# Mass parameters in the adiabatic time-dependent Hartree-Fock approximation. I. Theoretical aspects; the case of a single collective variable

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A self-consistent method for evaluation of mass parameters is presented in the framework of the adiabatic limit of the time-dependent Hartree-Fock approximation, reduced to a single collective variable. The corresponding collective path is assumed to be given either by solving a constrained Hartree-Fock problem with a given time-even constraining operator $Q$, or by scaling a static Hartree-Fock equilibrium solution. In the former case, once the path is given, a method for solving the equation of motion (of the Hamilton type) is provided, which reduces to a double-constrained Hartree-Fock problem with the time-even constraint $Q$ and with a time-odd constraining operator $P$. In the case of the scaling path, an analytical solution of the Hamilton equation is discussed and the adiabatic mass for the particular case of an isoscalar quadrupole $Q_{20}$ mode is given. The operator $P$, which is uniquely determined from the knowledge of $Q$, has the physical meaning of a momentum operator; it satisfies, together with $Q$, a weak quantal conjugation relation. Finally, the connection between the two paths is discussed in terms of generalized random-phase approximation sum rules.

[NUCLEAR STRUCTURE Evaluation of mass parameters within time-dependent Hartree-Fock approximation in adiabatic limit for single collective variable motion. Discussion and comparison of constrained Hartree-Fock and scaling paths. Expression as a doubly constrained Hartree-Fock problem with momentum operator uniquely defined from coordinate operator. Connection with sum rule and Inglis cranking approaches.]

## I. INTRODUCTION

During the last few years, significant progress has been made in the theoretical description of collective phenomena in nuclei. Most of the work in this direction had the same purpose: to find a coherent microscopic foundation for the Copenhagen phenomenological collective model,[1] and at the same time to get free of several too restrictive hypotheses underlying the existing microscopic theories [random phase approximation (RPA), cranking model, ...]. Reaching this goal would also considerably increase the predictive character of the collective model by allowing one to calculate, from the nucleon-nucleon interaction, the values of its adjustable parameters. The Inglis cranking model[2] was a first attempt in this respect; however, it suffers from a lack of self-consistency. Thouless and Valatin[3] gave a self-consistent version of the cranking formula in the particular case of a slowly rotating nucleus. For a long time, one has had at one's disposal another microscopic formalism, the RPA; this approximation can be very efficient for the description of several collective properties (especially of giant resonances), but it is clearly not adequate for large amplitude motions, such as fusion, fission, and other nonharmonic nuclear phenomena such as those encountered, for instance, in soft nuclei.

The time-dependent Hartree-Fock approximation, with the additional hypothesis of small collective velocities (compared to some characteristic single-particle velocities), has been the foundation of recent theoretical formulation. The main interest of the adiabatic approximation, besides its physical content, is to allow a connection with the phenomenological collective model. The Villars approach[4] deals with a single collective variable; the collective path is formally defined by an iterative procedure, with some "reasonable" guess for the starting point. Baranger and Véneroni[5] have obtained two sets of coupled equations of motion which, in the adiabatic limit, are equivalent to the time-dependent Hartree-Fock (TDHF) equation. As shown in Ref. 6, these equations are equivalent to Hamilton-like equations derived from a variational principle similar to a classical least action condition. The solution of these equations would in principle provide both the mass parameters and the collective paths for the collective degrees of freedom. It is clear, however, that the practical implementation of this problem would require a considerable amount of numerical effort.

To bypass some of these difficulties, one may decide in a first step to make an ansatz for the collective trajectories. It then becomes possible to solve the first set of Hamilton equations of motion providing the mass parameters. This is the ap-

 

proach adopted in the present paper, the formal framework being the adiabatic time-dependent Hartree-Fock (ATDHF) formalism as presented in Refs. 5 and 6, reduced to a single collective variable. This approach lies between the exact ATDHF solution and phenomenological calculations such as those using Nilsson single-particle wave functions to compute inertial parameters by the Inglis cranking formula. In other words, we shall compute in a consistent way the inertial parameters. We shall not study the dynamical validity of the path, which will be chosen *a priori*. We shall, however, compare the properties of two different choices for this path. Moreover, we shall present a method for the computation of the masses which we believe to be particularly convenient and accurate.

All the matter is presented at a very general level. In an accompanying paper[7] (hereafter referred as II), we specialize to the isoscalar $Q_{20}$ quadrupole mode, and give results obtained for large and small amplitude motions for the corresponding mass parameters, calculated with several Skyrme interactions. We would like to emphasize that the present work has been carried out entirely in the line of Refs. 5 and 6, and that the quotations of other work which will be found here constitutes a step towards a better understanding of the connections between different formulations of collective theories[4,8-10] and towards their unification.

## II. THE ADIABATIC TIME-DEPENDENT HARTREE-FOCK APPROXIMATION

In the independent particle approximation, one describes the physical system only in terms of its one-body reduced density operator $\rho$. For a pure $A$-body state, the operator $\rho$ writes

$$\rho=\sum_{i=1}^{A}|i\rangle\langle i|\,, \tag{2.1}$$

where $\{|i\rangle;\ i=1,\ldots,A\}$ is an orthonormal set of single-particle (SP) states. The projector character of $\rho$,

$$\rho^2=\rho\,, \tag{2.2}$$

clearly follows from Eq. (2.1). In other words, the corresponding wave function $\Psi$ is a Slater determinant built with the $A$ single-particle states $|i\rangle$.

Given a Hamiltonian $H$ composed of a kinetic energy operator $T$ and a two-body interaction $V$,[11] the dynamical evolution of $\rho$ is governed, in terms of $W(\rho)$, the so-called Hartree-Fock Hamiltonian (which is the one-body reduction of $H$ with respect to $\Psi$)

$$W(\rho)=T+\mathrm{Tr}_2\tilde{V}(1,2)\rho(2)\,, \tag{2.3}$$

by the TDHF equation[12]:

$$i\hbar\dot{\rho}=[W(\rho),\rho]\,, \tag{2.4}$$

which is the one-body reduction of the Liouville-Von Neumann equation.

The total TDHF energy, easily shown to be a constant of the motion, is given by

$$\langle\Psi|H|\Psi\rangle=E[\rho]=\mathrm{Tr}(T\rho)+\tfrac{1}{2}\,\mathrm{Tr}\,\mathrm{Tr}\rho\tilde{V}\rho\,. \tag{2.5}$$

The notation of Eqs. (2.3) and (2.5) is standard (see, e.g., Ref. 5).

The TDHF equation (2.4) can be derived in various ways, and, in particular, from the stationarity principle:

$$\delta\int_{t_1}^{t_2}\left\langle\Psi\left|i\hbar\frac{\partial}{\partial t}-H\right|\Psi\right\rangle dt=0\,, \tag{2.6}$$

where $\Psi$ and $\Psi^*$, restricted to be Slater determinants, should be varied independently, with fixed end points for $\Psi$.

*The adiabaticity assumptions.* To give a simple formulation of the ATDHF formalism, Baranger and Véneroni have introduced the following decomposition of the density operator $\rho$:

$$\rho=e^{i\chi}\rho_0 e^{-i\chi}\,. \tag{2.7}$$

The justification for such a decomposition is given by the following theorem, studied in Ref. 5, and further investigated in Refs. 13–15.

*Decomposition theorem.*[16] Given a Hermitian projection operator $\rho$ and its time-reversal conjugate $\rho_T$,

(i) *There exists* a projection operator $\rho_0$ and an operator $\chi$, both Hermitian and time-even:

$$\rho_0=\rho_0^{\dagger}=(\rho_0)_T=\rho_0{}^2\,, \tag{2.8}$$

$$\chi=\chi^{\dagger}=\chi_T \tag{2.9}$$

such as Eq. (2.7) is fulfilled, *provided* $\rho$ and $\rho_T$ do not have any common eigenvector corresponding to different eigenvalues of $\rho$ and $\rho_T$.

(ii) In addition to the requirements (2.8) and (2.9), *the supplementary conditions*

$$\rho_0\chi+\chi\rho_0=\chi\,, \tag{2.10}$$

$$\lambda_i\in\left]-\frac{\pi}{4},\frac{\pi}{4}\right[\,, \tag{2.11}$$

where $\lambda_i$ is any eigenvalue of $\chi$, *ensure the uniqueness* of the decomposition (2.7).

One can easily show that there cannot exist any decomposition (2.7) satisfying (2.8) and (2.9) for the one-body reduced density operator of an odd system of fermions; consequently, the ATDHF formalism as presented in Refs. 5 and 6 is restricted to even-even nuclei. When dealing with a sp density operator built from states $|i\rangle$ [see Eq.

(2.1)] which are eigenstates of the spin projection $s_z$, the (sufficient) condition for the existence of the decomposition to be satisfied by $\rho$ and its time-reversed $\rho_T$ requires the same number of spin-up and spin-down occupied states $\{|i\rangle;\ i=1,\ldots,A\}$.[14,15] This sufficient condition formulated in the decomposition theorem will be satisfied in all physical situations considered in this work (see also II); this allows us to make use of the decomposition (2.7) without any further justification.

Following Baranger and Véneroni, we call "natural" the particular decomposition unequivocally defined by Eqs. (2.7), (2.8), (2.9), and by the additional conditions (2.10) and (2.11). Notice that the condition (2.10) can be written equivalently (see Appendix A) as

$$\rho_0 \chi \rho_0 = \sigma_0 \chi \sigma_0 = 0 , \tag{2.12}$$

where $\sigma_0 = 1 - \rho_0$. Defining the hole (or particle) states as eigenvectors of $\rho_0$ (or $\sigma_0$) associated with the eigenvalue 1, it appears from Eq. (2.12) that the operator $\chi$ of the "natural" decomposition has only particle-hole and hole-particle matrix elements.

In the summary of the ATDHF formalism which follows we will make use of the natural decomposition of $\rho$. The apparent lack of generality due to this peculiar choice of the decomposition (2.7) will be discussed below.

The hypothesis of slow motion is introduced by the assumption that $\chi$ and its time derivative $\dot{\chi}$ are small.[17] Leaving for a moment the physical content of such conditions, we expand the exponential operators in Eq. (2.7) and truncate the resulting expression of $\rho$ at second order in $\chi$:

$$\rho(t) = \rho_0(t) + \rho_1(t) + \rho_2(t) , \tag{2.13}$$

with

$$\rho_1 = i[\chi, \rho_0] , \tag{2.14}$$

$$\rho_2 = -\tfrac{1}{2}[\chi, [\chi, \rho_0]] . \tag{2.15}$$

It is worth recalling here that the zero-order term $\rho_0$ depends on time, and may deviate considerably from a static Hartree-Fock solution, allowing thus the description of large amplitude motions. In this respect, the ATDHF expansion (2.13) differs basically from the one usually made in the derivation of RPA equations around the static Hartree-Fock (HF) equilibrium (see, e.g., Ref. 18).

*Classical Hamiltonian formulation*

By inserting the expansion (2.13) into the expression (2.5) for the TDHF energy, Baranger and Véneroni have obtained a division of the adiabatic energy into a potential and a kinetic part. The corresponding Lagrange equations have then been shown to be equivalent to the equations obtained directly by inserting the expansion (2.13) into the time-even and time-odd parts of the TDHF equation (2.4). Adopting the alternative point of view of a Hamiltonian formulation, Brink, Giannoni, and Véneroni[6] have directly introduced the expansion (2.13) into the variational principle (2.6) source of the TDHF equation. As a result, they have found

$$\delta \int_{t_1}^{t_2} \{\mathrm{Tr}(\hbar \chi \dot{\rho}_0) - E_a[\rho_0, \chi]\}\, dt = 0 , \tag{2.16}$$

where $E_a[\rho_0, \chi]$, which is a functional of $\rho_0$ and $\chi$, is the total energy of the system in the adiabatic approximation, i.e., is obtained by replacing $\rho$ in (2.5) by its adiabatic expansion (2.13). This allows us to write the adiabatic energy $E_a$ as

$$E_a = E_0 + E_2 , \tag{2.17}$$

where the term $E_2$ is quadratic in $\chi$, and where the zero-order part $E_0$ is the energy for the time-dependent determinant $\phi_0$ associated with the density operator $\rho_0$:

$$E_0 = \langle \phi_0 | H | \phi_0 \rangle = E[\rho_0] . \tag{2.18}$$

The integrand in Eq. (2.16) has therefore the same structure as the Lagrangian of a classical system, with a kinetic energy quadratic in the momenta and a coordinate-dependent metric tensor:

$$\mathfrak{L}_{\mathrm{cl}} = \sum_i p_i \dot{q}_i - \tfrac{1}{2} \sum_{i,j} [\mathfrak{M}^{-1}(q_k)]_{ij} p_i p_j - V(q_k) . \tag{2.19}$$

In this analogy, the matrix elements of $\rho_0$ and $\hbar\chi$ in a time-independent basis play respectively the roles of the coordinate and their conjugate momenta. As is well known, the condition of stationarity for the classical action $\int_{t_1}^{t_2} \mathfrak{L}_{\mathrm{cl}} dt$ with respect to independent variations of the $p$'s and $q$'s leads to Hamilton's equations.[19] Therefore, Hamilton-like equations should emerge from the stationarity equation (2.16) if the coordinates and the conjugate momenta are taken as independent variables. The situation is, however, complicated by the existence of two constraints to be taken into account during the variation. The first is the holonomic constraint expressing the projector character of $\rho_0$. The second is the algebraic relation (2.12) between coordinates and momenta. A complete discussion of these constraints would exceed the scope of this paper, and can be found in Ref. 20. It should be noted, however, that these constraints can be satisfied implicitly, i.e., without the introduction of Lagrange multipliers. The two sets of Hamilton

equations read

$$i\hbar\sigma_0\dot{\rho}_0\rho_0=\sigma_0\{[W_0^D,\rho_1]+[W_1,\rho_0]\}\rho_0\,, \tag{2.20a}$$

$$\hbar\sigma_0\dot{\chi}\rho_0=\sigma_0\{-W_0-iW_1\sigma_0\chi+i\chi\rho_0W_1-W_2\}\rho_0\,, \tag{2.20b}$$

where $W_0$, $W_1$, and $W_2$ are the three first terms of the expansion of the Hartree-Fock Hamiltonian in powers of $\chi$:

$$W_0=T+\mathrm{Tr}\tilde{V}\rho_0 \tag{2.21}$$

[its diagonal part $W_0^D$ is defined in Eq. (2.30)],

$$W_1=\mathrm{Tr}\tilde{V}\rho_1\,, \tag{2.22}$$

$$W_2=\mathrm{Tr}\tilde{V}\rho_2\,. \tag{2.23}$$

Notice[11] that $W_0$ and $W_2$, like $\rho_0$ and $\rho_2$, are time-even, whereas $W_1$, like $\rho_1$, is time-odd.

One sees that the two Hamilton equations (2.20a) and (2.20b) have only particle-hole matrix elements. This reduction of the number of dynamical equations results from the constraint $\rho_0^2=\rho_0$. The advantage of the choice of the natural decomposition is now understandable, since its operator $\chi$, whose matrix elements are the momenta, contains the right number of degrees of freedom.

One can also write the first Hamilton equation as

$$i\hbar\dot{\rho}_0=[\rho_0W_0\rho_0+\sigma_0W_0\sigma_0,\rho_1]+[W_1,\rho_0]\,. \tag{2.24}$$

Equation (2.24) [or (2.20a)], which provides a linear relation between the velocities and the momenta similar to the corresponding classical equation,

$$\dot{q}_i=\sum_j[\mathfrak{M}^{-1}(q_h)]_{ij}p_j\,, \tag{2.25}$$

can be rewritten in form

$$\hbar\begin{pmatrix}\underline{\dot{\rho}}_0\\ \underline{\dot{\rho}}_0^*\end{pmatrix}=\mathfrak{M}^{-1}\begin{pmatrix}\underline{\chi}\\ \underline{\chi}^*\end{pmatrix}\,, \tag{2.26}$$

where $\underline{\dot{\rho}}_0$ and $\underline{\chi}$ stand for vectors whose components are the particle-hole matrix elements of $\dot{\rho}_0$ and $\chi$ in the time-dependent basis defined by the eigenvectors of $\rho_0$. The inertia matrix is defined by

$$\mathfrak{M}=\begin{pmatrix}A[\rho_0] & -B[\rho_0]\\ -B^*[\rho_0] & A^*[\rho_0]\end{pmatrix}^{-1}\,, \tag{2.27}$$

with

$$A_{ph,p'h'}=(\epsilon_p-\epsilon_h)\delta_{pp'}\delta_{hh'}+\frac{\delta^2E[\rho_0]}{\delta\rho_{hp}\delta_{p'h'}}\,, \tag{2.28}$$

$$B_{ph,p'h'}=\frac{\delta^2E[\rho_0]}{\delta\rho_{hp}\delta_{h'p'}} \tag{2.29}$$

(where there is no possible confusion between the Kronecker and functional derivative symbols).

The energy functional $E[\rho_0]$ in (2.28) and (2.29) is given by Eq. (2.5); the single-particle states, labeled by $p$, $p'$ (particle) and $h$, $h'$ (hole), are defined as the common eigenvectors of $\rho_0$ and of the diagonal part of $W_0$ (see below the discussion of Inglis cranking):

$$W_0^D=\rho_0W_0\rho_0+\sigma_0W_0\sigma_0\,, \tag{2.30}$$

and the single-particle energies $\epsilon_p$, $\epsilon_h$ are the eigenvalues of $W_0^D$. One can notice that the submatrices $A$ and $B$ have the same formal definition as in the RPA theory, but they are represented in a time-dependent particle-hole basis defined by $\rho_0$ instead of the static equilibrium operator $\rho_{st}$. Moreover, one should not confuse the matrix $\mathfrak{M}^{-1}$, which is Hermitian, with the matrix giving the RPA eigensolutions [see Eq. (6.3)].

For the purpose of the present paper we need not discuss in great details the second Hamiltonian equation (2.20b), although its role is crucial since, when solved together with the first Hamilton equation, it determines the collective path $\rho_0(t)$. It allows also to give a different formulation of the second adiabaticity condition ($\hbar\dot{\chi}$ small). Indeed, Eq. (2.20b) shows that if the motion if adiabatic, the commutator $[W_0,\rho_0]$ (or equivalently the anti-diagonal part of $W_0$: see Appendix A) should be small, at least of first order in $\chi$. This condition means that at all times the system is in a "quasi-static" equilibrium since the static Hartree-Fock equation

$$[W_{st},\rho_{st}]=0 \tag{2.31}$$

is nearly satisfied. The meaning of the assumptions on $\chi$ and $\dot{\chi}$ can now be formulated as follows: Since $\chi$ is the "conjugate momentum" of the "coordinate" $\rho_0$, the first hypothesis (smallness of $\chi$) expresses simply a condition of small velocities; the second assumption (smallness of $\hbar\dot{\chi}$) prevents the system from getting large accelerations, and therefore preserves the slow character of the motion along the whole path.

At this point one should distinguish between two limiting cases according to whether $[W_0,\rho_0]$ is of first or second order in $\chi$. The first case corresponds to the RPA, i.e., to the small amplitude limit. The second corresponds to the large amplitude limit. Let us note in this respect that, as in Ref. 5, we use the term adiabaticity in a somewhat misleading way since with our definition ($\chi$ and $\hbar\dot{\chi}$ small) it encompasses these two limiting cases, whereas traditionally[21] it is only attached to the second situation.

By use of the first Hamilton equation, it can be shown that the collective kinetic energy, which is the quadratic part in $\chi$ of $E_a[\rho_0,\chi]$, can be expressed as

$$\mathcal{K}=\tfrac{1}{2}\hbar\,\mathrm{Tr}(\chi\dot{\rho}_0)=\tfrac{1}{2}\hbar^2(\dot{\underline{\rho}}_0^*,\dot{\underline{\rho}}_0)\mathfrak{M}\begin{pmatrix}\dot{\underline{\rho}}_0\\ \dot{\underline{\rho}}_0^*\end{pmatrix}. \tag{2.32}$$

It is useful to give another expression for $\mathcal{K}$, in terms of the conjugate momentum $\chi$. By expanding at order two the average value of the full Hamiltonian $H$:

$$\langle\Psi|H|\Psi\rangle=\langle\phi_0|e^{-i\chi}He^{i\chi}|\phi_0\rangle, \tag{2.33}$$

one gets

$$E_a[\rho_0,\chi]=E[\rho_0]+\tfrac{1}{2}\langle\phi_0|[\chi,[H,\chi]]|\phi_0\rangle, \tag{2.34}$$

and Eq. (2.17) leads to

$$E_2[\rho_0,\chi]=\tfrac{1}{2}\langle\phi_0|[\chi,[H,\chi]]|\phi_0\rangle=\mathcal{K}. \tag{2.35}$$

As for the potential energy

$$\mathcal{V}=E_a[\rho_0,\chi]-\mathcal{K}, \tag{2.36}$$

which is only a function of the coordinate $\rho_0$, it is simply

$$\mathcal{V}=E[\rho_0]. \tag{2.37}$$

In the preceding, we have thus put the total energy in a classical Hamiltonian form:

$$\mathcal{H}=\mathcal{K}+\mathcal{V}, \tag{2.38}$$

which will allow us to make the connection between this TDHF approach and the Bohr collective Hamiltonian approach.[1]

As already mentioned, the variational approach to ATDHF formalism presented here has been obtained in the case where the natural decomposition of $\rho$ into $\rho_0$ and $\chi$ is chosen. For the more general case of any other choice for the decomposition (2.7), Hamiltonlike equations can still be derived. but with some more difficulties[20]; all the equations (2.17) to (2.20a) and (2.21) to (2.38) remain valid. The only equation affected by a different choice of $\rho_0$ and $\chi$ is the second Hamilton equation (2.20b). Since this equation is supposed to define the adiabatic path, it may be argued that the natural choice for $\chi$ brings some arbitrariness into the whole approach. [Indeed, it is well known in some particular cases[5] that $\rho$ may be decomposed as in Eqs. (2.7), (2.8), and (2.9) without fulfillment of Eq. (2.10)]. In this respect, it is worth recalling the important result of Ref. 5: *In the adiabatic limit*, all decompositions fulfilling Eq. (2.7) with $\rho_0$ and $\chi$ Hermitian and time-even are dynamically equivalent.

*"Constrained forms" for the TDHF and first ATDHF equations.* As an immediate consequence of the projector character of $\rho$ [see Appendix A, Eq. (A18)], one can write[22] the TDHF equation (2.4) as

$$[W-i\hbar[\dot{\rho},\rho],\rho]=0. \tag{2.39}$$

This is formally a constrained Hartree-Fock equation for the external field $F=-i\hbar[\dot{\rho},\rho]$.

Inserting the expansion (2.13) into Eq. (2.39), one gets for the time-odd part of the adiabatic limit of (2.39)

$$i\hbar[[\dot{\rho}_0,\rho_0],\rho_0]=[W_0,\rho_1]+[W_1,\rho_0]. \tag{2.40}$$

The left-hand side and the last right-hand side terms in Eq. (2.40) have clearly vanishing diagonal (particle-particle and hole-hole) matrix elements. The diagonal part of the second term is $[W_0^A,\rho_1]$, which, due to the smallness of $[W_0,\rho_0]$, is at least of second order in $\chi$ (see Appendix A). Neglecting this term in the first order equation (2.40) leads to

$$i\hbar[[\dot{\rho}_0,\rho_0],\rho_0]=[W_0^D,\rho_1]+[W_1,\rho_0]. \tag{2.41}$$

Eq. (2.41) is nothing but the first Hamilton equation (2.24) in which the operator $\dot{\rho}_0$ has been written under its double commutator form.

This equation can also be viewed as the time-odd part[23] of the following constrained Hartree-Fock (CHF) equation:

$$[W_0^D+W_1-i\hbar[\dot{\rho}_0,\rho_0],\rho_0+\rho_1]=0. \tag{2.42}$$

In Eq. (2.42), the term which generates the time-odd part $\rho_1$ of the density is the time-odd external field:

$$-F_0=-i\hbar[\dot{\rho}_0,\rho_0]. \tag{2.43}$$

Therefore, the operator $F_0$ has the physical content of a "momentum" operator, times a velocity. Let us consider its mean value in the time-dependent state:

$$\langle F_0\rangle=\mathrm{Tr}\,F_0\rho. \tag{2.44}$$

By noticing that the only part of $\rho$ contributing to the trace is *time-odd* (due to the property of the product of two Hermitian operators having opposite parities under time reversal to have a vanishing trace), one obtains

$$\langle F_0\rangle=\mathrm{Tr}F_0\rho_1=\hbar\,\mathrm{Tr}[\dot{\rho}_0,\rho_0][\chi,\rho_0]. \tag{2.45}$$

A straightforward handling of Eq. (2.45) leads to

$$\langle F_0\rangle=\hbar\,\mathrm{Tr}\,\chi\dot{\rho}_0=2\mathcal{K}, \tag{2.46}$$

which further supports the interpretation of $F_0$ as the product of a momentum by a velocity.

The interest of the "constrained form" (2.42) of the first Hamilton equation and the reason for introducing the operator $F_0$ will appear in the next two sections.

*The Inglis cranking.* To close this section, we make some comments about the cranking model and its relation with the ATDHF approximation. The Inglis cranking approach[2] may be defined as a non-self-consistent solution of Eq. (2.24). More precisely, one neglects the effect of the time-odd

self-consistent field $W_1$ on the time-odd density $\rho_1$. The corresponding approximate equation of motion reads

$$i\hbar\dot{\rho}_0=[W_0^D,\rho_1], \tag{2.47}$$

whose inversion provides $\rho_1$ in terms of $\dot{\rho}_0$.

The Inglis formula can be deduced from (2.47) once a proper choice of the single-particle basis is made. A reasonable choice would consist in common eigenvectors of $\rho_0$ and of an "energy operator" commuting with $\rho_0$, as in the static Hartree-Fock case. Such an operator cannot be exactly the Hartree-Fock field $W_0$ constructed from $\rho_0$, which in general does not commute with $\rho_0$. However, the adiabaticity condition requires that $[W_0,\rho_0]$ should be small compared to some characteristic single-particle excitation energy; therefore, the eigenvectors of the diagonal part $W_0^D$ of $\rho_0$ [see Eq. (2.30)] are "nearly" eigenvectors of $W_0$. Since the operator $W_0^D$ clearly commutes with $\rho_0$, we can define the single-particle basis $\{|h\rangle, |p\rangle\}$ by

$$\rho_0|h\rangle=|h\rangle\,,\quad W_0^D|h\rangle=\epsilon_h|h\rangle\,, \tag{2.48}$$

$$\rho_0|p\rangle=0\,,\quad W_0^D|p\rangle=\epsilon_p|p\rangle\,. \tag{2.49}$$

Taking the matrix elements of Eq. (2.47) leads to

$$i\hbar\langle h|\dot{\rho}_0|p\rangle=(\epsilon_h-\epsilon_p)\langle h|\rho_1|p\rangle\,, \tag{2.50}$$

which gives, in terms of $\chi$ [see Eq. (2.14)],

$$\langle h|\chi|p\rangle=\frac{\hbar}{\epsilon_p-\epsilon_h}\langle h|\dot{\rho}_0|p\rangle\,. \tag{2.51}$$

The kinetic energy, given by Eq. (2.32), can then be written as

$$\mathcal{K}=\hbar^2\sum_{p,h}\frac{|\langle h|\dot{\rho}_0|p\rangle|^2}{\epsilon_p-\epsilon_h}\,, \tag{2.52}$$

which is the cranking formula.

## III. REDUCTION OF THE NUMBER OF DYNAMICAL VARIABLES

From now on, we will restrict the number of dynamical variables by assuming that the operator $\rho_0$ depends on time only through a few number of dynamical variables $q_i$. This implies in particular that

$$\dot{\rho}_0=\sum_i\dot{q}_i\frac{\partial\rho_0}{\partial q_i}\,. \tag{3.1}$$

For the sake of simplicity, we will consider the case of a single variable $q$. The generalization to several variables is straightforward.

From Eqs. (2.20a) and (2.22) one sees that $\rho_1$ (or equivalently $\chi$) is linear in $\dot{q}$, and therefore the kinetic energy $\mathcal{K}$ [see Eqs. (2.32)], such that

$$\mathcal{K}=\tfrac{1}{2}\dot{q}\,\mathrm{Tr}\left(\hbar\chi\frac{\partial\rho_0}{\partial q}\right), \tag{3.2}$$

is, as it should be, quadratic in $\dot{q}$. Equation (3.2) tells us that $p$ defined as

$$p=\hbar\,\mathrm{Tr}\,\chi\frac{\partial\rho_0}{\partial q}=\frac{\partial\mathcal{L}}{\partial\dot{q}}=2\frac{\partial\mathcal{K}}{\partial\dot{q}} \tag{3.3}$$

is the conjugate momentum of the coordinate $q$. This has also been checked directly in Ref. 6 by varying the adiabatic action. Since they are classical canonical variables, $p$ and $q$ satisfy the Poisson bracket relations:

$$\{q,p\}=1\,, \tag{3.4}$$

$$\dot{q}=\{q,\mathcal{H}\}\,, \tag{3.5}$$

$$\dot{p}=\{p,\mathcal{H}\}\,. \tag{3.6}$$

From Eq. (3.3) [or Eq. (3.2)], one defines an adiabatic mass $M(q)$ by

$$M(q)=\frac{p}{\dot{q}}=\frac{2\mathcal{K}}{\dot{q}^2}=\mathrm{Tr}\,\frac{\hbar\chi}{\dot{q}}\frac{\partial\rho_0}{\partial q}\,, \tag{3.7}$$

which is of course independent of $\dot{q}$.

Let us now consider the time-odd Hermitian operator:

$$P=i\hbar\left[\frac{\partial\rho_0}{\partial q},\rho_0\right], \tag{3.8}$$

which is just [see Eq. (2.43)]

$$P=F_0/\dot{q}\,. \tag{3.9}$$

From Eq. (2.46) and the definition (3.3) of $p$, we deduce that the expectation value of the operator $P$ in the time-dependent state $\Psi$ is the conjugate momentum $p$ of $q$:

$$\langle P\rangle=\frac{1}{\dot{q}}\langle F_0\rangle=\frac{2\mathcal{K}}{\dot{q}}=p\,. \tag{3.10}$$

It happens frequently that the coordinate $q$ is chosen to be the expectation value of some time-even observable $Q$:

$$q=\langle Q\rangle=\mathrm{Tr}\rho Q\simeq\mathrm{Tr}\rho_0 Q\,. \tag{3.11}$$

(The last equality has been obtained by using time-reversal properties of the operators under the trace, and by neglecting terms of second order in $\chi$.) Whereas we have just seen that the expectation values of $P$ and $Q$ are classical conjugate variables, it can be proved that $P$ and $Q$, as quantal variables, are canonically conjugate in a weak sense precised below. To show this, we compute the mean value of their commutator:

$$\langle\Psi|[Q,P]|\Psi\rangle=\mathrm{Tr}\rho[Q,P]\,. \tag{3.12}$$

Using again well known properties of the trace and neglecting second order terms in $\chi$, we get

$$\mathrm{Tr}\rho[Q,P]\simeq\mathrm{Tr}\rho_0[Q,P]=\mathrm{Tr}Q[P,\rho_0]\,. \tag{3.13}$$

After inserting the definition (3.8) of $P$ and the ex-

pression (A18) of Appendix A transposed to $\partial\rho_0/\partial q$, Eq. (3.13) leads to

$$\mathrm{Tr}\rho[Q,P]=i\hbar\,\mathrm{Tr}Q\frac{\partial\rho_0}{\partial q}=i\hbar\frac{\partial}{\partial q}\mathrm{Tr}Q\rho_0=i\hbar\frac{\partial}{\partial q}\langle Q\rangle\,, \tag{3.14}$$

which provides the canonical relation

$$\langle\Psi|[Q,P]|\Psi\rangle=i\hbar. \tag{3.15}$$

Of course, such a relation is valid for any time-even Hermitian operator $Q$; therefore, it does not provide any criterion for the choice of a "good" collective path. This is not surprising, since it is valid whether the second Hamilton equation (2.20b) is satisfied or not. Nevertheless, once a choice for $Q$ has been made, the weak conjugation relation (3.15) does support the definition (3.8) for $P$.

Some authors (see, e.g., Refs. 4 and 10) define the conjugate momentum $\hat{P}$ of $Q$ as:

$$\hat{P}\Psi(q)=i\hbar(\partial/\partial q)\Psi(q)\,. \tag{3.16}$$

Such a $\hat{P}$ is clearly not equal to the operator $P$ considered in the present work, which has only particle-hole matrix elements in the sp basis of $\rho_0$ [see Appendix A, Eq. (A16)], whereas $\hat{P}$ can have nonvanishing diagonal matrix elements. Indeed, one can easily see that

$$P|h\rangle=\sigma_0 P|h\rangle=\sigma_0\hat{P}|h\rangle\neq\hat{P}|h\rangle\,, \tag{3.17}$$

$$P|p\rangle=\rho_0 P|p\rangle=\rho_0\hat{P}|p\rangle\neq\hat{P}|p\rangle\,. \tag{3.18}$$

However, if one considers the time-dependent state ($|\psi\rangle=e^{i\chi}|\phi_0\rangle$) built from the natural decomposition[24] one can show that these two operators have the same expectation value:

$$\langle\hat{P}\rangle=\langle P\rangle\,. \tag{3.19}$$

Let us finally comment about the evolution with time of $\langle P\rangle$ and $\langle Q\rangle$. As for the expectation value of any one-body operator $G$ (having no explicit dependence on time), their TDHF equations of motion are of the general form

$$\frac{d}{dt}\langle G\rangle=\frac{i}{\hbar}\langle\Psi|[H,G]|\Psi\rangle\,. \tag{3.20}$$

The latter is easily demonstrated as follows: Since

$$\frac{d}{dt}\langle G\rangle=\mathrm{Tr}\dot{\rho}G\,, \tag{3.21}$$

one gets from the TDHF equation of motion (2.4)

$$\frac{d}{dt}\langle G\rangle=-\frac{i}{\hbar}\{G[W(\rho),\rho]\}, \tag{3.22}$$

where $W(\rho)$ is the one-body reduction with respect to $\rho$ of the one-body plus two-body operator $H$. From the general property of one-body reductions $O(\rho)$ of many-body operators $\mathcal{O}$,[25]

$$\langle\Psi|[\mathcal{O},C_m^\dagger C_n]|\Psi\rangle=-\langle m|[O(\rho),\rho]|n\rangle \tag{3.23}$$

(where $\rho$ is the density matrix defining the independent particle state $|\Psi\rangle$, and $C_i^\dagger$ are creation operators on the single-particle states $|i\rangle$), one gets readily Eq. (3.20). Using Eqs. (3.5) and (3.6), together with Eq. (3.20) applied to $G=Q$ and $G=P$ leads to

$$\{q,\mathcal{H}\}=\langle\Psi|\frac{1}{i\hbar}[Q,H]|\Psi\rangle\,, \tag{3.24}$$

$$\{p,\mathcal{H}\}=\langle\Psi|\frac{1}{i\hbar}[P,H]|\Psi\rangle\,. \tag{3.25}$$

The approximation consisting in reducing the number of dynamical variables, together with the preceding ones (existence of a mean field, adiabaticity of the motion), are the basis for the unified model description of low energy nuclear excitations.[1] However, a further approximation is generally associated to this approach. One decides *a priori*, i.e., without solving the equations of motion, what the dynamical variables should be. In other words, one chooses a special family $\rho_0(q)$. Possible choices for such families will be discussed in Secs. IV and V.

In this case, one has only to solve the first Hamilton equation, providing the pass parameter $M(q)$

$$i\hbar\dot{q}\frac{\partial\rho_0}{\partial q}=[W_0^D,\rho_1]+[W_1,\rho_0]\,. \tag{3.26}$$

It is worth noticing that this equation is not capable of determining the diagonal part of $\chi$ in terms of $\partial\rho_0/\partial q$. In other words, the mass parameter $M(q)$ does not depend on the diagonal part $(\rho_0\chi\rho_0+\sigma_0\chi\sigma_0)$ of $\chi$. This can also be seen directly on the expression (3.7) of $M(q)$. Since the operator $\partial\rho_0/\partial q$ has only particle-hole matrix elements, the particle-particle and hole-hole parts of $\chi$ do not contribute to the trace.

Let us finally deduce, from the Inglis formula (2.52) for the kinetic energy, the usual cranking formulae for the mass parameter $M(q)$. The first one is obtained by replacing $\dot{\rho}_0$ by $\dot{q}\,\partial\rho_0/\partial q$ in Eq. (2.52):

$$M(q)=2\hbar^2\sum_{p,h}\frac{|\langle h|\partial\rho_0/\partial q|p\rangle|^2}{\epsilon_p-\epsilon_h} \tag{3.27}$$

$$=2\hbar^2\sum_{p,h}\frac{|\langle h|\partial/\partial q|p\rangle|^2}{\epsilon_p-\epsilon_h}\,. \tag{3.28}$$

By use of

$$(\partial/\partial q)[W_0^D,\rho_0]=0\,, \tag{3.29}$$

one can also express the mass parameter as

$$M(q)=2\hbar^2\sum_{p,h}\frac{|\langle h|\partial W_0^D/\partial q|p\rangle|^2}{(\epsilon_p-\epsilon_h)^3}, \tag{3.30}$$

which is an alternative form for the cranking formula.

## IV. CONSTRAINED HARTREE-FOCK PATHS

As a possible prescription, the trajectory $\rho_0(q)$ is assumed to be given by the solution of a CHF equation

$$\delta\langle\phi_0|H-\lambda Q|\phi_0\rangle=0, \tag{4.1}$$

where $\phi_0$ is a Slater determinant minimizing the total energy of the system under the action of the time-even external field $(-\lambda Q)$. In terms of the density operator $\rho_0(q)$, Eq. (4.1) can be written equivalently as

$$[W_0-\lambda Q,\ \rho_0(q)]=0. \tag{4.2}$$

The operator $W_0$ is the Hartree-Fock Hamiltonian built from the density matrix $\rho_0$, and the collective coordinate $q$ is the expectation value of the constraining operator

$$q=\langle Q\rangle=\mathrm{Tr}\rho_0 Q. \tag{4.3}$$

The equations of motion form, as noticed before, a linear homogeneous system [see the matrix formulation (2.26) of the first ATDHF equation (2.20a)], and could be solved by a matrix inversion. For technical reasons, we prefer to proceed in a rather different way, i.e., take advantage of the "constrained form" (2.42) of the first Hamilton equation:

$$[W_0^D+W_1-\dot{q}P,\ \rho_0+\rho_1]=0, \tag{4.4}$$

with $P$ defined by

$$P=i\hbar\left[\frac{\partial\rho_0}{\partial q},\rho_0\right]. \tag{4.5}$$

As a consequence of Eq. (4.2), the operators $W_0$ and $\lambda Q$ have identical particle-hole (and hole-particle) matrix elements:

$$\sigma_0 W_0\rho_0=\sigma_0(\lambda Q)\rho_0, \tag{4.6}$$

$$\rho_0 W_0\sigma_0=\rho_0(\lambda Q)\sigma_0. \tag{4.7}$$

Denoting by $Q^A$ the antidiagonal (off-diagonal) part of $Q$,

$$Q^A=\sigma_0 Q\rho_0+\rho_0 Q\sigma_0,$$

we deduce from (4.6) and (4.7) the following expression of $W_0^D$:

$$W_0^D(=W_0-W_0^A)=W_0-\lambda Q^A. \tag{4.8}$$

Inserted into (4.4), Eq. (4.8) leads to

$$[W_0+W_1-\lambda Q^A-\dot{q}P,\ \rho_0+\rho_1]=0, \tag{4.9}$$

which is the doubly constrained Hartree-Fock equation:

$$\delta\langle\Psi|H-\lambda Q^A-\dot{q}P|\Psi\rangle=0. \tag{4.10}$$

The determinant $\Psi$ built from the occupied states of the density operator $\rho=\rho_0+\rho_1$ is not time-reversal invariant, due to the presence in the external field of the time-odd part $(-\dot{q}P)$. In the limiting case of small velocities $\dot{q}$, the time-odd part $\rho_1$ of $\rho$ is, as it should be [see Eq. (3.26)], proportional to $\dot{q}$ [linear response in Eq. (4.10)]. Since the adiabatic mass parameter $M(q)$ has no dependence on $\dot{q}$, its knowledge require only the computation of $\rho_1/\dot{q}$, or equivalently of $\chi/\dot{q}$, as seen in Eq. (3.7). The determination of $\rho_1/\dot{q}$ as given by Eq. (3.26) can thus be performed by solving Eq. (4.10) with an arbitrary value of $\dot{q}$, small enough to fulfill the linear response condition.

Equation (4.10) is composed, of course, of two distinct equations. The time-odd part

$$i\hbar\dot{q}\frac{\partial\rho_0}{\partial q}=[W_0^D,\rho_1]+[W_1,\rho_0]=\dot{q}[P,\rho_0] \tag{4.11}$$

is the equation which we actually want to solve. The time-even part is

$$[W_0-\lambda Q^A,\rho_0]+[W_1-\dot{q}P,\rho_1]=0, \tag{4.12}$$

and is therefore automatically satisfied up to first order in the doubly constrained Hartree-Fock process. This equation does not coincide exactly with Eq. (4.2), and it induces thus a slight change in the path $\rho_0(q)$. However, by choosing a sufficiently small $\dot{q}$ value, the second term of Eq. (4.12) responsible for this modification of the path is negligible. A quantitative discussion concerning the range of the choice of $\dot{q}$ in numerical applications will be given in II.

We have already noticed that the smallness of $\dot{q}$ is a necessary condition to ensure a linear response. Since this implies also the smallness of $\rho_1$, it is related to the first adiabaticity condition (smallness of $\chi$). On the other hand, the second adiabaticity assumption ($\hbar\dot{\chi}$ small) constrains the Lagrange multiplier $\lambda$ to be small; indeed, the smallness of $\hbar\dot{\chi}$ corresponds to the smallness of the commutator $[W_0,\rho_0]$, as mentioned in Sec. II. Using the definition (4.2) of the path $\rho_0$

$$[W_0,\rho_0]=\lambda[Q,\rho_0],$$

one sees how the smallness of $\lambda$ is imposed by the second adiabaticity assumption. Thus in our double CHF approach for which the external field is $(-\lambda Q^A-\dot{q}P)$, *both* $\lambda$ and $\dot{q}$ should be small. These conditions are connected to the adiabaticity assumptions, but *they clearly do not imply any small amplitude hypothesis*. A simple example of cases where $\lambda$ is small but where a large ampli-

tude motion occurs is given by nuclei having a soft behavior with respect to deformations. Their potential energy curve is very flat in a large region around the HF minimum, corresponding to a small value of the slope $\lambda(q)$ (see, e.g., Fig. 7 of II). The authors of Ref. 26 identify the limiting case $\lambda \to 0$ with small amplitude motion, which is in contradiction with the previous statement; it is likely that they have in mind a definition of small vibrations different from the usual RPA hypothesis ($\| \rho - \rho_{st} \| \ll 1$).

The method of computation of mass parameters described in the present section has been first proposed in Ref. 22, where the first numerical applications were also presented. Up to now, it has been applied to the calculation of mass parameters for quadrupole vibrations[7,22] and for heavy ion collisions.[27]

To conclude this presentation of the CHF path, we will discuss briefly the connection of the preceding with different approaches of the same problem.

(i) The Inglis cranking formula is obtained, as seen in Sec. II, by neglecting $W_1$ in the first ATDHF equation of motion. Starting from a solution $\rho_0$ of the time-even CHF problem, one gets simply the Inglis cranking value of $\rho_1$ from the solution $(\rho_0 + \rho_1)^1$ of the first iteration of the CHF equation (4.10) (i.e., the solution of the Schrödinger equation for the one-body Hamiltonian $W_0 - \lambda Q^A - \dot{q}P$). The Inglis adiabatic mass is thus obtained very easily as a byproduct of the full solution of the ATDHF problem.

(ii) In the particular case of rotational collective motion (rotations of the nucleus as a whole), Thouless and Valatin[3] have already shown that the solution of the TDHF equation could be cast into the form of a CHF problem, with the time-odd constraining field $(-\omega \hat{n} \cdot \vec{J})$ ($\omega$ being the angular velocity, $\hat{n}$ the unit vector defining the rotation axis, and $\vec{J}$ the angular momentum operator). This result can be easily deduced from our more general formalism, since in this case the family $\rho_0(\theta)$ (where $\theta$ is the collective coordinate specifying the angular position) is simply given by

$$\rho_0(\theta) = \exp(-i\theta \hat{n} \cdot \vec{J}/\hbar) \rho_{st} \exp(i\theta \hat{n} \cdot \vec{J}/\hbar), \quad (4.13)$$

where $\rho_{st}$ correspond to a static HF solution. From the definition (4.5) of $P$, one gets readily

$$P = (\hat{n} \cdot \vec{J})^A . \quad (4.14)$$

Our time-odd constraining field $P$ is therefore the antidiagonal part of the Thouless-Valatin's time-odd field; however, it is easily seen that the moments of inertia obtained by these two methods are equal. Indeed, one could add to the "momentum operator" $P$ in the time-odd equation (4.11) any particle-particle plus hole-hole part $P^D$ without any change in the result, since any diagonal operator commutes with $\rho_0$. Thus the value of $\rho_1$ would not be affected by such a change of $P$. Moreover, the mean value of $P' = P + P^D$ would remain unchanged, since

$$\langle P' \rangle = i\hbar \, \mathrm{Tr} \rho P' = i\hbar \, \mathrm{Tr} \rho_1 (P + P^D) = i\hbar \, \mathrm{Tr} \rho_1 P = \langle P \rangle . \quad (4.15)$$

In the above equalities, we have used the property $\mathrm{Tr} \rho_1 P^D = 0$, which comes from the antidiagonal character of $\rho_1$ (see Appendix A). Of course, a similar result is available for uniform translational motion, and one gets for the mass parameter the nucleus mass, as in the Thouless-Valatin method.

(iii) The present approach bears some similarities with a formalism presented by Villars in Ref. 8. In this paper, the author considers also a doubly constrained Hartree-Fock equation of the type of our Eq. (4.10), where the operators $P$ and $Q$ satisfy the canonical relation (3.15). However, once the choice of $Q$ is made, we do have a prescription to determine $P$, while in Ref. 8 an ambiguity in the choice of $P$ is explicitly acknowledged. This ambiguity stems from the fact that $P$ is only subject to the weak canonical relation (3.15). It may be noted that in our case it is the adiabatic approximation (via the first Hamiltonian equation) which leads to the unequivocal determination of $P$.

Rowe and Bassermann[9] have also proposed a double CHF approach to nuclear dynamics, giving explicit expressions for the $P$ and $Q$ operators in terms of a set of local normal coordinates and momenta. Such a general formalism does not assume any adiabaticity.

In fact, these approaches,[8,9] and several other attempts[4,10,28] to derive the collective path (problem which we do not touch in the present contribution) do correspond in practice to a tremendous numerical effort which, to the best of our knowledge, has not yet been mastered in nontrivial cases.

## V. SCALING PATH

The choice of a dynamical path defined by a scaling of equilibrium wave functions has been recently considered by several authors either in the framework of the ATDHF formalism[22,29] or within a slightly different context.[30-34] Our aim here is to study is some detail the scaling hypothesis as a possible prescription for the ATDHF path $\rho_0(q)$.

The scaling approximation consists in constructing from a static equilibrium HF solution defined by its density matrix $\rho_{st}$ a family of density opera-

tors $\rho_0(\beta)$ by

$$\rho_0(\beta)=e^{i\beta\hat{\theta}}\rho_{st}e^{-i\beta\hat{\theta}}, \tag{5.1}$$

where $\hat{\theta}$ is a local time-odd Hermitian spin-independent one-body operator whose $\vec{r}$ representation is such that

$$\forall f(\vec{r}),\quad 2i\hat{\theta}f(\vec{r})=2\vec{\nabla}\theta(\vec{r})\cdot\vec{\nabla}f(\vec{r})+f(\vec{r})\vec{\nabla}^2\theta(\vec{r}). \tag{5.2}$$

In Eqs. (5.1) and (5.2), $\beta$ is a small number (compared to one) and $\theta(\vec{r})$ is a given real function of the space coordinate chosen to reproduce the studied collective motion. One may consider, for instance,

$$\theta=r^2 \quad \text{(isoscalar monopole vibrations)}, \tag{5.3}$$

$$\theta=2z^2-x^2-y^2 \quad \text{(isoscalar quadrupole vibrations)}, \tag{5.4}$$

$$\theta=\hat{n}\cdot\vec{r} \quad \text{(translations defined by the unit vecor } \hat{n}). \tag{5.5}$$

The well known example of translations, studied extensively in Ref. 5, suggests to try as a solution of the first ATDHF equation (2.24) for the most general mode.

$$\chi=-(m/\hbar)\dot{\beta}\theta(\vec{r}). \tag{5.6}$$

In fact, it is shown in Appendix B that the operators $\rho_0$ and $\chi$ defined in Eqs. (5.1) and (5.6) do satisfy Eq. (2.24) provided the two-body interaction $V$ is gauge invariant with respect to $\theta(\vec{r})$:

$$[V,\theta(\vec{r})]=0. \tag{5.7}$$

This gauge invariance property is trivially fulfilled for velocity-independent interactions. For velocity-dependent forces of the Skyrme type, it can be shown (see Appendix A of II) that the gauge invariance is ensured, even for the spin-orbit part, but *only for isoscalar modes*.

From now on we will restrict ourselves to isoscalar modes and assume the gauge invariance property. In this case, we may write a continuity equation

$$\dot{\rho}_0(\vec{r})+(\hbar/m)\vec{\nabla}\cdot\vec{j}(\vec{r})=0, \tag{5.8}$$

where the current vector $\vec{j}$ is given by

$$\vec{j}(\vec{r})=\rho_0(\vec{r})\vec{\nabla}\chi(\vec{r}). \tag{5.9}$$

In order to get it, one can, for instance, represent the first Hamilton equation (2.24) in configuration space and take its limit when $\vec{r}'\to\vec{r}$.[35] Consider now the classical adiabatic kinetic energy

$$\mathcal{K}=\tfrac{1}{2}\hbar\,\mathrm{Tr}\chi\dot{\rho}_0. \tag{5.10}$$

Using the continuity equation, we get for $\mathcal{K}$

$$\mathcal{K}=-\frac{\hbar^2}{2m}\int\chi(\vec{r})\vec{\nabla}\cdot\vec{j}(\vec{r})d^3r \tag{5.11}$$

$$=\frac{\hbar^2}{2m}\int\rho_0(\vec{r})[\vec{\nabla}\chi(\vec{r})]^2d^3r, \tag{5.12}$$

after integration by parts. From the definition (5.6) for $\chi$ one obtains finally

$$\mathcal{K}=\tfrac{1}{2}M_{SC}(\beta)\dot{\beta}^2, \tag{5.13}$$

where the scaling mass parameter $M_{SC}(\beta)$ is given by

$$M_{SC}(\beta)=m\int\rho_0(\vec{r})[\vec{\nabla}\theta(\vec{r})]^2d^3r. \tag{5.14}$$

To illustrate the preceding we will now concentrate on a specific isoscalar collective mode, namely the quadrupole motion. In this case since

$$(\vec{\nabla}\theta)^2=4(x^2+y^2+4z^2), \tag{5.15}$$

one gets for the mass parameter $M_{SC}(\beta)$

$$M_{SC}(\beta)=4m(2\langle r^2\rangle+\langle Q_{20}\rangle), \tag{5.16}$$

where $r^2$ and $Q_{20}$ are the operators:

$$r^2=x^2+y^2+z^2, \tag{5.17}$$

$$Q_{20}=2z^2-x^2-y^2. \tag{5.18}$$

Since we would like to compare the scaling path with the CHF one, we must choose the same collective variable $q=\langle Q_{20}\rangle$ in the two cases. For this purpose we expand each orbital $\psi_i^0(\beta;x,y,z)$ of $\rho_0$ around the corresponding orbital $\psi_i^{st}$ of $\rho_{st}$ to first order in $\beta$, which leads to

$$\psi_i^0(\beta;x,y,z)\simeq(1+i\beta\hat{\theta})\psi_i^{st}(x,y,z). \tag{5.19}$$

For $\theta(\vec{r})$ given by Eq. (5.4),

$$\vec{\nabla}^2\theta(\vec{r})=0, \tag{5.20}$$

and thus one gets from Eq. (5.19)

$$\psi_i^0(\beta;x,y,z)=\psi_i^{st}(x,y,z)+\beta\vec{\nabla}\theta\cdot\vec{\nabla}\psi_i^{st}(x,y,z)$$
$$=\psi_i^{st}\left\{x(1-2\beta),y(1-2\beta),z\frac{1}{(1-2\beta)^2}\right\}. \tag{5.21}$$

It is clear from the preceeding that the operator $\beta\hat{\theta}$ acts as a scaling operator *only for small values of* $\beta$, that is, for small amplitude motions. The quadrupole moment $q(\beta)$ of $\psi_i^0(\beta;x,y,z)$ can be easily expressed as

$$\langle Q_{20}\rangle=q(\beta)=\frac{(1-2\beta)^2}{3}(q_{st}-2Ar_{st}^2)$$
$$+\frac{2}{3(1-2\beta)^4}(Ar_{st}^2+q_{st}), \tag{5.22}$$

where $q_{st}$ and $Ar_{st}^2$ are the expectation values of $Q_{20}$ and $r^2$ for the equilibrium state $\rho_{st}$, $a$ being

the number of particles. Similarly, one gets for the radius $r(\beta)$ the expression

$$\langle r^2\rangle = Ar^2(\beta) = -\frac{(1-2\beta)^2}{3}(q_{st} - 2Ar_{st}^2) + \frac{1}{3(1-2\beta)^4}(Ar_{st}^2 + q_{st}). \quad (5.23)$$

Therefore, the mass $M_{SC}(\beta)$ is given by

$$M_{SC}(\beta) = 4m\left[-\frac{(1-2\beta)^2}{3}(q_{st} - 2Ar_{st}^2) + \frac{4}{3(1-2\beta)^4}(Ar_{st}^2 + q_{st})\right] \quad (5.24)$$

$$= m(1-2\beta)\frac{dq}{d\beta}, \quad (5.25)$$

which for small values of $\beta$ leads to

$$dq/d\beta \simeq M_{SC}(\beta)/m. \quad (5.26)$$

Now the mass $M_{SC}(q)$ can be deduced from the mass $M_{SC}(\beta)$ as

$$M_{SC}(q) = M_{SC}(\beta)\left(\frac{d\beta}{dq}\right)^2, \quad (5.27)$$

that is, in the small $\beta$ limit,

$$M_{SC}(q) = \frac{m^2}{M_{SC}(\beta)} = \frac{m}{4(2\langle r^2\rangle + \langle Q_{20}\rangle)}. \quad (5.28)$$

One may note incidentally that the operator $P$ defined in Eq. (3.8) writes

$$P = i\hbar\left[\frac{\partial\rho_0}{\partial q}, \rho_0\right] = -\hbar\frac{dq}{d\beta}\hat{\theta}^A. \quad (5.29)$$

We have heuristically used the result obtained for translations to find a solution to the first ATDHF equation in the most general scaling case. However, the latter is significantly different from the translational case. Indeed, the second ATDHF equation is exactly fulfilled for uniform translational motion as a consequence of the Galilean invariance.[5] Such a fulfillment is not achieved *a priori* for an arbitrary scaling transformation.

The operator $\chi$ considered in this section is *not* the natural one since it has obviously nonvanishing $p$-$p$ and $h$-$h$ matrix elements. (In this respect it has been shown that the natural $\chi$ cannot be local.[14]) We recall that the expressions (2.20a) for the first Hamilton equation and (3.7) for the mass parameter are valid for any (natural or non-natural) decomposition (2.7). Therefore, it was legitimate to calculate the scaling mass parameter from a local $\chi$ solution of Eq. (2.20a). Whereas the p-h representation is most convenient to derive the general ATDHF formalism, the $\vec{r}$ representation is undoubtedly more appropriate when $\chi$ is local. In this case, most of the mechanical properties will pertain more to classical fluid dynamics than to point particle Hamiltonian mechanics.

We have presented the cases of scaling variables and of CHF variables in separate sections. It should be noticed, however, that the scaling path for a multipole operator $Q$ can also be given by a CHF equation[26]:

$$\delta\langle H - \lambda[H,[H,Q]']'\rangle = 0. \quad (5.30)$$

In Eq. (5.30), the prime indicates one-body reductions of operators. According to the prescription given in Sec. IV, the definition of the collective coordinate $q$ corresponding to the path provided by (5.30) would be

$$q = \langle[H,[H,Q]']'\rangle, \quad (5.31)$$

which is proportional to the variable $\beta$ considered in the present section (see, e.g., Ref. 33). The definition (5.30) for the collective path has of course a purely formal interest, since mass and stiffness parameters can be numerically calculated in a much simpler way.

## VI. SUM RULES

During the last few years, the language of sum rules has been extensively used (see, e.g., Ref. 31) for the description of collective states. In this section, we briefly recall some results which can be of some help to better understand our study, and discuss the physical content of the two kinds of paths presented before.

The energy-weighted moments of any one-body operator $Q$ are defined by

$$m_k(Q) = \sum_{n>0} |\langle n|Q|0\rangle|^2(\epsilon_n - \epsilon_0)^k, \quad (6.1)$$

where $k$ is integer, and $n$ (or 0) labels excited (or ground) states.

These moments are often evaluated within the RPA approximation for the excitation energies $(\epsilon_n - \epsilon_0)$ and for the transition matrix elements $\langle n|Q|0\rangle$ defined as

$$\langle n|Q|0\rangle = \sum_{ph}\{(\underline{X}_n)^*_{ph}Q_{ph} + (\underline{Y}_n)^*_{ph}Q_{hp}\}, \quad (6.2)$$

where the $Q_{ph}$'s are the particle-hole matrix elements of $Q$ in the static Hartree-Fock basis, and the vectors $\underline{X}_n$ and $\underline{Y}_n$ [whose components are $(\underline{X}_n)_{ph}$ and $(\underline{Y}_n)_{ph}$] satisfy the RPA eigenvalue equation

$$\begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix}\begin{bmatrix} \underline{X}_n \\ \underline{Y}_n \end{bmatrix} = (\epsilon_n - \epsilon_0)\begin{bmatrix} \underline{X}_n \\ \underline{Y}_n \end{bmatrix}. \quad (6.3)$$

In Eq. (6.3), $A$ and $B$ are the standard RPA matrices defined by (2.28) and (2.29) in the static

Hartree-Fock basis.

When the Hartree-Fock solution is a true local minimum of the total energy, the stability RPA condition[37] ensures that the excitation energies $(\epsilon_n - \epsilon_0)$ are real; this leads to positive moments $m_k$.[38]

By straightforward use of Schwarz inequality, one can deduce various inequalities for the moments,[30,31] in particular,

$$E_k \leq E_{k+1}\,, \tag{6.4}$$

$$E_1 \leq \bar{E} = \frac{m_1}{m_0} \leq E_2\,, \tag{6.5}$$

where the energies $E_k$ are defined by

$$E_k = \left(\frac{m_k}{m_{k-2}}\right)^{1/2}. \tag{6.6}$$

Moments evaluated according to RPA prescriptions can be expressed, at least for odd $k$, in the following form[26]:

$$m_{2n+1}(Q) = \tfrac{1}{2}(\tilde{\underline{Q}}^*\tilde{\underline{Q}}) \begin{bmatrix} A & B \\ -B^* & -A^* \end{bmatrix}^{2n+1} \begin{bmatrix} \underline{Q} \\ -\underline{Q}^* \end{bmatrix}, \tag{6.7}$$

where the components of the vector $\underline{Q}$ are the particle-hole matrix elements of the operator $Q$ in the static Hartree-Fock basis. Formula (6.7) holds for positive or negative $n$.

If one does no longer consider a static Hartree-Fock solution $\rho_{st}$, but instead some point of an "adiabatic path" $\rho_0(q)$, one can still define "generalized local RPA moments" by Eq. (6.7). But now, while the matrices $A$ and $B$ keep the same formal expressions (2.28) and (2.29) as previously, they are expressed in the ATDHF particle-hole basis composed of common eigenvectors of $\rho_0$ and $(W_0)^D$ [as in Eq. (2.27)]. Since these generalized matrices $A$ and $B$ are not related to the static HF equilibrium, they do not *a priori* satisfy the stability condition. Therefore, the positiveness of $m_k$ and the inequalities (6.4) and (6.5) are no longer guaranteed in this case. However, sum rules can still be obtained by standard procedures; in particular, the adiabatic mass parameters $M_{CHF}(q)$ and $M_{sc}(q)$ calculated respectively for a "constrained Hartree-Fock" coordinate and for a scaling coordinate can be expressed in terms of generalized moments along the whole path $q(t)$. In both cases, the adiabatic mass is the nuclear polarizability with respect to the momentum operator $P$ generating the motion $[M = 2m_{-1}(P)]$. Let us now express $M$ in terms of generalized moments of the operator $Q$ defining the path.

*(a) Scaling path.* To get a sum rule for the scaling mass parameter, we introduce the expression (5.6) of $\chi$ into Eq. (2.35) for the kinetic energy. This leads to

$$\mathcal{K} = \tfrac{1}{2}\dot{\beta}^2\left(\frac{m}{\hbar}\right)^2 \langle \phi_0 | [\theta, [H, \theta]] | \phi_0 \rangle\,. \tag{6.8}$$

As is well known, the expectation value of the double commutator $[\theta, [H, \theta]]$ in the static Hartree-Fock state $\phi_{st}$ is related to the first RPA moment, provided $\theta$ is a one-body operator:

$$m_1(\theta) = \tfrac{1}{2}\langle \phi_{st} | [\theta, [H, \theta]] | \phi_{st} \rangle\,. \tag{6.9}$$

This linear energy-weighted sum rule studied by Thouless[39] has been recently extended to density-dependent interactions.[31] Similarly, it can be shown that the generalized first moment satisfies the relation

$$m_1(\theta, \beta) = \tfrac{1}{2}\langle \phi_0(\beta) | [\theta, [H, \theta]] | \phi_0(\beta) \rangle \tag{6.10}$$

along the whole path $\rho_0(\beta)$. For multipole modes, $\theta$ is the corresponding multipole operator $Q$ [see Eqs. (5.3), (5.4), and (5.5)], and the scaling mass parameter writes

$$M_{SC}(\beta) = 2\left(\frac{m}{\hbar}\right)^2 m_1(Q, \beta)\,, \tag{6.11}$$

or, in terms of the coordinate $q = \langle Q \rangle$,

$$M_{SC}(q) = \frac{\hbar^2}{2}\,\frac{1}{m_1(Q, q)}\,. \tag{6.12}$$

To evaluate the excitation energy in the small amplitude limit, one needs the stiffness parameter at the static Hartree-Fock equilibrium point $q_{st}$:

$$K_{SC} = \frac{\partial^2 \mathcal{V}_{SC}}{\partial q^2}\Big]_{q_{st}} = \frac{\partial^2 E[\rho_0(q)]}{\partial q^2}\Big]_{q_{st}}. \tag{6.13}$$

From the expansion of the potential energy

$$E[\rho_0] = \langle \phi_0 | H | \phi_0 \rangle = \langle \phi_{st} | e^{-i\beta\hat{\theta}} H e^{i\beta\hat{\theta}} | \phi_{st} \rangle \tag{6.14}$$

to leading order in $\beta$, one gets

$$\frac{\partial^2 \mathcal{V}_{SC}}{\partial \beta^2}\Big]_{st} = \langle \phi_{st} | [\hat{\theta}, [H, \hat{\theta}]] | \phi_{st} \rangle$$

$$= 2m_1(\hat{\theta}) = 2m_3(Q)\,. \tag{6.15}$$

The demonstration of the last equality in Eq. (6.15) can be found in Ref. 30. This leads for the stiffness parameter $K_{SC}$ to the value

$$K_{SC} = \frac{m_3(Q)}{[m_1(Q)]^2}\,, \tag{6.16}$$

and for the ATDHF excitation energy corresponding to a scaling path $\rho_{SC}(q)$ in the small amplitude limit:

$$E_{SC} = \hbar\left(\frac{K_{SC}}{M_{SC}(q_{st})}\right)^{1/2} = \left(\frac{m_3(Q)}{m_1(Q)}\right)^{1/2} = E_3\,. \tag{6.17}$$

The latter expression for the excitation energy has already been considered by several authors. In

Ref. 30, it is used as a prescription for an estimation of the isoscalar resonance energy, the operator $Q$ being the corresponding multipole operator. As mentioned in these references, the evaluation of $E_{SC}$ through formula (6.17) involves only a static Hartree-Fock calculation at the equilibrium point. The authors of Ref. 33 get the same expression of the excitation energy by a method offering some similarity with the ATDHF approach. They also use a scaling hypothesis for the wave function, and they construct a collective Hamiltonian in the small amplitude limit of TDHF approximation.

*(b) Constrained Hartree-Fock path.* The mass parameter obtained by solving the first ATDHF equation for a path $\rho_0(q)$ solution of Eq. (4.2) can also be expressed in terms of the previously defined generalized moments as[26,40]

$$M_{CHF}(q)=\tfrac{1}{2}\hbar^2\frac{m_{-3}(Q,q)}{[m_{-1}(Q,q)]^2}\,. \tag{6.18}$$

Although it would be meaningless to make the small amplitude approximation if the ATDHF motion is found to be anharmonic, let us give the expression of the excitation energy in this very restrictive hypothesis. As is well known, the stiffness of the deformation energy curve at the static HF minimum is related to the polarizability sum rule:

$$K_{CHF}=\frac{\partial^2 v_{CHF}}{\partial q^2}\Big]_{q_{st}}=\frac{\partial^2 E[\rho_0(q)]}{\partial q^2}\Big]_{q_{st}}$$
$$=\frac{\partial^2 E_0}{\partial\lambda^2}\Big]^{-1}_{\lambda_{st}}=\frac{1}{2m_{-1}(Q)}\,. \tag{6.19}$$

Therefore, *in the small amplitude limit,* the excitation energy writes

$$E_{CHF}=\hbar\left(\frac{K_{CHF}}{M_{CHF}(q_{st})}\right)^{1/2}=\left(\frac{m_{-1}(Q)}{m_{-3}(Q)}\right)^{1/2}=E_{-1}\,. \tag{6.20}$$

It should be emphasized that the latter expression for the excitation energy is given only for indication, and does not represent, in general, the true ATDHF result for a constrained path. Indeed, it can happen that such a path corresponds to a large amplitude motion, as illustrated in II. In this case, the calculation of the ATDHF excitation energy would require a quantization of the collective Hamiltonian:

$$\mathcal{H}=\frac{p^2}{2M_{CHF}(q)}+v_{CHF}(q)\,, \tag{6.21}$$

which may be very different from an harmonic oscillator Hamiltonian.

The expressions (6.12) and (6.18) of $M_{SC}(q)$ and $M_{CHF}(q)$ already allow us to draw some conclusions. Let us consider for the discussion the example of isoscalar quadrupole modes, and make for the operator $Q$ the choice $Q=Q_{20}$. As a first important remark, we note that the presence of negative moments in the CHF path gives more weight to low energy particle-hole excitations, whereas the linear sum rule of Eq. (6.12) for $M_{SC}(q)$ favors 2-$\hbar\omega$ excitations. As a consequence, we expect significant differences between the two paths for non-spin-saturated nuclei.

To develop the preceding comment, let us restrict the comparison to the static Hartree-Fock equilibrium point, where the two mass parameters can be expressed in terms of the usual RPA moments

$$M_{CHF}(q_{st})=\tfrac{1}{2}\hbar^2\frac{m_{-3}(Q)}{[m_{-1}(Q)]^2}\,,$$
$$M_{SC}(q_{st})=\tfrac{1}{2}\hbar^2\frac{1}{m_1(Q)}\,. \tag{6.22}$$

By use of Eqs. (6.4), (6.6), and (6.22), one gets the following property for the ratio of the two mass parameters:

$$\frac{M_{CHF}(q_{st})}{M_{SC}(q_{st})}=\frac{E_1}{E_{-1}}\geq 1\,. \tag{6.23}$$

Moreover, one knows that the inequalities (6.4) are reduced to equalities only in the case where the whole strength of the excitation operator $Q$ is concentrated in one collective state. Equation (6.23) thus means that the two paths considered here lead to the same mass parameter at the equilibrium Hartree-Fock point if and only if the RPA sum rules are exhausted by a single excited state; otherwise, the CHF mass is always greater than the scaling mass.

The fact that the CHF path takes into account low energy excitations, whereas the scaling path is completely dominated by the giant resonance, is confirmed by the values $E_{-1}$(CHF) and $E_3$ (scaling) of the excitation energies in the small amplitude limit.

All the preceding arguments will be illustrated and supported in II, but henceforth it is possible to conclude that these two paths are adapted to different physical situations. The scaling path, as is well known, is convenient for the description of giant resonances, whereas the CHF path with the constraint $(-\lambda Q_{20})$ seems appropriate to the study of *low lying collective states*. The discussion of the matter presented here will be completed by the calculations reported in II to which we reserve general conclusions.

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## APPENDIX A: PARTICLE-HOLE ALGEBRA

In this Appendix, we derive some useful properties resulting from the idempotency of $\rho_0$ (or of the TDHF density operator $\rho$):

$$\rho_0^2=\rho_0 . \tag{A1}$$

We introduce the projector $\sigma_0=1-\rho_0$ orthogonal to $\rho_0$

$$\sigma_0\rho_0=0 , \tag{A2}$$

and recall that the hole and particle states are defined, with respect to $\rho_0$, as

$$\rho_0|h\rangle=|h\rangle \quad (\text{thus } \sigma_0|h\rangle=0) , \tag{A3}$$

$$\rho_0|p\rangle=0 \quad (\text{thus } \sigma_0|p\rangle=|p\rangle) . \tag{A4}$$

Let us decompose any one-body operator $R$ as

$$R=(\rho_0+\sigma_0)R(\rho_0+\sigma_0) \tag{A5}$$

or

$$R=R^A+R^D , \tag{A6}$$

with

$$R^A=\sigma_0R\rho_0+\rho_0R\sigma_0 , \tag{A7}$$

$$R^D=\rho_0R\rho_0+\sigma_0R\sigma_0 . \tag{A8}$$

It is clear from (A3) and (A4) that the operator $R^A$ is antidiagonal in the particle-hole basis (it has vanishing p-p and h-h matrix elements), whereas the operator $R^D$ is diagonal (it has vanishing p-h and h-p matrix elements).

Many operators involved in the present work are antidiagonal. Let us consider, for instance, an operator $R$ such that

$$\rho_0R+R\rho_0=R . \tag{A9}$$

Writing (A9) as

$$\rho_0R(\rho_0+\sigma_0)+(\rho_0+\sigma_0)R\rho_0=(\rho_0+\sigma_0)R(\rho_0+\sigma_0) \tag{A10}$$

leads immediately to

$$\rho_0R\rho_0=\sigma_0R\sigma_0=0 , \tag{A11}$$

which means that

$$R=R^A . \tag{A12}$$

As examples of operators satisfying (A9), we know

(i) the natural $\chi$ [see Eq. (2.10)], which therefore fulfills Eq. (2.12), and

(ii) any first derivative of the density $\rho_0$. For instance,

$$\frac{\partial}{\partial\alpha}\rho_0=\frac{\partial}{\partial\alpha}(\rho_0^2)=\rho_0\frac{\partial\rho_0}{\partial\alpha}+\frac{\partial\rho_0}{\partial\alpha}\rho_0 . \tag{A13}$$

Consequently, the operator $\dot\rho_0$ has only p-h and h-p matrix elements

$$\dot\rho_0=\sigma_0\dot\rho_0\rho_0+\rho_0\dot\rho_0\sigma_0 , \tag{A14}$$

and the same property holds for $\partial\rho_0/\partial q$.

Let us consider the commutator of any operator $R$ with $\rho_0$

$$[R,\rho_0]=[R^D+R^A,\rho_0]=[R^A,\rho_0] , \tag{A15}$$

since the diagonal operator $R^D$ commutes with $\rho_0$. Making (A15) explicit leads to

$$\begin{aligned}[R,\rho_0]=[R^A,\rho_0]&=[\rho_0R\sigma_0+\sigma_0R\rho_0,\rho_0]\\&=\sigma_0R\rho_0-\rho_0R\sigma_0 .\end{aligned} \tag{A16}$$

From (A16), we see that the commutator of any operator with $\rho_0$ has only p-h and h-p matrix elements. This is the case for $\rho_1=i[\chi,\rho_0]$, $F_0=i\hbar[\dot\rho_0,\rho_0]$, $P=F_0/\dot q$. and $[W_0,\rho_0]$. Notice also [see Eq. (A15)] that the antidiagonal part of $R$ is the only one contributing to the commutator. We have used this property for the operator $\chi$, which enters into the first Hamilton equation (2.24) only through $\rho_1$; therefore, this equation gives access only to the antidiagonal part $\chi^A$ of $\chi$. As another consequence of Eq. (A15), the second adiabaticity hypothesis (small acceleration) can be formulated equivalently by the smallness of $[W_0,\rho_0]$ or by the smallness of $W_0^A$.

In the same way followed to obtain Eq. (A16), we get

$$\begin{aligned}[[R^A,\rho_0],\rho_0]&=[\sigma_0R\rho_0-\rho_0R\sigma_0,\rho_0]\\&=\sigma_0R\rho_0+\rho_0R\sigma_0 ,\end{aligned} \tag{A17}$$

that is,

$$[[R^A,\rho_0],\rho_0]=R^A . \tag{A18}$$

This latter property has been used for the antidiagonal operators $\dot\rho$ and $\dot\rho_0$ to derive the "constrained forms" of the TDHF and first ATDHF equations.

We finally remark that the product of a diagonal operator with a diagonal one is antidiagonal,

$$(\rho_0R\rho_0+\sigma_0R\sigma_0)(\rho_0S\sigma_0+\sigma_0S\rho_0)=\rho_0RS\sigma_0+\sigma_0RS\rho_0 , \tag{A19}$$

and therefore has a vanishing trace

$$\mathrm{Tr}\, R^D S^A = 0 . \tag{A20}$$

In particular, this applies to the product of $\rho_1$ with a diagonal operator $P^D$ [see Eq. (4.15)], and also for the product of $\chi$ with $\dot{\rho}_0$,

$$\mathrm{Tr}\, \chi \dot{\rho}_0 = \mathrm{Tr}\, \chi^A \dot{\rho}_0 ,$$

since $\dot{\rho}_0 = (\dot{\rho}_0)^A$. Therefore, the only part of $\chi$ contributing to the collective kinetic energy is its antidiagonal part.

## APPENDIX B: THE FIRST HAMILTON EQUATION FOR THE SCALING PATH

Here we show explicitly that the operators

$$\rho_0(\beta) = e^{i\beta\hat{\theta}} \rho_{\mathrm{st}} e^{-i\beta\hat{\theta}} \tag{5.1}$$

and

$$\chi = -(m/\hbar)\dot{\beta}\theta(\vec{\mathbf{r}}) \tag{5.6}$$

satisfy the first Hamilton equation

$$\hbar\dot{\rho}_0 + i[W_0^D, \rho_1] + i[W_1, \rho_0] = 0 , \tag{B1}$$

provided the gauge invariance

$$[V, \theta(\vec{\mathbf{r}})] = 0 \tag{B2}$$

is fullfilled.

The operators $\theta$ and $\hat{\theta}$ are defined in Sec. V, and $V$ is the two-body interaction.

First, we will use Eq. (B2) to find a new expression for $W_1$. To explicit the gauge invariance, we expand the two-body force as a sum of tensor products

$$V(1,2) = \sum_i V_1^i(1) \otimes V_2^i(2) \tag{B3}$$

and define

$$\chi(1) = \chi \otimes \underline{1} , \tag{B4}$$

$$\chi(2) = \underline{1} \otimes \chi . \tag{B5}$$

Equation (B2) can also be written as

$$[V(1,2), \chi(1) + \chi(2)] = 0 , \tag{B6}$$

which leads to

$$\sum_i [V_1^i, \chi] \otimes V_2^i + \sum_i V_1^i \otimes [V_2^i, \chi] = 0 . \tag{B7}$$

By right-multiplying this equation by $\underline{1} \otimes \rho_0$, one gets

$$\sum_i [V_1^i, \chi] \otimes V_2^i \rho_0 + \sum_i V_1^i \otimes [V_2^i, \chi] \rho_0 = 0 . \tag{B8}$$

We now consider the definition of $W_1$ (Ref. 41)

$$W_1 = i\,\mathrm{Tr}_2 V(1,2)[\chi(2), \rho_0(2)] , \tag{B9}$$

which leads to

$$W_1 = i\,\mathrm{Tr}_2 \sum_i V_1^i \otimes V_2^i [\chi, \rho_0] , \tag{B10}$$

by inserting the definition (B5) of $\chi(2)$ and the expansion (B3) of $V(1,2)$. By use of the cyclic property of the trace, this equation writes

$$W_1 = i\,\mathrm{Tr}_2 \sum_i V_1^i \otimes [V_2^i, \chi] \rho_0 . \tag{B11}$$

From Eq. (B8), we get

$$W_1 = -i\,\mathrm{Tr}_2 \sum_i [V_1^i, \chi] \otimes V_2^i \rho_0 \tag{B12}$$

$$= -i\,\mathrm{Tr}_2 \left[ \sum_i V_1^i \otimes V_2^i \rho_0 , \chi \otimes \underline{1} \right] , \tag{B13}$$

which gives

$$W_1 = -i[W_0 - T, \chi] . \tag{B14}$$

Using the definition (5.6) of $\chi$, we easily obtain

$$[T, \chi] = i\hbar\dot{\beta}\hat{\theta} . \tag{B15}$$

Equations (B14) and (B15) lead finally to

$$-iW_1 = [\chi, W_0] + i\hbar\dot{\beta}\hat{\theta} . \tag{B16}$$

This equation will be used to transform the particle-hole matrix elements of Eq. (B1):

$$\sigma_0 \{ i[W_0^D, \rho_1] + i[W_1, \rho_0] \} \rho_0$$

$$= \sigma_0 \chi W_0^D \rho_0 - \sigma_0 W_0^D \chi \rho_0 + i\sigma_0 W_1 \rho_0 \tag{B17}$$

$$= \sigma_0 \chi W_0^D \rho_0 - \sigma_0 W_0^D \chi \rho_0 - \sigma_0 [\chi, W_0^A + W_0^D] \rho_0 - i\hbar\dot{\beta}\sigma_0\hat{\theta}\rho_0 \tag{B18}$$

$$= -\sigma_0 \chi W_0^A \rho_0 + \sigma_0 W_0^A \chi \rho_0 - i\hbar\dot{\beta}\sigma_0\hat{\theta}\rho_0 . \tag{B19}$$

Since the operator $W_0^A$ (or equivalently the commutator $[W_0, \rho_0]$) is at least of first order in $\chi$, we obtain, by keeping only terms of first order in Eq. (B19),

$$\sigma_0 \{ i[W_0^D, \rho_1] + i[W_1, \rho_0] \} \rho_0 = -i\hbar\dot{\beta}\sigma_0\hat{\theta}\rho_0 . \tag{B20}$$

Now since

$$\sigma_0(\hbar\dot{\rho}_0)\rho_0 = i\hbar\dot{\beta}\sigma_0\hat{\theta}\rho_0 , \tag{B21}$$

[which is a trivial consequence of Eq. (5.1)], all the particle-hole matrix elements of Eq. (B1) vanish, at least as far as we neglect second order terms in $\chi$. Since all terms of this equation have trivially vanishing particle-particle and hole-hole matrix elements, the fulfilling of the first Hamilton equation by $\rho_0$ and $\chi$ given by Eqs. (5.1) and (5.6) is established.

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