bigg] \\
+ \frac{1}{2} & \frac{\hat{L}_Q \hat{L}_R}{4\pi} \begin{bmatrix} L_Q & L_R & L' \\ 0 & 0 & 0 \end{bmatrix}^2 F^{L'}_{\alpha_p\alpha_h} \int_0^{\infty} dr\, r^2 R_{\alpha_p}(r) R_{\alpha_h}(r) \frac{d^2U}{d\rho^2}\bigg|_{\rho=\rho_0} 2 \frac{\rho_Q(r)}{2} \frac{\rho_R(r)}{2} \, .
\end{aligned}
\tag{C4}
$$

Note that in these equations, only the matrix B appears and not the matrix A. This is due to the fact that we consider a simplified Skyrme interaction.

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