PHYSICAL REVIEW C VOLUME 18, NUMBER 4 OCTOBER 1978

Adiabaticity of time-dependent Hartree-Fock solutions

P. Bonche*
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125

P. Quentin†
Theoretical Division, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico 87545
(Received 29 March 1978)

A tractable method is presented for the study of the adiabaticity of a given time-dependent Hartree-Fock solution. In terms of the Baranger-Véneroni approach, this amounts to extracting the two operators ρ_0 and χ, for which rather simple expressions are derived. These explicit formulas are exploited to illustrate some implications of the adiabatic approximation itself and several related approximations. In particular, the incompatibility of two current hypotheses for the χ operator (locality and absence of particle-particle, hole-hole matrix elements) is pointed out. Finally, the whole discussion is exemplified by the simple case of uniform translational motion.

[NUCLEAR STRUCTURE Discussion of adiabatic limit of TDHF approximation, derivation of practical method of study adiabaticity of collective motion from TDHF solutions.]

I. INTRODUCTION

Long after Dirac[1] introduced the time-dependent Hartree-Fock (TDHF) approximation, its adiabatic limit (ATDHF) was extensively studied in the context of nuclear collective motion, even though TDHF solutions in the most general case were not yet available. Since the TDHF equations have been recently solved numerically,[2] it is now possible to check within the TDHF framework the validity of the adiabatic and related assumptions in any physical situation where they are invoked. In this paper, we present an explicit formalism to implement this program in an easy practical way.

It is important to bear in mind that by no means do we intend to discuss the validity of the TDHF approximation versus the exact time-dependent Schrödinger equation. Therefore when we examine the validity of the ATDHF equations of motion, we mean its validity with regard to the TDHF equations of motion.

The organization of this paper is as follows. An introductory discussion of the approximations to be tested is given in Sec. II. The derivation of relevant formulas is performed in Sec. III for the most general case. In Sec. IV, we explicitly take into account the spin degree of freedom to demonstrate some properties of the operators ρ_0 and χ. In addition, we study important limiting cases corresponding to extreme situations. A methodological survey on how to check the relevant approximations is given in Sec. V, whereas Sec. VI is devoted to the discussion of a simple illustrative example. Appendix A is concerned with a proof of existence for the decomposition of a density matrix. In Appendix B, we work out this decomposition while taking into account the spin degree of freedom. Finally, Appendix C provides a detailed derivation of the adiabatic collective kinetic energy.

II. SURVEY OF THE ATDHF APPROXIMATIONS

The TDHF approximation provides a simplified yet relevant framework within which the interplay between collective and single-particle degrees of freedom in a nucleus can be studied. If adiabaticity is assumed, one is led to specific equations of motion which have recently been the subject of many detailed studies.[3-8] For simplicity, two further assumptions are usually made as follows:

(i) The dynamical evolution of the nuclear system is governed by a few collective variables.
(ii) These variables are known *a priori*.

Under these circumstances, one may derive from the ATDHF equations of motion rather tractable expressions for the adiabatic mass parameter.[9] A non-self-consistent version of such a formalism is known as the Inglis cranking formula.[10] Corrections to the Inglis cranking mass parameters arise from the change in the self-consistent Hartree-Fock field due to the nonstatic part of the ATDHF solutions. They have been exhibited first in the particular case of collective rotation by Thouless and Valatin[11] and were recently

 © 1978 The American Physical Society

studied for more general modes.[9] Furthermore, the ATDHF formalism is capable of describing another interesting limiting case of TDHF equations, the random phase approximation (RPA).[7,12] Fully self-consistent RPA calculations are now available, where both Hartree-Fock single-particle states and coherent particle-hole excitations are determined from the same nucleon-nucleon effective interactions.[13-15] The ATDHF formalism has therefore proven to be a useful tool in a variety of physical processes.

Obviously, the relevance of all these studies is contingent upon the smallness of the collective velocities with respect to the single-particle motion. This is expected to be so for low energy collective motions and is particularly supported by the considerable sucess of phenomenological descriptions of such motion (as those described in Ref. 16), which are implicitly based upon some type of adiabatic, mean-field assumption.

For the low energy fission process (spontaneous or neutron-induced fission) the question of how adiabatic is the descent from saddle to scission remains rather open. The comparison of experimental fission-fragment kinetic energies with the results of various liquid drop calculations has led to the conclusion that some internal excitation may take place before scission[17,18] and therefore invalidate a purely adiabatic description of the fission process to the scission point. However, this amount of internal excitation would imply a transition away from a superfluid phase, which in turn would make an explanation of the odd-even effect[19] difficult in the fission fragment kinetic energy. It is therefore desirable to study in great detail how the available energy is shared between a few collective degrees of freedom and the internal motion. Finally, in the collision between two heavy ions, it is not yet completely clear how far one may describe the physical process as an adiabatic one.

In all these situations, a double study needs to be carefully undertaken. First, we want to know when the adiabatic assumption is no longer valid. Then, when this is the case, we want to know how fast nonadiabatic effects develop and how important they are. For these purposes, it is useful to work within the expansion framework developed by Baranger and Véneroni.[7] They have proved (under a restrictive condition discussed below), that given a one-body reduced density matrix ρ, one can find a set of two Hermitian time-even operators (ρ_0, χ) such that

$$\rho = e^{i\chi} \rho_0 e^{-i\chi} . \tag{1}$$

Since the operator ρ_0 satisfies the projector identity $\rho_0^2 = \rho_0$, it can also be viewed as the one-body reduced density matrix of an independent particle system. We will refer to eigenstates of ρ_0 with eigenvalue 1 as occupied or hole states, whereas those with eigenvalue 0 will be called unoccupied or particle states. The proof of the existence and uniqueness of the set (ρ_0, χ) relies only upon the assumption that the eigenvalues of χ lie within the open interval $]-\pi/4, \pi/4[$ (see Appendix A). In this case, the operator χ has neither particle-particle (p-p) nor hole-hole (h-h) matrix elements. In their proof of these results, the authors of Ref. 7 have explicitly discarded the "ambiguous" case where at least one eigenvalue of χ is equal to $\pm\pi/4$, as being too far from adiabaticity. We believe, however, that this case deserves a detailed study (see Sec. IV).

The expansion of the right-hand side of Eq. (1) in powers of χ yields

$$\rho = \sum_{q=0}^{\infty} \rho_q , \tag{2}$$

where ρ_q is given by the q-fold commutator

$$\rho_q = \frac{(i)^q}{q!} [\chi, [\chi, \ldots [\chi, \rho_0] \ldots]] . \tag{3}$$

We may insert this expansion in the TDHF equation for the density matrix ρ:

$$i\hbar \dot{\rho} = [h, \rho] , \tag{4}$$

where the dot denotes time derivative and h is the Hartree-Fock one-body Hamiltonian associated with ρ. The truncation of Eq. (4) to second order in χ provides the so-called ATDHF set of two coupled equations.[7,8] Similarly, the corresponding truncated expansion of the TDHF energy, written as a functional of ρ, $E[\rho]$, leads to

$$E[\rho] = E[\rho_0] + K + O(\chi^4) , \tag{5}$$

where the energies $E[\rho_0]$ and K are identified as the adiabatic potential and collective kinetic energy, respectively. Due to time-reversal symmetry, there are no odd terms in χ in the expansion (5), and K is therefore quadratic in χ. From the ATDHF equations, one can derive the explicit expression for K (Ref. 8):

$$K = \tfrac{1}{2} \hbar \, \mathrm{Tr} \, (\chi \dot{\rho}_0) . \tag{6}$$

Since $\dot{\rho}_0$ is linear in χ, K is indeed quadratic in χ. The identification of $E[\rho_0]$ and K as potential and kinetic energy is further confirmed by the fact that the ATDHF equations have been shown to be of the canonical Hamiltonian form; the matrix elements of ρ_0 and χ play the role of coordinates and momenta, respectively.[8] Testing the adiabaticity of a TDHF solution then amounts to exhibiting the smallness of χ, for instance through its eigenvalues. The difference between the TDHF

energy, which is a conserved quantity, and the sum $E[\rho_0]+K$ may also be used as a measure of the rate at which adiabaticity is violated by exhibiting the contributions of higher order terms in χ to the energy.

All practical calculations performed so far within the adiabatic limit of the TDHF approximation assume in one way or another that the dynamical evolution of the whole system can be expressed in terms of a limited set of collective variables, and that the corresponding operators are known *a priori*. The most common "guess" for these in the literature has been the standard multipole operators. Under the condition χ small, the extraction of ρ_0 then provides a direct test of these assumptions.

The method we present in this paper is capable of answering all the above-raised questions. Together with a check of adiabaticity, it provides a direct and easy way to extract the adiabatic path (when adiabaticity turns out to be a good approximation) as well as a measure of the rate at which nonadiabatic effects build up.

We will also discuss the limiting case where χ is a local operator, for it has been demonstrated that the TDHF equations then reduce to a set of hydrodynamical equations.[20] However, we will see that the two assumptions: χ local and having p – h matrix elements only, are exclusive.

III. CONSTRUCTION OF ρ_0 AND χ

Baranger and Véneroni have shown[7] that one may always define (see Appendix A) a time-even operator χ by

$$e^{4i\chi} = (2\rho - 1)(2\bar{\rho} - 1), \tag{7}$$

where $\bar{\rho}$ is the time reversal of ρ. From this expression, the method we will follow is straightforward. We first diagonalize $e^{4i\chi}$, then extract χ under the assumption that all the eigenvalues χ^λ of χ belong to $[-\pi/4, \pi/4]$, paying special attention to the case $|\chi^\lambda| = \pi/4$. When the latter does not occur, Baranger and Véneroni have proven that ρ_0 can be constructed by inverting Eq. (1) and that χ has only particle-hole matrix elements, namely,

$$\chi\rho_0 + \rho_0\chi = \chi. \tag{8}$$

This method is by far more explicit and useful for practical calculations than that proposed by Ring and Schuck[21] using Thouless' theorem.

In this section we exclude the cases $\chi^\lambda = 0$ and $\chi^\lambda = \pm\pi/4$, postponing their analysis to the following one.

Let us call S the subspace onto which ρ is a projector and $\{\mu\}$ the orthonormal basis which diagonalizes ρ in S with eigenvalues 1. The choice of this basis is quite natural for practical applications since actual TDHF calculations provide directly the time evolution of such states, rather than the matrix elements of ρ in some arbitrary basis. The orthonormal set $\{\bar{\mu}\}$, corresponding to the time-reversed determinant, diagonalizes $\bar{\rho}$ with eigenvalues 1 and spans the subspace $\bar{S}$ onto which $\bar{\rho}$ is a projector. The complete basis $(\{\mu\}+\{\bar{\mu}\})$ in the space $S+\bar{S}$ is bi-orthogonal, since the two sets $\{\mu\}$ and $\{\bar{\mu}\}$ are separately orthonormal, but not between themselves. This bi-orthogonal basis plays an important role, since in the complement of $S+\bar{S}$, $e^{4i\chi}$ is the unit operator and χ is therefore zero. Consequently, we only have to diagonalize $e^{4i\chi}$ within the subspace $S+\bar{S}$. For this purpose, we first orthonormalize the basis $(\{\mu\}+\{\bar{\mu}\})$, using the method developed by Gogny[22] for bi-orthogonal bases.

The overlap matrix A between the basis states of S and $\bar{S}$ is defined as

$$A_{ij} = \langle \mu_i | \bar{\mu}_j \rangle . \tag{9}$$

The matrix elements of $AA^\dagger$ describe the restriction onto S of the projector on $\bar{S}$,

$$(AA^\dagger)_{ij} = \sum_k \langle \mu_i | \bar{\mu}_k \rangle \langle \bar{\mu}_k | \mu_j \rangle = \langle \mu_i | \bar{\rho} | \mu_j \rangle . \tag{10}$$

The matrix $AA^\dagger$ is thus Hermitian, positive definite and with eigenvalues between 0 and 1. We will denote its orthonormalized eigenstates by $|1\lambda\rangle$ and corresponding eigenvalues by $\cos^2\varphi_\lambda$, where φ_λ is contained in the interval $[0, \pi/2]$:

$$AA^\dagger |1\lambda\rangle = \cos^2\varphi_\lambda |1\lambda\rangle . \tag{11}$$

Upon left multiplying Eq. (11) by $A^\dagger$, we immediately solve the diagonalization problem for $A^\dagger A$:

$$A^\dagger A\ |2\lambda\rangle = \cos^2\varphi_\lambda |2\lambda\rangle , \tag{12}$$

where the orthonormalized states $|2\lambda\rangle$ correspond to the same eigenvalues $\cos^2\varphi_\lambda$ and are related to the previous ones by the following transformation between components:

$$\langle \bar{\mu}_i | 2\lambda \rangle = \frac{1}{\cos\varphi_\lambda} \sum_j A^\dagger_{ij} \langle \mu_j | 1\lambda \rangle . \tag{13}$$

Note that the state $|1\lambda\rangle$ ($|2\lambda\rangle$) is completely defined in the space S ($\bar{S}$) by its components on the set $\{\mu\}$ ($\{\bar{\mu}\}$). This new bi-orthogonal basis ($\{1\lambda\}+\{2\lambda\}$) is such that

$$\langle 1\lambda | 2\lambda' \rangle = \cos\varphi_\lambda \delta_{\lambda\lambda'} , \tag{14}$$

as can be shown from Eqs. (11) and (13).

Let us define for each value of λ two states $|h\lambda\rangle$ and $|p\lambda\rangle$ as

$$|h\lambda\rangle = \frac{1}{2\cos(\frac{1}{2}\varphi_\lambda)}\,(|1\lambda\rangle + |2\lambda\rangle), \tag{15a}$$

$$|p\lambda\rangle = \frac{1}{2\sin(\frac{1}{2}\varphi_\lambda)}\,(|1\lambda\rangle - |2\lambda\rangle), \tag{15b}$$

This notation anticipates the fact that these states will turn out to be hole and particle states for ρ_0. The set $(\{h\lambda\}+\{p\lambda\})$ constitutes an orthonormal basis spanning the subspace $S+\bar{S}$, in which $e^{4i\chi}$ can now be expressed. The unitary transformation which diagonalizes $AA^\dagger$ in S changes the density matrix ρ

$$\rho = \sum_i |\mu_i\rangle\langle\mu_i|, \tag{16}$$

into

$$\rho = \sum_\lambda |1\lambda\rangle\langle 1\lambda|. \tag{17}$$

Similarly we have

$$\bar{\rho} = \sum_\lambda |2\lambda\rangle\langle 2\lambda|. \tag{18}$$

Therefore, upon inverting Eqs. (15), the operator $e^{4i\chi}$ reduces to a simple (2×2) block diagonal form. Each block B_λ corresponds to a single eigenvalue φ_λ and reads

$$B_\lambda = \begin{pmatrix} \cos 2\varphi_\lambda & -\sin 2\varphi_\lambda \\ \sin 2\varphi_\lambda & \cos 2\varphi_\lambda \end{pmatrix}. \tag{19}$$

The eigenstates of B_λ are

$$\begin{aligned} |+\lambda\rangle &= \frac{1}{\sqrt{2}}\,(|h\lambda\rangle - i|p\lambda\rangle), \\ |-\lambda\rangle &= \frac{1}{\sqrt{2}}\,(|h\lambda\rangle + i|p\lambda\rangle), \end{aligned} \tag{20}$$

associated with eigenvalues

$$m_+^\lambda = m_-^{\lambda *} = e^{2i\varphi_\lambda}. \tag{21}$$

This yields the following eigenvalues for χ

$$\chi_+^\lambda = -\chi_-^\lambda = \tfrac{1}{2}\varphi_\lambda. \tag{22}$$

Using the spectral decomposition theorem, we then get

$$\chi = \sum_\lambda \tfrac{1}{2}\varphi_\lambda\,(|+\lambda\rangle\langle+\lambda| - |-\lambda\rangle\langle-\lambda|). \tag{23}$$

From Eq. (1), ρ_0 is given by

$$\rho_0 = e^{-i\chi}\,\rho\,e^{i\chi} \tag{24}$$

and can be expressed in terms of the eigenstates of χ:

$$\begin{aligned} \rho_0 = \sum_\lambda (&|+\lambda\rangle\langle+\lambda|\langle+\lambda|\rho|+\lambda\rangle + |-\lambda\rangle\langle-\lambda|\langle-\lambda|\rho|-\lambda\rangle \\ &+ e^{i\varphi_\lambda}|-\lambda\rangle\langle+\lambda|\langle-\lambda|\rho|+\lambda\rangle \\ &+ e^{-i\varphi_\lambda}|+\lambda\rangle\langle-\lambda|\langle+\lambda|\rho|-\lambda\rangle). \end{aligned} \tag{25}$$

Upon evaluating the matrix elements of ρ and re-expressing the states $|\pm\lambda\rangle$ in terms of $|h\lambda\rangle$ and $|p\lambda\rangle$ through Eqs. (20), ρ_0 takes the simple form

$$\rho_0 = \sum_\lambda |h\lambda\rangle\langle h\lambda|, \tag{26}$$

which shows that the states $|h\lambda\rangle$ ($|ph\rangle$) are nothing but the hole (particle) states for ρ_0. The procedure we have followed thus provides directly with the basis diagonalizing ρ_0. In this basis, χ is

$$\chi = \sum_\lambda \tfrac{1}{2} i\varphi_\lambda\,(|h\lambda\rangle\langle p\lambda| - |p\lambda\rangle\langle h\lambda|), \tag{27}$$

which clearly exhibits its lack of p-p and h-h matrix elements.

States very close to the particle states $|p\lambda\rangle$ have already been considered in Ref. 23. Indeed, the states $|\eta\lambda\rangle$ in Sec. 7 of that reference are the states $|p\lambda\rangle$, apart for a factor $\frac{1}{2}i\varphi_\lambda$.

IV. PROPERTIES OF ρ_0 AND χ, LIMITING CASES

Hermiticity and time-reversal properties

In the previous section, we have described a simple method to diagonalize the operators ρ_0 and χ and given their representation in the particle-hole basis. Although we know *a priori* that they are both Hermitian and time-even from general considerations,[7] we will show from their explicit forms that they indeed have these two properties. Hermiticity is directly seen from their expressions (26) and (27). On the other hand, their time-even character is less transparent and requires taking into account the spin degrees of freedom.

As a result of the analysis of the time-even behavior of ρ_0 and χ, we will learn how to generalize ATDHF to odd-even nuclei and how to treat correctly the extreme nonadiabatic case where some φ_λ is equal to $+\pi/2$ (i.e., some eigenvalues of χ equal to $\pm\pi/4$).

From now on, we shall limit ourselves to the consideration of TDHF single particle states $\{\mu_i\}$ which are eigenstates of the third component, s_z, of the spin operator. A similar discussion can be carried out when the TDHF single particle states are eigenvalues of j_z. The set $\{\mu_i\}$ is composed of n_+ spin-up states (eigenvalue $+\frac{1}{2}$) and n_- spin-down states (eigenvalue $-\frac{1}{2}$). We show in Appendix B that if n_+ and n_- are not equal, at least $|n_+ - n_-|$ eigenvalues of $AA^\dagger$ vanish, i.e., are such that $\varphi_\lambda = \pi/2$. When this is not the case, we also show that, to solve the eigenproblem for $AA^\dagger$, one needs only to diagonalize the restriction $MM^\dagger$ of this matrix to either one of the spin-up or spin-down subspace. To each eigensolution characterized by φ_λ, $|1\lambda\rangle$, and $|2\lambda\rangle$ in a given spin subspace, there corresponds in the other

one an eigensolution characterized by the same eigenvalue φ_λ and by the eigenvectors $|1'\lambda\rangle$ and $|2'\lambda\rangle$ related to the previous ones by time-reversal conjugation:

$$|1'\lambda\rangle = |\overline{2\lambda}\rangle\,, \qquad |2'\lambda\rangle = |\overline{1\lambda}\rangle\,. \tag{28}$$

Due to the time-reversal properties for fermions, we also have

$$|\overline{1'\lambda}\rangle = -|2\lambda\rangle\,, \qquad |\overline{2'\lambda}\rangle = -|1\lambda\rangle\,. \tag{29}$$

Consequently, the states $|h\lambda\rangle$ and $|p\lambda\rangle$ built from $|1\lambda\rangle$ and $|2\lambda\rangle$ by Eqs. (15) are related to the states $|h'\lambda\rangle$ and $|p'\lambda\rangle$ built from $|1'\lambda\rangle$ and $|2'\lambda\rangle$, by

$$|\overline{h\lambda}\rangle = |h'\lambda\rangle\,, \quad |\overline{h'\lambda}\rangle = -|h\lambda\rangle\,, \qquad |\overline{p\lambda}\rangle = -|p'\lambda\rangle\,, \quad |\overline{p'\lambda}\rangle = |p\lambda\rangle\,. \tag{30}$$

It immediately follows from Eqs. (26) and (27) that ρ_0 and χ are indeed time-even operators. In addition, we have found that for each non-vanishing eigenvalue $\cos^2\varphi_\lambda$ ($\varphi_\lambda \neq \pi/2$) of $MM^\dagger$ (or $AA^\dagger$), there are two orthogonal eigenstates $|1\lambda\rangle$ and $|1\lambda'\rangle$ in the subspace S. The same thing occurs in $\bar{S}$ where both $|2\lambda\rangle$ and $|2\lambda'\rangle$ are eigenstates of $A^\dagger A$ with eigenvalue $\cos^2\varphi_\lambda$. This is to be related to the following result of Ref. 7: If a state $|a\rangle$ is an eigenstate of χ, the state $(2\rho-1)|a\rangle$ is also an eigenstate with the same eigenvalue. Indeed, the two eigenstates of χ, $|\pm\lambda\rangle$, constructed from $|p\lambda\rangle$ and $|h\lambda\rangle$ by means of Eq. (20), are related to each other through

$$(2\rho-1)|\pm\lambda\rangle = e^{\pm i\varphi_\lambda}|\mp\lambda\rangle\,. \tag{31}$$

Finally, we note the time-reversal properties of the eigenstates of χ:

$$|\overline{+\lambda}\rangle = |+'\lambda\rangle\,, \qquad |\overline{-\lambda}\rangle = |-'\lambda\rangle\,, \tag{32}$$

where the states $|\pm'\lambda\rangle$ are constructed from $|h'\lambda\rangle$ and $|p'\lambda\rangle$ according to Eq. (20).

Limiting cases

In both cases, $\varphi_\lambda = 0$ and $\varphi_\lambda = \pi/2$, we have to go back to the basic definition of $e^{4i\chi}$ [Eq. (7)] and ρ_0 [Eq. (24)]; the method derived in Sec. III fails because of the denominators in Eqs. (13) and (15b).

We first deal with the case $\varphi_\lambda = 0$. When φ_λ vanishes, the corresponding eigenvalue of $AA^\dagger$, $\cos^2\varphi_\lambda$, is equal to 1. Due to the projector character of $AA^\dagger$ [Eq. (10)], the corresponding eigenstate $|a\rangle$ belongs to both S and $\bar{S}$, thus

$$(2\rho-1)|a\rangle = (2\bar{\rho}-1)|a\rangle = |a\rangle\,. \tag{33}$$

Therefore, as seen in Eq. (7), $|a\rangle$ is an eigenstate of $e^{4i\chi}$ with eigenvalue 1 and an eigenstate of χ with eigenvalue 0. It contributes neither to χ nor to any dynamical quantity (like K) and, according to Eq. (24), is an occupied state of ρ_0. According to Eq. (33), the twofold degeneracy discussed above still applies and there exists a second eigenstate which is nothing but the time reversal of $|a\rangle$, so that the total contribution to ρ_0 is time-even: $|a\rangle\langle a| + |\bar{a}\rangle\langle\bar{a}|$.

On the other hand, $\cos^2\varphi_\lambda = 0$ ($\varphi_\lambda = \pi/2$) means that some eigenvalues of the projector-like operator $AA^\dagger$ vanishes. This implies that there exists a subspace $\mathcal{O}$ of S orthogonal to $\bar{S}$. Let us call $\{\omega\}$ a set of orthonormalized vectors spanning $\mathcal{O}$. The time-reversed space $\bar{\mathcal{O}}$ spanned by the set $\{\bar{\omega}\}$ is orthogonal to S, and thus:

$$(2\rho-1)|\omega\rangle = |\omega\rangle\,, \quad (2\bar{\rho}-1)|\omega\rangle = -|\omega\rangle\,, \qquad (2\bar{\rho}-1)|\bar{\omega}\rangle = |\bar{\omega}\rangle\,, \quad (2\rho-1)|\bar{\omega}\rangle = -|\bar{\omega}\rangle\,. \tag{34}$$

Therefore, again from Eq. (7), both $|\omega\rangle$ and $|\bar{\omega}\rangle$ are eigenstates of $e^{4i\chi}$ with eigenvalues -1, i.e., $4\chi = \pm\pi$, which is indeed the ambiguous case quoted in Ref. 7. Let us decide that the corresponding eigenvalue χ_ω of χ is $+\pi/4$, the phases $4\chi_\omega$ are then contained within the semiopen interval $]-\pi, +\pi]$. We also denote the restriction of operators to the subspace $\mathcal{O}+\bar{\mathcal{O}}$ by $\tilde{\rho}, \tilde{\chi}, \ldots$. It is clear that the sum $\tilde{\tau}\tilde{\chi} + \tilde{\chi}\tilde{\tau}$ does not vanish any more. Thus, we cannot define from the expression (7) of $e^{4i\tilde{\chi}}$, a time-even Hermitian operator $\tilde{\rho}_0$ such that Eq. (1) is fulfilled (cf. Appendix A). However, as a formal extension of the choice made in Ref. 7, it is natural to make use of Eq. (24) to define an Hermitian operator $\tilde{\rho}_0$ from $\tilde{\rho}$ and $\tilde{\chi}$ as

$$\tilde{\rho}_0 = \tilde{\rho} = \sum_\omega |\omega\rangle\langle\omega|\,. \tag{35}$$

Clearly, $\tilde{\rho}_0$ is not time-even. The states $|\omega\rangle$ diagonalizing $\tilde{\rho}_0$ with eigenvalues 1 are hole states and the states $|\bar{\omega}\rangle$ particle states. The operator $\tilde{\chi}$ may be written

$$\tilde{\chi} = e^{i\pi/4}\tilde{e} + e^{-i\pi/4}\bar{\tilde{e}} = \sum_\omega \left(e^{i\pi/4}|\omega\rangle\langle\omega| + e^{-i\pi/4}|\bar{\omega}\rangle\langle\bar{\omega}|\right) \tag{36}$$

Contrary to the previous case, $\tilde{\chi}$ has only p – p and h – h matrix matrix elements. There is no contradiction with Ref. 7 where the assumption made about the eigenvalues of χ implied the vanishing of those p – p and h – h matrix elements for χ. In fact, we have simply proposed a possible generalization of the decomposition (1) to cases ($\chi^\lambda = \pi/4$) which were not explicitly taken into account. Such cases may be encountered in two different instances: first for systems such that $n_+ \neq n_-$ (as is the case for odd nuclei), second,

whether or not $n_+ = n_-$, there may be accidental zero eigenvalues of the matrix $AA^\dagger$.

It would be rather inconvenient if the adiabatic collective energy were to depend on the choice of phase for the eigenvalues of $\tilde{\chi}$. Actually, this is not the case, the potential energy part depends only upon ρ_0 whose restriction to $\mathcal{O} + \bar{\mathcal{O}}$, $\tilde{\rho}_0$, is independent of the choice of phase, as seen in Eq. (35). On the contrary, the kinetic energy part K does depend upon χ [cf. Eq. (6)]; however, the contribution to K arising from $\tilde{\chi}$ vanishes for it involves only p-p and h-h matrix elements of $\tilde{\rho}_0$ which are known to be zero in the most general case. As a result, the collective adiabatic energy is not affected at all by the phase choice for the χ_ω eigenvalues.

The expansion of the TDHF energy in terms of $\tilde{\rho}$ provides an additional justification for our choice of $\tilde{\rho}_0$:

$$E(\rho) = E(\rho - \tilde{\rho}) + \mathrm{Tr}\,\mathrm{Tr}[(\rho - \tilde{\rho})\, V\, \tilde{\rho}] + E(\tilde{\rho}) . \quad (37)$$

In Eq. (37), the first term can be approximated in the adiabatic limit according to standard techniques.[7] The second one is the coupling energy between $|\omega\rangle$ and the other states $|\mu\rangle$, whereas the third is a correction term arising only from the subspace $\mathcal{O}$. Our choice of $\tilde{\rho}_0$ and $\tilde{\chi}$ is therefore consistent with a restriction of the adiabatic approximation to the $(S - \mathcal{O})$ subspace. In addition, it provides a framework for further approximations in the dynamical treatment of the states $|\omega\rangle$ and their coupling to the other states $|\mu\rangle$.

Practical derivation; Summary

Unless ρ is built from states which already diagonalize s_z, we follow the method given in Sec. III. When the overlap matrix A is built and $AA^\dagger$ diagonalized, we have to classify its eigenvalues:

(i) $\cos^2\varphi_\lambda = 1$, eigenstates $|a\rangle$, then

$$\chi(a) = 0 , \quad (38)$$

$$\rho_0(a) = \sum_a |a\rangle\langle a| . \quad (39)$$

There is no contribution to K.

(ii) $0 < \cos^2\varphi_\lambda < 1$, eigenstates $|1\lambda\rangle$. We have to construct the states $|2\lambda\rangle$ through Eq. (13), and $|p\lambda\rangle$ and $|h\lambda\rangle$ according to Eq. (15), then

$$\chi(ph) = \sum_\lambda \tfrac{1}{2} i\varphi_\lambda (|h\lambda\rangle\langle p\lambda| - |p\lambda\rangle\langle h\lambda|) , \quad (40)$$

$$\rho_0(ph) = \sum_\lambda |h\lambda\rangle\langle h\lambda| . \quad (41)$$

(iii) $\cos^2\varphi_\lambda = 0$, eigenstates $|\omega\rangle$:

$$\chi(\omega) = \tilde{\chi} = \sum_\omega (e^{\pm i\pi/4}|\omega\rangle\langle\omega| + e^{\mp i\pi/4}|\bar{\omega}\rangle\langle\bar{\omega}|) , \quad (42)$$

$$\rho_0(\omega) = \tilde{\rho}_0 = \sum_\omega |\omega\rangle\langle\omega| . \quad (43)$$

There is no contribution to K.

Only $\rho_0(a)$ and $\rho_0(ph)$ are time-even, whereas χ is time-even in any case. The final expressions for ρ_0 and χ are

$$\rho_0 = \rho_0(a) + \rho_0(ph) + \rho_0(\omega) , \quad (44)$$

$$\chi = 0 + \chi(ph) + \chi(\omega) . \quad (45)$$

V. TEST OF THE VALIDITY OF SOME CURRENT ASSUMPTIONS

At the end of Sec. II, three different questions concerning the motion represented by a TDHF solution have been listed:

(i) Is the motion adiabatic?

(ii) If so, what is the adiabatic path?

(iii) Is χ local?

In this section, we will further develop some implications of the formulas which have been derived in the two previous sections, in the context of these three questions. For the sake of simplicity, we assume that none of the eigenvalues of $e^{4i\chi}$ correspond to the limiting cases studied in the previous section and we adopt the notation of Sec. III.

Adiabaticity of the motion

Let us first reexpress the adiabatic collective kinetic energy, as given by Eq. (6) in the basis which diagonalizes ρ_0. Using Eq. (27) we get

$$K = \frac{i\hbar}{4} \sum_\lambda \varphi_\lambda (\langle p\lambda|\dot{\rho}_0|h\lambda\rangle - \langle h\lambda|\dot{\rho}_0|p\lambda\rangle) , \quad (46)$$

which can be rewritten as

$$K = \frac{\hbar}{2} \sum_\lambda \varphi_\lambda \,\mathrm{Im}\langle \dot{h}\lambda|p\lambda\rangle , \quad (47)$$

where $|\dot{h}\lambda\rangle$ stands for the time derivative of $|h\lambda\rangle$. In terms of the states $|1\lambda\rangle$ and $|2\lambda\rangle$, K reads as

$$K = \frac{\hbar}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda} \,\mathrm{Im}\,(\langle \dot{1}\lambda|1\lambda\rangle + \langle 2\lambda|\dot{2}\lambda\rangle) . \quad (48)$$

Note that there is no $\dot{\varphi}_\lambda$ dependence in this expression. According to Appendix C, we have

$$K = \frac{1}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda} (\langle 1\lambda|h|1\lambda\rangle + \langle 2\lambda|\bar{h}|2\lambda\rangle)$$

$$- \frac{1}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin 2\varphi_\lambda} (\langle 2\lambda|h + \bar{h}|1\lambda\rangle + \langle 1\lambda|h + \bar{h}|2\lambda\rangle) . \quad (49)$$

where $\bar{h}$ is the time-reverse HF Hamiltonian. The

time derivative of the eigenvalues of χ are given by

$$\frac{\dot{\varphi}_\lambda}{2} = \frac{i}{2\hbar \sin 2\varphi_\lambda} \langle 1\lambda | [\bar{p}, (h+\bar{h})] | 1\lambda \rangle . \tag{50}$$

We can also calculate the qth term ρ_q in the expansion of ρ in terms of χ [cf. Eq. (3)]. First we notice that all ρ_q operators are diagonal in terms of 2×2 blocks corresponding to a given λ. We restrict ourselves to such a block, and evaluate the contribution ρ_q^λ to ρ_q coming from λ. The full ρ_q will be simply the sum over λ of each of the ρ_q^λ. From Eq. (3) we derive the recursion relations:

$$\rho_q^\lambda = \frac{-\varphi_\lambda}{2q} [X, \rho_{q-1}^\lambda] \tag{51}$$

and

$$\rho_q^\lambda = \frac{\varphi_\lambda^{\,2}}{4q(q-1)} [X, [X, \rho_{q-2}^\lambda]] \tag{52}$$

where

$$X = \frac{-2i}{\varphi_\lambda} \chi . \tag{53}$$

The solution of Eq. (52) for odd values of q is

$$\rho_{2n+1}^\lambda = \frac{(-1)^n \varphi_\lambda^{2n+1}}{2(2n+1)!} (|h\lambda\rangle\langle p\lambda| + |p\lambda\rangle\langle h\lambda|) , \tag{54}$$

with $n \geq 0$. Using the recursion relation (51) once, we obtain for even value of q:

$$\rho_{2n}^\lambda = \frac{(-1)^n \varphi_\lambda^{2n}}{2(2n)!} (|h\lambda\rangle\langle h\lambda| - |p\lambda\rangle\langle p\lambda|) \tag{55}$$

with $n \geq 1$. In the above expressions, it is easy to check the p-h character of $\rho_{2n+1} = \sum_\lambda \rho_{2n+1}^\lambda$ and the p-p, h-h character of $\rho_{2n} = \sum_\lambda \rho_{2n}^\lambda$. Also, from Eq. (30) we immediately see that the even terms ρ_{2n} are time-even and the odd ones ρ_{2n+1} are time-odd under time-reversal conjugation.

Moreover, Eqs. (51) and (52) provide an explicit measure of the convergence of the expansion (2) for ρ. These expressions could have also been obtained in another way. Indeed ρ can be directly expressed in terms of particle and hole states:

$$\rho = \rho_0 + \sum_\lambda \tfrac{1}{2} \sin\varphi_\lambda (|h\lambda\rangle\langle p\lambda| + |p\lambda\rangle\langle h\lambda|) \cdot$$

$$+ \sum_\lambda \tfrac{1}{2} (1 - \cos\varphi_\lambda) (|p\lambda\rangle\langle p\lambda| - |h\lambda\rangle\langle h\lambda|) \tag{56}$$

which is also readily obtained by resumming ρ from Eqs. (51) and (52).

We have thus given explicit and rather simple expressions for both the operator ρ and the adiabatic kinetic collective energy K. Such expressions allow a direct study of the adiabaticity of any given TDHF solution. Moreover, by simple inspection of the time derivative of the eigenvalues of χ [cf. Eq. (50)], one can tell at any time how nonadiabatic effects may develop.

Adiabatic path

The knowledge of ρ_0 is in principle sufficient to characterize the adiabatic path. However, for practical purposes one needs to analyze it through the time behavior of the expectation values of a sufficient set of operators such as multipole moments, total Hamiltonian, etc. For instance, the expectation value of a one-body operator Q is given by

$$\mathrm{Tr}(Q\rho_0) = \frac{1}{4} \sum_\lambda \frac{1}{\cos^2 \tfrac{1}{2}\varphi_\lambda} (\langle 1\lambda | Q | 1\lambda \rangle + \langle 2\lambda | Q | 2\lambda \rangle + \langle 1\lambda | Q | 2\lambda \rangle + \langle 2\lambda | Q | 1\lambda \rangle) . \tag{57}$$

In the particular case where Q is invariant under time-reversal conjugation and where the original TDHF set $\{\mu\}$ diagonalizes the operator s_z, it is readily seen from Eq. (29) that the summation in Eq. (57) can be done only on spin-up states, upon replacing the factor $\frac{1}{4}$ by $\frac{1}{2}$, since contributions from spin-up and spin-down states are equal.

It is also possible to evaluate the HF Hamiltonian h_0 constructed from the reduced density matrix ρ_0. This defines the external field U_{ext} necessary to constrain the system to be described by the Slater determinant corresponding to ρ_0. The equation

$$[h_0, \rho_0] = -[U_{\mathrm{ext}}, \rho_0] \tag{58}$$

provides the p-h matrix elements of the external field U_{ext}. From this equation, one may easily check the current hypothesis[9] stating that the adiabatic path is given by a series of HF calculations under a constraint on a single time-independent operator Q, or in other words, whether or not

$$U_{\mathrm{ext}} \simeq -\lambda(t) Q. \tag{59}$$

However, even if it turns out that this approximation is justified, it still remains to determine the operator Q precisely. On the other hand, Eq. (59) may very well be not valid. This may be the case in a large amplitude motion if the adiabatic path experiences a sudden turn in the multidimensional space whose coordinates are expectation values of a set of operators $\{Q_i\}$. Such a drastic change in the constraining field has been advocated for instance in connection with the fission process, where during the descent from the saddle point to the scission point, the elongation motion seems to transform suddenly

into a necking motion.[24]

At last, it is also worthwhile to study the differences between the expectation values of some operators for the reduced density matrices ρ and ρ_0. If the considered operators are Hermitian and time-even, their trace with a time-odd operator like ρ_{2n+1} is zero.[7] For a one-body operator, this implies that its expectation value will only involve its p-p and h-h matrix elements. Furthermore, for such an operator Q, the difference $\mathrm{Tr}[Q(\rho-\rho_0)]$ is at least of second order in χ. This is in particular true for the total energy $E\{\rho\}$ which can be written as

$$E[\rho]=E[\rho_0]+T_2+V_2+\cdots, \tag{60}$$

where T_2 and V_2 are the second order terms in the expansion of the kinetic and potential energies, respectively. The sum T_2+V_2 is the adiabatic collective kinetic energy K defined in Eq. (6) and $E[\rho_0]$ the potential energy.[7,8]

Locality of the operator χ

Let us assume that ρ may be formally written as in Eq. (1) with an operator χ local and independent of spin and isospin. If in addition, the effective nucleon-nucleon potential is gauge invariant under the unitary transformation $e^{i\chi}$, then it has been demonstrated[20] that the TDHF equations of motion can be transformed into an equation of state for the nuclear medium, supplemented by a continuity equation and a Euler's equation corresponding to an irrotational flow.

An application of this, in a rather restricted case, has been made within the ATDHF framework by assuming a particular form for the adiabatic path and is often referred to as the scaling approximation.[9,23,25]

It is particularly important to notice that the demonstration made in Ref. 20 does not at all postulate that the operator χ appearing in Eq. (1) should have only p-h matrix elements (restriction referred to as the "natural choice" for χ in Ref. 7). We show below that, with this choice for χ, the additional condition of locality implies its vanishing.

Let us then assume that χ is given by Eq. (27) which clearly assesses its "natural" character, and postulate its locality, namely,

$$\langle\vec{r}\,|\chi|\,\vec{r}'\rangle=\chi(\vec{r})\delta(\vec{r}-\vec{r}'). \tag{61}$$

From Eq. (27), we have

$$\chi\,|p\lambda\rangle=\tfrac{1}{2}i\varphi_\lambda\,|h\lambda\rangle \tag{62}$$

and

$$\chi\,|h\lambda\rangle=-\tfrac{1}{2}i\varphi_\lambda\,|p\lambda\rangle. \tag{63}$$

Upon left multiplying Eq. (62) by χ and using Eq. (63), we readily see that χ is a constant operator. Then projecting Eq. (63) on $|h\lambda\rangle$, the vanishing of χ follows from the orthogonality of the states $|h\lambda\rangle$ and $|p\lambda\rangle$. Therefore the assumption χ local makes sense only if we abandon the "natural" choice for χ.

Indeed, in the calculations using the scaling approximation, the local operator χ was "non-natural": for the study of monopole vibrations,[25] χ was chosen to be proportional to r^2 while it was proportional to $(2z^2-x^2-y^2)$ for quadrupole vibrations.[9,25]

Note that there is a case where one knows the exact TDHF solution in the form of Eq. (1) with a non-natural operator. This is the uniform translation of a Slater determinant which will be studied in some detail in the next section.

VI. UNIFORM TRANSLATION

Consider a set of N static single-particle orthonormalized wave functions $\{\phi_j(\vec{r})\}$ defining a static density matrix ρ_s by

$$\rho_s(\vec{r},\vec{r}')=\langle\vec{r}\,|\rho_s|\,\vec{r}'\rangle=\sum_j\phi_j(\vec{r})\phi_j^*(\vec{r}'), \tag{64}$$

and let these wave functions satisfy the following set of static Hartree-Fock equations

$$h_s\phi_j(\vec{r})=e_j\phi_j(\vec{r}), \tag{65}$$

where h_s is the Hartree-Fock Hamiltonian associated with the density matrix ρ_s.

We define the translated wave functions corresponding to a translational velocity $\vec{v}$ (or to a momentum per nucleon $\vec{k}=m\vec{v}/\hbar$), by

$$\psi_j(\vec{r},t)=e^{-ie_jt/\hbar}\,e^{-i\hbar k^2t/2m}\,e^{i\vec{k}\cdot\vec{r}}\,\phi_j(\vec{r}-\vec{v}t), \tag{66}$$

and correspondingly a translated density matrix ρ, by

$$\begin{aligned}\rho(\vec{r},\vec{r}',t)&=\sum_j\psi_j(\vec{r},t)\,\psi_j^*(\vec{r}',t)\\&=e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\,\rho_s(\vec{r}-\vec{v}t,\vec{r}'-\vec{v}t).\end{aligned} \tag{67}$$

This definition of translated states is natural due to Galilean invariance, since the wave functions ψ_j satisfy the following set of TDHF equations[11]

$$i\hbar\dot{\psi}_j(\vec{r},t)=h\psi_j(\vec{r},t), \tag{68}$$

where h is the Hartree-Fock Hamiltonian associated with the density matrix ρ [cf. Eq. (67)]. The Slater determinant Ψ constructed from the single-particle states ψ_j simply represents the uniformly translated Slater determinant Ψ_s (with velocity $\vec{v}$) constructed from the ϕ_j's.

We multiply the states ψ_j by the time-independent phase factor $\exp[i(e_j/\hbar-\vec{k}\cdot\vec{v}/2)t]$ thus defining the new set of wave functions $\theta_j(\vec{r},t)$

$$\theta_j(\vec{r},t)=\theta_j(\vec{s})=e^{i\vec{k}\cdot\vec{s}}\,\phi_j(\vec{s}), \tag{69}$$

where $\vec{s}=\vec{r}-\vec{v}t$. The density matrix ρ can be reexpressed as

$$\rho(\vec{r},\vec{r}',t)=\sum_j \theta_j(\vec{s})\theta_j^*(\vec{s}'). \tag{70}$$

The states θ_j diagonalize ρ and can be taken as the starting states μ_j. We may further assume that they also diagonalize s_z, which implies that θ_j^* contains implicitly a bra in the spin space. The matrix elements of A are

$$A_{ij}=\langle\theta_i|\bar{\theta}_j\rangle=\int d\vec{s}\; e^{-2i\vec{k}\cdot\vec{s}}\,\theta_i^*(\vec{s})\bar{\theta}_j(\vec{s}). \tag{71}$$

Neither A, nor $A^\dagger$, depends upon time. As a consequence, all $\cos\varphi_\lambda$ are time-independent.

Let us define X_i^λ and Y_i^λ as the components of the eigenvectors $|1\lambda\rangle$ and $|2\lambda\rangle$ which diagonalize $AA^\dagger$ and $A^\dagger A$:

$$X_i^\lambda=\langle\theta_i|1\lambda\rangle,\quad Y_i^\lambda=\langle\bar{\theta}_i|2\lambda\rangle. \tag{72}$$

According to Eq. (13), we have (from now on, we exclude the case $\varphi_\lambda=\pi/2$)

$$Y_i^\lambda=\frac{1}{\cos\varphi_\lambda}\sum_j A_{ij}^\dagger X_j^\lambda. \tag{73}$$

These X's and Y's do not depend upon time due to the time independence of $AA^\dagger$ and $A^\dagger A$. From Eq. (15a), we obtain the hole wave functions

$$h^\lambda(\vec{r},t)=\frac{1}{2\cos\frac{1}{2}\varphi_\lambda}\sum_i[X_i^\lambda\,\theta_i(\vec{s})+Y_i^\lambda\bar{\theta}_i(\vec{s})] \tag{74}$$

and a similar equation for the particle states. From the right-hand side of Eq. (74), it can be seen that h^λ depends upon time only through the vector $\vec{s}=\vec{r}-\vec{v}t$.

The density matrix ρ_0 is given by

$$\rho_0(\vec{s},\vec{s}')=\sum_\lambda\frac{1}{2(1+\cos\varphi_\lambda)}\sum_{ij}[X_i^\lambda X_j^{\lambda*}\theta_i(\vec{s})\theta_j^*(\vec{s}')+X_i^\lambda Y_j^{\lambda*}\theta_i(\vec{s})\bar{\theta}_j^*(\vec{s}')$$
$$+Y_i^\lambda X_j^{\lambda*}\bar{\theta}_i(\vec{s})\theta_j^*(\vec{s}')+Y_i^\lambda Y_j^{\lambda*}\bar{\theta}_i(\vec{s})\bar{\theta}_j^*(\vec{s}')]. \tag{75}$$

As shown in Sec. IV, the assumption that no φ_λ are equal to $\pi/2$ implies the vanishing of half the X_i^λ and Y_i^λ for any given λ, in such a way that $\rho_0(\vec{s},\vec{s}')$ does not exhibit any spin vector component. Similarly, $\chi(\vec{s},\vec{s}')$ reads as

$$\chi(\vec{s},\vec{s}')=\sum_\lambda\frac{i\varphi_\lambda}{2\sin\varphi_\lambda}\sum_{ij}[Y_i^\lambda X_j^{\lambda*}\bar{\theta}_i(\vec{s})\theta_j^*(\vec{s}')$$
$$-X_i^\lambda Y_j^{\lambda*}\theta_i(\vec{s})\bar{\theta}_j^*(\vec{s}')], \tag{76}$$

where the second term in the sum over i and j is nothing but the complex conjugate of the first one, except for an implicit spin operator.

α particle

To illustrate in a simple manner the properties of χ and ρ_0 for translational motion, we now restrict the discussion to the case of a spin-isospin symmetric α particle, assuming the single wave function ϕ to be real. The matrix M [see Eq. (B1)] is the following 2 by 2 matrix

$$M=\begin{pmatrix}a & 0\\ 0 & a\end{pmatrix}, \tag{77}$$

where a is given by

$$a=\int\phi^2(\vec{s})\,e^{-2i\vec{k}\cdot\vec{s}}\,d\vec{s}=\cos\varphi\,e^{i\alpha}. \tag{78}$$

We will assume even parity of ϕ, which is natural for an α particle. Therefore, the phase α vanishes. Since [cf. Eq. (11)]

$$AA^\dagger X=\cos^2\varphi\,X, \tag{79}$$

and [cf. Eq. (13)]

$$Y=\frac{A^\dagger}{\cos\varphi}X, \tag{80}$$

we get for each spin-isospin state

$$X=1,\quad Y=1. \tag{81}$$

Therefore

$$h(\vec{s})=\frac{\cos(\vec{k}\cdot\vec{s})}{\cos(\frac{1}{2}\varphi)}\,\phi(\vec{s}),$$
$$p(\vec{s})=i\,\frac{\sin(\vec{k}\cdot\vec{s})}{\sin(\frac{1}{2}\varphi)}\,\phi(\vec{s}), \tag{82}$$

where the spin-isospin dependence is implicit for each of the four states. The density matrix ρ_0 is given in terms of ρ_s by

$$\rho_0(\vec{s},\vec{s}')=\frac{1}{1+\cos\varphi}\{\cos[\vec{k}\cdot(\vec{s}-\vec{s}')]$$
$$+\cos[\vec{k}\cdot(\vec{s}+\vec{s}')]\}\rho_s(\vec{s},\vec{s}') \tag{83}$$

and the operator χ is

$$\chi(\vec{s},\vec{s}') = \frac{\varphi}{\sin\varphi} \sin[\vec{k}\cdot(\vec{s}+\vec{s}')]\rho_s(\vec{s},\vec{s}'). \quad (84)$$

Taking advantage of the time independence of φ, the expression (47) for the adiabatic collective kinetic energy reduces to

$$K = 4\frac{\varphi}{\sin\varphi} \tfrac{1}{2} m |\vec{v}|^2. \quad (85)$$

Discussion

In the case of collective translation, the time-dependent density (67) may be written in the form of Eq. (1) with

$$\langle \vec{r}|\hat{\rho}_0|\vec{r}'\rangle = \rho_s(\vec{s},\vec{s}'), \quad (86)$$

$$\langle \vec{r}|\hat{\chi}|\vec{r}'\rangle = \vec{k}\cdot\vec{r}\,\delta(\vec{r}-\vec{r}'). \quad (87)$$

Such a choice for $\hat{\rho}_0$ and $\hat{\chi}$ is not "natural" according to the Baranger and Véneroni notation,[7] since $\hat{\chi}$ has nonvanishing p-p and h-h matrix elements. Moreover, this new decompositon of ρ provides a local operator χ.

We now compare the two sets of operators (ρ_0, χ) and $(\hat{\rho}_0, \hat{\chi})$ in the adiabatic limit. If $|\vec{k}|$ is small, φ is small, as seen from Eq. (78), and therefore χ is also small, which is indeed the adiabatic limit. From Eq. (83), ρ_0 then approaches ρ_s, i.e., $\hat{\rho}_0$, as $|\vec{k}|$ goes to zero, and the adiabatic translation energy given in Eq. (85) is equal to the exact translational energy, up to second order in φ.

The comparison between χ and $\hat{\chi}$ is slightly more complicated since it implies a comparison between matrix elements. Owing to parity symmetry, the p-p and h-h matrix elements of $\hat{\chi}$ are identically zero. In the adiabatic limit ($|\vec{k}| \to 0$), Eq. (78) provides the leading term in φ^2 as

$$\tfrac{1}{4}\varphi^2 \simeq \int (\vec{k}\cdot\vec{s})^2 \phi^2(\vec{s})\, d\vec{s}. \quad (88)$$

The p-h- matrix elements of $\hat{\chi}$ and χ are equal at the same order.[7] Therefore, the operators χ and $\hat{\chi}$, in the subspace $S+\bar{S}$, are identical in the adiabatic limit.

Apparently, $\hat{\chi}$ is local and at the same time has only p-h matrix elements; therefore, according to the discussion of Sec. V, it seems that it should be identically zero. However, this result was proven for χ only when the relevant particle and hole states were those corresponding to ρ_0. In other words, $\hat{\chi}$ would be identically zero if the states $h(\vec{s})$ and $p(\vec{s})$ altogether with $\hat{\chi}$ were to fulfill Eqs. (62) and (63), which is not the case:

$$\hat{\chi}(\vec{s})h(\vec{s}) = -\tfrac{1}{2} i\varphi\, p(\vec{s}), \quad (89)$$

corresponds to Eq. (63), but

$$\chi(\vec{s})p(\vec{s}) = \frac{2i}{\varphi}(\vec{k}\cdot\vec{s})^2 h(\vec{s}), \quad (90)$$

differs from Eq. (62).

We have therefore shown explicitly in the α particle case that the ATDHF formalism specified by the "natural" choice for χ is capable of describing exactly uniform translational collective motion in the limit of small velocities. However, this "natural" decomposition of ρ is not quite appropriate for translation where one would rather use the decomposition given by Eqs. (86) and (87).

Conversely, one may take advantage of this situation to eliminate in a simple way the overall center-of-mass motion of a nucleus to be studied. Let us assume that an excited nucleus is in uniform translation. Its center of mass is moving with a constant velocity $\vec{v}(=\hbar\vec{k}/m)$ defined by

$$\vec{v} = \frac{\hbar}{m}\frac{1}{N}\int \vec{j}(\vec{r})\, d\vec{r}, \quad (91)$$

where N is the total number of particles and $\vec{j}$ the usual current. Provided the effective Hamiltonian is Galilean invariant, we define a new set of wave functions ϕ_j by means of the gauge transformation

$$\phi_j(\vec{r},t) = e^{-i\hbar k^2 t/2m}\, e^{-i\vec{k}\cdot\vec{r}}\, \psi_j(\vec{r}-\vec{v}t). \quad (92)$$

While the evolution of the nucleus was known by the corresponding time evolution of the Ψ_j states, this transformation allows us to study its behavior in its rest frame, the overall translational kinetic energy being exactly removed.

VII. CONCLUSION

We have proposed a tractable method to obtain the operators ρ_0 and χ of the ATDHF method from a numerical TDHF solution. One of the formal aspects of our derivation is the fact that we have been able to express all relevant quantities in the particle-hole basis associated with ρ_0 which plays an important role in the ATDHF formalism. Moreover, such an explicit formulation has allowed us not only to illustrate some of the general statements of Refs. 7 and 8 but also to give further insight into the ATDHF approximations. For instance, we have given simple closed expressions for all the terms of the expansion of ρ in terms of χ as well as for the adiabatic collective kinetic energy. Furthermore, we have been able to clarify the discussion about the locality of χ and prove its incompatibility with the natural choice for χ.

More generally, we have extended the discussion of the authors of Ref. 7 to cases discarded therein. Indeed, the case where some eigenvalues of χ are equal to $\pm\pi/4$ have been found to be of practical importance in the study of collective motion of

odd nuclei. A natural formal extension of the standard formalism has provided a working framework for such studies. Another limiting case (vanishing part of the spectrum of χ) has also been studied. It corresponds to a situation where the dynamical treatment can be restricted to a subgroup of nucleons, the others then stand as spectators.

The whole formalism has been illustrated in the particularly simple case of uniform translation. In such cases, the exact TDHF solution is known and the validity of the ATDHF solution has been explicitly demonstrated in the limit of a small velocity. A practical method has been proposed to extract the adiabatic vibrational collective motion from possibly highly nonadiabatic translational motion, as may be encountered in final stages of heavy ion collisions.

Note that in practical calculations, if N is the number of single-particle wave functions evolved by the TDHF equations of motion, the dimensionality of the matrix $e^{4i\chi}$ to be diagonalized is *a priori* $2N$. We have shown that one has to diagonalize the N by N matrix $AA^\dagger$ and then to make rather trivial linear algebra manipulations. Furthermore, the dimension will be reduced to about $\frac{1}{2}N$ (matrix $MM^\dagger$) when the TDHF single-particle states are eigenstates of the spin operator s_z. This is the case when there is no spin-orbit term in the effective Hamiltonian and when dealing with even nuclei. As a matter of fact, most of the available TDHF calculations[26] are such. In addition, they impose an isospin degeneracy and the dimensionality is therefore reduced to $\frac{1}{4}N$. Any further symmetry (parity, axial symmetry, ...) implying a conservation of quantum numbers will result in the splitting of the $MM^\dagger$ matrix into a block diagonal form. These considerations provide further simplifications to practical calculations since they involve mainly the diagonalization of the matrix $MM^\dagger$.

Practical applications addressing themselves to the problem of low energy vibrations are under progress.[27]

ACKNOWLEDGMENTS

We gratefully acknowledge the hospitality enjoyed by us at the W. K. Kellogg Radiation Laboratory (P.B.) and at the theoretical division of the Los Alamos Scientific Laboratory (P.Q.). We have benefitted from many illuminating and challenging discussions, particularly with M. Véneroni and S. Koonin on the general problem, with D. Gogny on the orthonormalization procedure for bi-orthogonal basis and with J. R. Nix and C. Signarbieux on the adiabaticity of the low energy fission process. We also wish to thank M. Baranger and M. Véneroni for a manuscript of their forthcoming article, which was an inspiration for this work. Special thanks are due S. Koonin for many comments and a critical reading of the final manuscipt. This research was supported in part by the National Science Foundation [PHY76-83685] at Caltech, and by the U. S. Department of Energy [W-7450-ENG-36] at Los Alamos.

APPENDIX A: PROOF OF EXISTENCE FOR THE DECOMPOSITION OF A DENSITY MATRIX

Under a specific restriction discussed below, Baranger and Véneroni (Ref. 7) have given a proof of the existence and uniqueness of two Hermitian time-even operators ρ_0 and χ, satisfying Eq. (1):

$$\rho = e^{i\chi}\rho_0 e^{-i\chi},$$

given a one-body density matrix ρ. To substantiate the discussion of some important points of our present work, we reproduce and discuss in this Appendix the main steps of their proof.

Defining the Hermitian operator τ as

$$\tau = 2\rho - 1, \tag{A1}$$

the projector identity for ρ implies that τ is also unitary:

$$\tau^2 = 1. \tag{A2}$$

In the same way, the time-reversed operator $\bar{\tau}$ is also Hermitian and unitary, so that the operator $\tau\bar{\tau}$ is unitary and may be written as

$$\tau\bar{\tau} = e^{4i\chi}, \tag{A3}$$

where χ is an Hermitian operator. The adjoint of $\tau\bar{\tau}$ is

$$\bar{\tau}\tau = e^{-4i\chi} \tag{A4}$$

and its time reverse is

$$\bar{\tau}\tau = e^{-4i\bar{\chi}}. \tag{A5}$$

It immediately follows that χ is time-even ($\chi = \bar{\chi}$). Left multiplying Eq. (A4) by τ yields

$$e^{4i\chi}\tau = \tau e^{-4i\chi}. \tag{A6}$$

So far, no assumptions have been made about χ. At this point, Baranger and Véneroni introduce an assumption which defines, in their words, the "natural choice" for χ. Specifically, they fix the phase $4\chi^\lambda$ of each eigenvalue of $\tau\bar{\tau}$ to lie within one of the two semiopen intervals $]-\pi, +\pi]$, $[-\pi, +\pi[$. Since their main concern was the study of small χ values, they have discarded the ambiguous case where $|\chi^\lambda| = \pi/4$. This limiting case is discussed in Sec. IV. In this Appendix, we assume that χ^λ lies strictly between $-\pi/4$ and $+\pi/4$ for any λ.

From the consideration of the matrix elements of $e^{4i\chi}\tau - \tau e^{-4i\chi}$ and $\chi\tau + \tau\chi$, the vanishing of the former implies the vanishing of the latter, i.e.,

$$\chi\tau + \tau\chi = 0 \tag{A7}$$

or, in terms of ρ:

$$\chi\rho + \rho\chi = \chi . \tag{A8}$$

This expression implies that χ has neither p-p nor h-h matrix elements, where particle and hole refer to unoccupied and occupied states of ρ. As a consequence of Eq. (A7), one has, for any complex number α:

$$e^{i\alpha\chi}\tau = \tau e^{-i\alpha\chi} . \tag{A9}$$

Let us consider the operator

$$\tau_0 = e^{-2i\chi}\tau . \tag{A10}$$

Independently of the phase convention for $e^{4i\chi}$, this operator can easily be proven to be time-even and unitary. It is also Hermitian, as can be seen from Eq. (A9) with $\alpha = -2$. This latter property is therefore a direct consequence of the phase convention. Let us define a Hermitian time-even operator ρ_0 by

$$\tau_0 = 2\rho_0 - 1 . \tag{A11}$$

Note that ρ_0 satisfies the projector identity and therefore defines a time-even independent-particle state. In addition τ_0 satisfies an equation similar to Eq. (A7):

$$\tau_0\chi + \chi\tau_0 = 0 , \tag{A12}$$

which shows that χ has neither p-p nor h-h matrix elements, where now p and h refer to unoccupied and occupied states of ρ_0. From Eqs. (A9) and (A10), one has

$$\tau = e^{i\chi}\tau_0 e^{-i\chi} , \tag{A13}$$

and finally

$$\rho = e^{i\chi}\rho_0 e^{-i\chi} . \tag{A14}$$

Since the operators ρ_0 and χ are both Hermitian and time-even and since, in addition, ρ_0 is idempotent, this provides a proof of existence of the set (ρ_0, χ) under the only condition that the eigenvalues of χ lie within the open interval $]-\pi/4, +\pi/4[$. This condition implies the natural choice for χ[cf. Eq. (A8)].

The proof of uniqueness is not essential for our purpose, and we do not derive it here, it can be found in Ref. 7.

APPENDIX B: DIAGONALIZATION OF THE AA^+ MATRIX WHEN BUILT FROM EIGENSTATES OF s_z

Let us consider a set $\{\nu_i\}$ of TDHF solutions which are eigenstates of the spin-operator s_z. This set is composed of n_+ spin-up states and n_- spin-down states. The spin-up states will be written as $|u\rangle|+\rangle$, where $|u\rangle$ and $|+\rangle$ are, respectively, the space and spin parts of the state $|\nu\rangle$. In the same way, the spin-down states will be denoted by $|d\rangle|-\rangle$. The overlap matrix A then has zero matrix elements between different spin states. Similarly, ρ, $\bar{\rho}$, and therefore $e^{4i\chi}$ do not modify a given spin state. We can thus separate $S + \bar{S}$ into the spin up subspace $(\{|u\rangle|+\rangle\} + \{|\bar{d}\rangle|\bar{-}\rangle\})$ and the spin-down subspace $(\{|d\rangle|-\rangle\} + \{|\bar{u}\rangle|\bar{+}\rangle\})$.

First we consider the spin-up subspace, in which the A and A^+ matrices read as

$$\begin{aligned} A &= M\langle +|\bar{-}\rangle , \\ A^\dagger &= M^\dagger\langle\bar{-}|+\rangle , \end{aligned} \tag{B1}$$

where M is the overlap matrix $\langle u|\bar{d}\rangle$. The dimensions of the A and $A^\dagger$ matrices are $n_+ \times n_-$ and $n_- \times n_+$, respectively. From Eq. (B1), the $n_+ \times n_+$ square matrix $AA^\dagger$ becomes

$$AA^\dagger = MM^\dagger , \tag{B2}$$

since, irrespective of the phase convention for the time-reversed state $|\bar{-}\rangle$,

$$|+\rangle\langle +| = |\bar{-}\rangle\langle\bar{-}| . \tag{B3}$$

Defining $|1\lambda\rangle$ as

$$|1\lambda\rangle = |x\lambda\rangle|+\rangle , \tag{B4}$$

the reduction of Eq. (11) to the spin-up subspace is

$$MM^\dagger|x\lambda\rangle = \cos^2\varphi_\lambda|x\lambda\rangle . \tag{B5}$$

We have thus obtained n_+ eigenvectors $|x\lambda\rangle$ associated to eigenvalues $\cos^2\varphi_\lambda$ which diagonalize the $n_+ \times n_+$ matrix $MM^\dagger$. Multiplying Eq. (B5) by $M^\dagger$, we get

$$M^\dagger M(M^\dagger|x\lambda\rangle) = \cos^2\varphi_\lambda(M^\dagger|x\lambda\rangle) . \tag{B6}$$

Therefore the n_+ states $M^\dagger|x\lambda\rangle$ diagonalize the $n_- \times n_-$ matrix $M^\dagger M$. If $n_+ > n_-$ this implies that some of the states $M^\dagger|x\lambda\rangle$ which are orthogonal:

$$\langle x'|MM^\dagger|x\rangle = \cos^2\varphi\langle x'|x\rangle = 0 \tag{B7}$$

have a zero norm, i.e., $M^\dagger|x\lambda\rangle = 0$. So, at least $n_+ - n_-$ vectors $M^\dagger|x\rangle$ must have a norm 0. Since their norm is nothing but $\cos^2\varphi_\lambda$, it means that $n_+ - n_-$ eigenvalues $\cos^2\varphi_\lambda$ must vanish. In the situation where $n_+ < n_-$ a similar demonstration in the spin-down subspace shows that $n_- - n_+$ eigenvalues are 0. Therefore if $n_+ \neq n_-$, at least $|n_+ - n_-|$ eigenvalues $\cos^2\varphi_\lambda$ must be zero (i.e., $\varphi_\lambda = \pi/2$).

From now on, we assume that there are no eigenvalues $\cos^2\varphi_\lambda$ of $MM^\dagger$ equal to zero (and therefore $n_+ = n_-$). The normalized states

$$|y\lambda\rangle = \frac{1}{\cos\varphi_\lambda} M^\dagger |x\lambda\rangle \tag{B8}$$

diagonalize $M^\dagger M$ with eigenvalue $\cos^2\varphi_\lambda$. According to Eq. (13), the states $|2\lambda\rangle$ are

$$|2\lambda\rangle = |y\lambda\rangle|+\rangle . \tag{B9}$$

In the spin-down subspace, the same demonstration can be carried out, and we have

$$A = (M^\dagger)^* \langle \mp | - \rangle , \tag{B10}$$

therefore

$$A^\dagger A = (MM^\dagger)^* . \tag{B11}$$

By comparing Eq. (B11) to Eq. (B2), we immediately see that the states $|2'\lambda\rangle$ which diagonalize $A^\dagger A$ can be deduced from the states $|1\lambda\rangle$ by

$$|2\lambda'\rangle = |x\lambda^*\rangle|\mp\rangle . \tag{B12}$$

The transformation (13) of $|1\lambda\rangle$ in $|2\lambda\rangle$ via $M^\dagger$ becomes in the spin-down subspace the transformation of $|1'\lambda\rangle$ in $|2'\lambda\rangle$ via $(M^\dagger)^*$, and then

$$|1'\lambda\rangle = |y^*\rangle|\mp\rangle . \tag{B13}$$

The comparison of Eqs. (B4) and (B12) implies

$$|\overline{1\lambda}\rangle = |2'\lambda\rangle . \tag{B14}$$

Similarly, from Eqs. (B9) and (B13)

$$|\overline{2\lambda}\rangle = |1'\lambda\rangle . \tag{B15}$$

APPENDIX C: DERIVATION OF THE ADIABATIC COLLECTIVE KINETIC ENERGY

The adiabatic collective kinetic energy K is given in Eq. (48) by

$$K = \frac{\hbar}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda} \operatorname{Im}[\langle \dot{1}\lambda|1\lambda\rangle + \langle 2\lambda|\dot{2}\lambda\rangle] , \tag{C1}$$

In this Appendix, we express the overlaps $\langle \dot{1}\lambda|1\lambda\rangle$ and $\langle 2\lambda|\dot{2}\lambda\rangle$ in terms of quantities which do not involve explicit time derivatives. For this purpose, we introduce the expansion of the states $|1\lambda\rangle$ and $|2\lambda\rangle$ in the spaces S and $\bar{S}$

$$\begin{aligned} |1\lambda\rangle &= \sum_\mu X_\mu^\lambda |\mu\rangle , \\ |2\lambda\rangle &= \sum_{\mu'} Y_{\mu'}^\lambda |\overline{\mu'}\rangle . \end{aligned} \tag{C2}$$

When taking the time derivatives of Eqs. (C2), one introduces the time derivatives of the states $|\mu\rangle$ and $|\bar{\mu}\rangle$ which are known from the TDHF equations (68). The time derivatives of the components X_μ^λ, $Y_{\mu'}^\lambda$ are also introduced and remain to be evaluated. These components generally vary in time, except in very particular cases such as translations (see Sec. VI).

From Eqs. (C2), we may express the two overlaps in Eq. (C1) as

$$\begin{aligned} i\hbar\langle \dot{1}\lambda|1\lambda\rangle &= -\sum_{\mu\mu'} X_\mu^{\lambda *} \langle \mu|h|\mu'\rangle X_{\mu'}^\lambda \\ &\quad + i\hbar \sum_\mu \dot{X}_\mu^{\lambda *} X_\mu^\lambda , \\ i\hbar\langle 2\lambda|\dot{2}\lambda\rangle &= -\sum_{\mu\mu'} Y_\mu^{\lambda *} \langle \bar{\mu}|\bar{h}|\bar{\mu}'\rangle Y_{\mu'}^\lambda \\ &\quad + i\hbar \sum_\mu Y_\mu^{\lambda *} \dot{Y}_\mu^\lambda , \end{aligned} \tag{C3}$$

where $\bar{h}$ is the time-reverse HF Hamiltonian. The energy K becomes thus

$$\begin{aligned} K &= \frac{1}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda} [\langle 1\lambda|h|1\lambda\rangle + \langle 2\lambda|\bar{h}|2\lambda\rangle] \\ &\quad + \frac{\hbar}{4} \sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda} \operatorname{Im}\left(\sum_\mu (\dot{X}_\mu^{\lambda *} X_\mu^\lambda + Y_\mu^{\lambda *} \dot{Y}_\mu^\lambda) \right) . \end{aligned} \tag{C4}$$

In order to derive a more convenient expression for the second term of the right-hand side of Eq. (C4), we write explicitly the eigenvalue problem for which the X's are solutions, namely [cf. Eqs. (10) and (11)]:

$$\sum_{\mu'\nu} \langle \mu|\bar{\nu}\rangle \langle \bar{\nu}|\mu'\rangle X_{\mu'}^\lambda = \cos^2\varphi_\lambda X_\mu^\lambda . \tag{C5}$$

Upon multiplying Eq. (C5) by $i\hbar$ and taking its time derivative, we get

$$\begin{aligned} \sum_{\mu'} \langle \mu|[\bar{\rho}, h + \bar{h}]|\mu'\rangle X_{\mu'}^\lambda + \sum_{\mu'} \langle \mu|\bar{\rho}|\mu'\rangle i\hbar \dot{X}_{\mu'}^\lambda , \\ = -i\hbar\dot{\varphi}_\lambda X_\mu^\lambda \sin 2\varphi_\lambda + i\hbar \dot{X}_\mu^\lambda \cos^2\varphi_\lambda . \end{aligned} \tag{C6}$$

The time derivative of φ_λ can be evaluated by multiplying the latter expression by $X_\mu^{\lambda *}$ and summing over μ, to obtain

$$\begin{aligned} \langle 1\lambda|[\bar{\rho}, h + \bar{h}]|1\lambda\rangle + \sum_{\mu\mu'\nu} X_\mu^{\lambda *} \langle \mu|\bar{\nu}\rangle \langle \bar{\nu}|\mu'\rangle i\hbar \dot{X}_{\mu'}^\lambda , \\ = -i\hbar\dot{\varphi}_\lambda \sin 2\varphi_\lambda + i\hbar \sum_\mu X_\mu^{\lambda *} \dot{X}_\mu^\lambda \cos^2\varphi_\lambda , \end{aligned} \tag{C7}$$

which, due to Eq. (C5), reduces to

$$i\hbar\dot{\varphi}_\lambda \sin 2\varphi_\lambda = \langle 1\lambda|[h + \bar{h}, \bar{\rho}]|1\lambda\rangle . \tag{C8}$$

Replacing $\dot{\varphi}_\lambda$ in Eq. (C6) by its value from Eq. (C8) would give a set of linear equations for $\dot{X}_\mu^\lambda$. However, as we shall see below, the solution to such equations is not needed for the evaluation of K.

Assuming the $\dot{X}_\mu^\lambda$ known, the time derivatives $\dot{Y}_\mu^\lambda$ are obtained by differentiating Eq. (13), written as

$$Y_\mu^\lambda = \frac{1}{\cos\varphi_\lambda} \sum_\nu \langle \bar{\mu}|\nu\rangle X_\nu^\lambda \tag{C9}$$

to get

$$i\hbar\dot{Y}_\mu^\lambda = i\hbar\dot{\varphi}_\lambda Y_\mu^\lambda \tan\varphi_\lambda + \frac{1}{\cos\varphi_\lambda}\sum_\nu \langle\bar{\mu}|(h+\bar{h})|\nu\rangle X_\nu^\lambda + \frac{i\hbar}{\cos\varphi_\lambda}\sum_\nu \langle\bar{\mu}|\nu\rangle\dot{X}_\nu^\lambda . \quad \text{(C10)}$$

In Eqs. (C9) and (C10) we have assumed that φ_λ is not equal to $\pi/2$. This restriction is perfectly justified since, as seen in Sec. IV, the corresponding states $|h\lambda\rangle$ and $|p\lambda\rangle$ are such that their contribution to K is identically zero.

As we do not need all the $\dot{Y}_\mu^\lambda$ individually, but rather the linear combination appearing in Eq. (C4), we multiply Eq. (C10) by $Y_\mu^{\lambda *}$ and sum over μ to obtain

$$i\hbar\sum_\mu Y_\mu^{\lambda *}\dot{Y}_\mu^\lambda = i\hbar\dot{\varphi}_\lambda \tan\varphi_\lambda + \frac{1}{\cos^2\varphi_\lambda}\langle 1\lambda|\bar{\rho}(h+\bar{h})|1\lambda\rangle + i\hbar\sum_\mu X_\mu^{\lambda *}\dot{X}_\mu^\lambda , \quad \text{(C11)}$$

where we have used Eqs. (C2), (C5), and (C9). The linear combination of $\dot{X}_\mu^{\lambda *}$ and $\dot{Y}_\mu^\lambda$ in Eq. (C4) is

$$i\hbar\sum_\mu (Y_\mu^{\lambda *}\dot{Y}_\mu^\lambda + \dot{X}_\mu^{\lambda *}X_\mu^\lambda) = i\hbar\dot{\varphi}_\lambda \tan\varphi_\lambda + \frac{1}{\cos^2\varphi_\lambda}\langle 1\lambda|\bar{\rho}(h+\bar{h})|1\lambda\rangle , \quad \text{(C12)}$$

where we have taken advantage of the fact that the states $|1\lambda\rangle$ are normalized to unity at all times, namely,

$$\sum_\mu (\dot{X}_\mu^{\lambda *}X_\mu^\lambda + X_\mu^{\lambda *}\dot{X}_\mu^\lambda) = 0 . \quad \text{(C13)}$$

If we now replace $\dot{\varphi}_\lambda$ in Eq. (C12) by the expression (C8), we obtain

$$i\hbar\sum_\mu (Y_\mu^{\lambda *}\dot{Y}_\mu^\lambda + \dot{X}_\mu^{\lambda *}X_\mu^\lambda) = \frac{1}{2\cos^2\varphi_\lambda}[\langle 1\lambda|\bar{\rho}(h+\bar{h})|1\lambda\rangle + \langle 1\lambda|(h+\bar{h})\bar{\rho}|1\lambda\rangle] = \frac{1}{2\cos\varphi_\lambda}[\langle 2\lambda|(h+\bar{h})|1\lambda\rangle + \langle 1\lambda|(h+\bar{h})|2\lambda\rangle] , \quad \text{(C14)}$$

and finally for K [see Eq. (C4)]

$$K = \frac{1}{4}\sum_\lambda \frac{\varphi_\lambda}{\sin\varphi_\lambda}(\langle 1\lambda|h|1\lambda\rangle + \langle 2\lambda|\bar{h}|2\lambda\rangle) - \frac{1}{4}\sum_\lambda \frac{\varphi_\lambda}{\sin 2\varphi_\lambda}[\langle 2\lambda|(h+\bar{h})|1\lambda\rangle + \langle 1\lambda|(h+\bar{h})|2\lambda\rangle] . \quad \text{(C15)}$$

This expresses the adiabatic collective kinetic energy K in a form directly calculable from the states $|1\lambda\rangle$ and $|2\lambda\rangle$, without having to extract explicitly their time derivatives. In addition, we have obtained a simple expression for the time derivatives of the eigenvalue $\frac{1}{2}\varphi_\lambda$ of the operator χ.

*Permanent address: Service de Physique Théorique, CEN-Saclay, B.P. No. 2, 91190 Gif-sur-Yvette, France.

†Permanent address: IPN Orsay, Division de Physique Théorique, B. P. No. 1, 91406 Orsay, France.

[1] P. A. M. Dirac, Proc. Cambridge Phil. Soc. 26, 376 (1930).

[2] P. Bonche, S. Koonin, and J. W. Negele, Phys. Rev. C 13, 1226 (1976).

[3] S. T. Belyaev, Nucl. Phys. 64, 17 (1965).

[4] F. Villars, in *Dynamical Structure of Nuclear States, proceedings of the 1971 Mont Tremblant International Summer School*, edited by D. J. Rowe *et al.* (University of Toronto Press, Toronto, 1972), p. 3.

[5] F. Villars, in *Nuclear Self Consistent Fields*, edited by G. Ripka and M. Porneuf (North-Holland, Amsterdam, 1975), p. 3.

[6] F. Villars, Nucl. Phys. A285, 269 (1977).

[7] M. Baranger and M. Véneroni, Ann. Phys. (N.Y.) (to be published). A preliminary presentation of the above work has been given at the 1972 European Physical Society Conference at Aix en Provence; M. Baranger, J. Phys. (Paris) 33, C5-61 (1972).

[8] D. M. Brink, M. J. Giannoni, and M. Veneroni, Nucl. Phys. A258, 237 (1976).

[9] M. J. Giannoni, F. Moreau, P. Quentin, D. Vautherin, M. Véneroni, and D. M. Brink, Phys. Lett. 65B, 305 (1976).

[10] D. R. Inglis, Phys. Rev. 96, 1059 (1954); 103, 1786 (1956).

[11] D. J. Thouless and J. G. Valatin, Nucl. Phys. 31, 211 (1962).

[12] H. Ehrenreich and M. H. Cohen, Phys. Rev. 115, 786 (1959); J. Goldstone and K. Gottfried, Nuovo Cimento 13, 849 (1959).

[13] J. P. Blaizot and D. Gogny, Nucl. Phys. A284, 429 (1977), and references therein; G. Saunier, J. Le Tourneux, B. Rouben, and R. Padjen, Can. J. Phys. 51, 629 (1973).

[14] G. Bertsch and S. F. Tsai, Phys. Rep. 18C, 125 (1975); K. F. Liu and G. E. Brown, Nucl. Phys. A265, 385 (1976).

[15] K. F. Liu and Nguyen Van Giai, Phys. Lett. 65B, 23 (1976); S. Krewald, V. Klemt, J. Speth, and A. Faess-

ler, Nucl. Phys. A281, 166 (1977).
[16]Å. Bohr and B. R. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. II.
[17]See, e.g., K. T. R. Davies, R. A. Managan, J. R. Nix, and A. J. Sierk, Phys. Rev. C 16, 1890 (1977).
[18]J. Blocki, Y. Boneh, J. R. Nix, J. Randrup, M. Robel, A. J. Sierk, and W. J. Swiatecki, Ann. Phys. (N.Y.) (to be published).
[19]H. Nifenecker, C. Signarbieux, R. Babinet, and J. Poitou, in *Physics and Chemistry of Fission 1973* (IAEA, Vienna, 1974), Vol. II, p. 117.
[20]M. J. Giannoni, D. Vautherin, M. Véneroni, and D. M. Brink, Phys. Lett. 63B, 8 (1976).
[21]P. Ring and P. Schuck, Nucl. Phys. A292, 20 (1977).
[22]D. Gogny, private communication.
[23]Y. M. Engel, D. M. Brink, K. Goeke, S. J. Krieger, and D. Vautherin, Nucl. Phys. A249, 215 (1975).
[24]U. Mosel and H. W. Schmitt, Nucl. Phys. A165, 73 (1971).
[25]D. Vautherin, Phys. Lett. 57B, 425 (1975).
[26]See, for instance, the review article by P. Bonche [J. de Phys. (Paris) 37, C5-213 (1976)] and also H. Flocard, S. E. Koonin, and M. Weiss [Phys. Rev. C 17, 1682 (1978)]; P. Bonche, B. Grammaticos, and S. E. Koonin, Phys. Rev. C 17, 1700 (1978).
[27]P. Bonche, H. Doubre, and P. Quentin (unpublished).