Lyapunov stability and Poisson structure of the thermal TDHF and RPA equations

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ABSTRACT

The thermal TDHF equation is analyzed in the Liouville representation of quantum mechanics, where the matrix elements of the single-particle (s.p.) density ρ behave as classical dynamical variables. By introducing the Lie-Poisson bracket associated with the unitary group of the s.p. Hilbert space, we show that TDHF has a hamiltonian, but non-canonical, classical form. Within this Poisson structure, either the s.p. energy or the s.p. grand potential $\Omega(\rho)$ act as a Hamilton function. The Lyapunov stability of both the TDHF and RPA equations around a HF state then follows, since the HF approximation for thermal equilibrium is determined by minimizing $\Omega(\rho)$. The RPA matrix in the Liouville space is expressed as the product of the Poisson tensor with the HF stability matrix, interpreted as a metric tensor generated by the entropy. This factorization displays the roles of the energy and entropy terms arising from $\Omega(\rho)$ in the RPA dynamics, and it helps to construct the RPA modes. Several extensions are considered.

1 INTRODUCTION

The formal structures of the time-independent and time-dependent Hartree-Fock theories and of the random-phase approximation, as well as the nature of their interrelations, have been discussed in many articles and text books. A sample is given in Refs.[1-5]. An especially clear treatment can be found in Chapter VII of the book by Amos de Shalit and Herman Feschbach [6]. Yet we believe that the vein is not exhausted and that some ores are worth assaying.

Most of the literature on TDHF, within the nuclear context, deals with the zero-temperature case. However, far from being more difficult, the finite temperature formalism simplifies several problems and even helps to the understanding of the zero-temperature limit. Two notable references are [4]. The finite temperature random-phase approximation (RPA) has become a fruitful tool to describe the collective modes of nuclei strongly excited through heavy ion collisions [7]. For large amplitude motions, the time-dependent Hartree-Fock (TDHF) equation has recently been used to study the evolution of hot compressed nuclei, with special emphasis on the emission of particles during the expansion and the ensuing separation between liquid and vapor phases [8]. We also recall earlier static HF calculations at finite temperature [9]. For all these reasons, we shall work with general density operators of the form (2.1) both for the static and the time-dependent HF methods.

Our main goal is to clarify a few questions which appeared somewhat obscure to us. As a first example, *entropy* does not seem to enter the finite temperature RPA equations, while it is a basic ingredient in the construction of the static HF state at thermal equilibrium. Why is it then absent from the RPA equations which provide stability conditions about this very HF state ? Another set of perplexing questions are related to the formal structure of the TDHF equations. These exhibit classical hamiltonian features, although we are dealing with a quantum problem.

We shall rely throughout on two main ideas. Firstly, we exhibit the essential role played by the HF *grand potential* $\Omega(\rho) = E - TS - \mu N$, in the dynamical TDHF equations as well as in the static HF method, and at zero temperature as well as at finite temperature. Indeed, while the effective

single-particle (s.p.) TDHF Hamiltonian (2.6) is usually expressed as the variation of the HF *energy* $E(\rho)$ with respect to the s.p. density matrix ρ, we note that the TDHF dynamics is alternatively generated by using $\Omega(\rho)$ instead of $E(\rho)$. By linearizing this new form of the TDHF equation, we recover the two well-known terms of the RPA as contributions from the internal energy E and from the entropy S, respectively. This allows us to disclose the *hidden role of the entropy* in RPA (Section 2.2), and to understand better the relation between the RPA and the HF thermal equilibrium. The replacement of the HF energy by the HF grand potential provides a more compact form for the RPA dynamics, in which entropy is embedded in a crucial way (even in the zero-temperature limit).

Our second tool is the use of the *Liouville representation* of quantum mechanics (Section 2.3). Namely, after having selected some set of relevant observables (here the s.p. operators $a_j^\dagger a_i$), we regard their expectation values (here the set ρ_{ij}) as the components of a time-dependent *vector* (rather than a matrix) governed by non-linear differential equations. In this scope, the TDHF equations get the simple formal structure of a classical dynamical system with coordinates ρ_{ij}.

Having thus inserted the TDHF and RPA equations in a classical frame raises questions about the stability of the motion. It is a well-known result of Thouless [3] that all the RPA modes around a HF solution have real frequencies if this HF solution corresponds to a minimum of the energy. This property has been extended to non-zero temperature HF states [4], the grand potential replacing the energy. However, from the viewpoint of dynamical systems, we are led to wonder under which conditions the TDHF dynamics around a HF state is *Lyapunov stable*. Indeed, the fact that the linearized motion defined by the RPA is a superposition of oscillations does *not* imply that a TDHF trajectory starting from a point close to the HF state will remain for ever in its neighbourhood, since non-linear terms may destabilize the motion. Actually, even if we stick to the RPA, the mere fact that the eigenfrequencies are real does not preclude unstable evolutions of the $t^m e^{-i\omega t}$ type if ω happens to be degenerate.

We address this problem in Section 3, where we examine the stability in the Lyapunov sense of a HF state against TDHF and RPA motions. There is no systematic approach to study the stability of non-linear dynamical

equations, except in one special circumstance. Let us quote in this respect from Ref. [11] : "The only effective way to establish stability of an equilibrium point of a hamiltonian system in many degrees of freedom is to find a conserved quantity with a local maximum or minimum point at the equilibrium." Fortunately such a quantity exists for the TDHF evolution, since the mean-field grand potential $\Omega(\rho)$ is both a *constant* of the TDHF motion and a *minimum* at the HF equilibrium point (in contrast to other conserved quantities such as the average particle number, the s.p. entropy or the HF energy). This allows us to establish the Lyapunov stability of the TDHF motion (Section 3.3). A similar proof holds for the RPA motion (Section 3.4). It provides, without any calculation, a result somewhat stronger than the reality of the eigenfrequencies. We also discuss vanishing eigenfrequencies, which result in differences between the stability conditions for TDHF and RPA.

Another puzzling question, the classical structure of the TDHF equations, has long been outstanding. At least at zero temperature, several studies [12-14]. suggest that the s.p. density can be parametrized by canonically conjugate variables. However, it seems that this has to be paid for by introducing either constraints or some approximation (such as adiabaticity). The present approach helps us to reconsider this problem in a general scope. Recognizing that the TDHF dynamics can be endowed with a hamiltonian or Poisson structure is of interest in several directions. Among the many uses for Poisson structures listed in Ref. [15], let us mention the possibilities of proving the existence of chaos, of better understanding the conservation laws, and of improving the numerical algorithms. However, the main incentive in the nuclear context is the search for "requantization" (see for instance chapter 11 of Ref. [5]).

Our concern in Section 4 has thus been to recast the TDHF dynamics into a classical hamiltonian framework without introducing constraints or using approximations, both at zero and non-zero temperature. The trick consists in using the concept of Poisson structure (see for instance the articles in Ref. [10]), already applied to exhibit the (non-canonical) hamiltonian nature of the Vlasov equation [16] . A Poisson structure is a generalization of the standard Poisson bracket in which the dynamical variables do not need to be generated from pairs of variables satisfying the

canonical relations $\{q_\alpha, p_\beta\} = \delta_{\alpha\beta}$. Here, the brackets $\{f, g\}$ need only to fulfill the main properties of Poisson brackets. From the Lie algebra of $a_j^\dagger a_i$ pairs of creation and annihilation operators, we have inferred a natural Poisson structure for the matrix elements $\rho_{ij} =< a_j^\dagger a_i >$ of the s.p. density, considered as classical variables in the Liouville space (Section 4.2). In this structure, the usual symplectic tensor is replaced by a Poisson tensor C, defined by (4.16) as the bracket between the ρ's. *With respect to this Lie-Poisson structure*(4.19), the TDHF dynamics turns out to be generated by $d\rho/dt = \{\rho, H\}$, where the self-consistent HF energy E (or the HF grand potential Ω) *plays the role of a classical hamiltonian* $H = E$ (or $H = \Omega$). Once this non-canonical hamiltonian form of the TDHF equations is recognized, a systematic research of pairs of canonical variables, possibly overabundant or satisfying constraints, becomes feasible [Section (4.3)].

The formalism is flexible enough to cover several extensions (Section 5), such as fermion systems with *pairing*, or *boson* systems. The only essential changes lie in the set of relevant observables of the Liouville representation, and in their commutation relations which induce different Lie-Poisson structures. We also discuss the connection between the TDHF equation and its classical counterpart, the *Vlasov* equation. It appears that in the Wigner representation, the quantum corrections only arise from a change in the structure of the Poisson tensor [Eqs.(5.5), (5.6)].

Finally, we have taken advantage of the hamiltonian structure of TDHF to cast formally the RPA equations (Section 2.3) into a general and attractive form

$$d\Delta\rho/dt = C_0 \mathcal{B} \Delta\rho \ , \tag{1.1}$$

where C_0 and $\mathcal{B}$ are matrices and $\Delta\rho$ is a vector in the Liouville space. The first matrix C_0, antisymmetric and defined by (2.26), is identified with the Poisson tensor (4.16), evaluated at the HF solution. The second matrix, $\mathcal{B}$, symmetric and positive, is the stability matrix (2.12) of the static HF theory. The occurence of these two matrices reflects the two ingredients entering our formulation of the TDHF equation, namely the Poisson tensor C and the Hamiltonian Ω. Expanding this equation to describe small motions around the HF state naturally gives rise to C_0 and to $\mathcal{B}$ (the matrix of second derivatives of Ω), both taken at the HF point. Since the same approach holds for more general problems, including the dynamics

of fermions with pairing or the dynamics of bosons (Sections 5.1 and 5.2), the factorization $\mathcal{C}_0\mathcal{B}$ of the RPA matrix into a product of simpler matrices appears as a general feature. In the appendices A and B, we take advantage of this factorization to revisit the construction of the RPA modes. It turns out that the eigenvalues and eigenvectors of the RPA matrix can be obtained by diagonalizing two real matrices, one symmetric and positive, the other antisymmetric.

The stability matrix $\mathcal{B}$ of the static HF theory entering the RPA equation (1.1) can also be given another interpretation. It has been shown quite generally [17] that minus the second differential of the entropy, $-d^2S$, defines a metric over the space of relevant variables on which S depends. Here, these variables are restricted to the matrix elements of the s.p. density ρ plus the overall energy. The latter, as well as the particle number, is fixed by means of a heat bath. As usual in thermodynamics, the inclusion of this bath amounts to adding $-T^{-1}(E-\mu N)$ to the entropy of the system. Hence, the metric $-d^2S$ generated by the entropy becomes $T^{-1}\partial^2\Omega/\partial\rho\partial\rho$, which is nothing but $T^{-1}\mathcal{B}$. Thus, $\mathcal{B}$ can be identified with a *metric tensor.*

Although they both rely on the classical structure of the TDHF equations, the Section 3, devoted to stability questions, and the Section 4, where TDHF is recognized as a Poisson system, can be read independently.

2 THE SINGLE-PARTICLE GRAND POTENTIAL IN THE TDHF AND RPA EQUATIONS

2.1 Résumé of HF and TDHF approximations

First we review the well-known formalism of static and dynamic Hartree-Fock theories and, at the same time, define the notations. Mean-field approximations are characterized by replacing the exact density operator by an *uncorrelated* one of the form

$$D = Z^{-1}\ \exp(-\sum_{ij} M_{ij}a_i^\dagger a_j)\ , \tag{2.1}$$

where $a_i^\dagger$ and a_i are creation and annihilation operators associated with a given single-particle basis i, and where Z accounts for the normalization

of D. The approximate state (2.1) can equally be parametrized by the single-particle (s.p.) density matrix

$$\rho_{ij} = \mathrm{Tr}\, D a_j^\dagger a_i \ , \tag{2.2}$$

which is related to the matrix M by

$$\rho = 1/(1+e^M) \ . \tag{2.3}$$

Let us recall the expressions for the energy, the average particle number and the entropy in the mean-field approximation (2.1). For a system of fermions interacting through two-body forces, the energy is

$$\mathrm{Tr}\, H\, D = \mathrm{tr}\, K\rho + \frac{1}{2}\mathrm{tr}\,\mathrm{tr}\, V\rho\rho \equiv E(\rho) \ , \tag{2.4}$$

where K denotes the kinetic energy and V the (antisymmetrized) two-body interaction. The traces in Fock-space and in single-particle space are denoted by Tr and tr, respectively. The variation of the Hartree-Fock energy (2.4) yields

$$\delta E(\rho) = \mathrm{tr}\, W(\rho)\ \delta\rho \ , \tag{2.5}$$

which defines the matrix $W_{ij} \equiv \partial E/\partial\rho_{ji}$ as

$$\frac{\partial E(\rho)}{\partial\rho} \equiv W(\rho) = K + \mathrm{tr}\, V\rho \ . \tag{2.6}$$

The average particle number is

$$\mathrm{Tr}\, N D = \mathrm{tr}\rho \equiv N(\rho) \ . \tag{2.7}$$

The von-Neumann entropy $S(D)$ corresponding to (2.1) is

$$S(D) = -\mathrm{Tr}\, D\log D = -\mathrm{tr}\,[\rho\log\rho + (1-\rho)\log(1-\rho)] \equiv S(\rho) \ , \tag{2.8}$$

and its variation is given by

$$\delta S(\rho) = \mathrm{tr}\,\delta\rho\log\frac{1-\rho}{\rho} = \mathrm{tr}\, M\delta\rho \ . \tag{2.9}$$

The static Hartree-Fock approximation for the grand potential $\Omega(T,\mu)$, which is a function of the temperature T and the chemical potential μ, relies on the minimization of the approximate s.p. expression

$$\mathrm{Tr}\, D(H-\mu N) - TS(D) = E(\rho) - \mu \mathrm{tr}\, \rho - TS(\rho) \equiv \Omega(\rho) \qquad (2.10)$$

with respect to the variations of the matrix elements M_{ij} parametrizing D, or equivalently with respect to the matrix elements of ρ. We denote the resulting s.p. density matrix by ρ_0, which satisfies

$$\frac{\partial \Omega(\rho_0)}{\partial \rho_0} = 0\ . \qquad (2.11)$$

This variational scheme is meaningful only for the *minima* of $\Omega(\rho)$. The absolute minimum is considered as the best s.p. approximation for the actual grand potential at equilibrium ; local minima may be interpreted as approximations to metastable states. Thus, the matrix $\mathcal{B}$, defined by

$$\mathcal{B}_{ij,k\ell} \equiv \frac{\partial^2 \Omega(\rho_0)}{\partial \rho_{0ji} \partial \rho_{0\ell k}}\ , \qquad (2.12)$$

should be non-negative. The usual explicit form for the Hartree-Fock equations is obtained by inserting (2.5) and (2.9) into (2.11), which yields the coupled equations (2.3) and

$$M_0 = \frac{W(\rho_0) - \mu}{T}\ . \qquad (2.13)$$

In the zero temperature limit, where D reduces to a projector on a Slater determinant, $S(\rho)$ approaches zero but $T\partial S/\partial \rho$ does not, and the coupled equations (2.3), (2.13) reduce to the standard equation $[W(\rho_0),\rho_0] = 0$ with $\rho_0^2 = \rho_0$ (and to the prescription of filling the lowest orbitals).

For dynamical problems, the matrices M and ρ [connected by (2.3)] depend on time. Within the time-dependent Hartree-Fock approximation, ρ evolves according to

$$\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}[W(\rho),\rho]\ , \qquad (2.14)$$

where the s.p. HF Hamiltonian $W(\rho)$ is again defined by (2.6). The equation (2.14) can be obtained in various ways ; a variational derivation is

given in Ref. [18]. During the TDHF evolution, the HF energy (2.4) is conserved as a consequence of (2.5), (2.14), since

$$\frac{dE}{dt} = \frac{1}{\mathrm{i}\,\hbar}\mathrm{tr}\, W(\rho)[W(\rho),\rho] = 0\ . \tag{2.15}$$

Moreover, the trace of any function of ρ, $\varphi(\rho)$, is also conserved ; indeed,

$$\frac{d}{dt}\mathrm{tr}\,\varphi(\rho) = \mathrm{tr}\,\varphi'(\rho)\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\,\mathrm{tr}\,\varphi'(\rho)[W(\rho),\rho] = 0 \tag{2.16}$$

vanishes because the function $\varphi'(\rho)$ of the matrix ρ is itself a matrix which commutes with ρ. In particular, the eigenvalues of ρ, the particle number (2.7) and the HF entropy (2.8) are constants of the motion. Accordingly, *the HF grand potential* $\Omega(\rho)$ [Eq.(2.10)] *is conserved by the TDHF evolution.*

2.2 Alternative forms of the TDHF and RPA equations

Using (2.6), the TDHF equation (2.14) can be written equivalently as

$$\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\,[\frac{\partial E(\rho)}{\partial\rho},\rho]\ . \tag{2.17}$$

Moreover, as just noted, both matrices $\partial N(\rho)/\partial\rho$ (the unit matrix in the s.p. space) and

$$\frac{\partial S(\rho)}{\partial\rho} = \log\frac{1-\rho}{\rho} = M \tag{2.18}$$

commute with ρ [from (2.9), (2.3)]. Hence, the TDHF equation (2.17) can as well be expressed as

$$\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\,[\frac{\partial\Omega(\rho)}{\partial\rho},\rho]\ . \tag{2.19}$$

Although the usual form (2.14) is the most convenient for a direct solution, the form (2.19) *in terms of the grand potential* offers conceptual advantages which we proceed to explore.

In particular, Eq.(2.19) allows for a concise writing of the RPA equation of motion. The usual form,

$$\frac{d\Delta\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\,[W(\rho_0), \Delta\rho] + \frac{1}{\mathrm{i}\,\hbar}[\mathrm{tr}\, V\,\Delta\rho, \rho_0]\ , \tag{2.20}$$

is obtained from (2.14) by expanding $\rho(t) = \rho_0 + \Delta\rho(t)$ around a static HF solution and by keeping only the first-order terms in $\Delta\rho$. [The zeroth-order term vanishes as a consequence of (2.3), (2.13).] However, we can also write the RPA equation by expanding (2.19). Owing to the stationarity of $\Omega(\rho)$ at the thermal static HF solution $\rho = \rho_0$ [Eq.(2.11)], the linearization of (2.19) yields

$$\frac{d\Delta(\rho)}{dt} = \frac{1}{\mathrm{i}\,\hbar}[\mathrm{tr}\,\frac{\partial^2\Omega}{\partial\rho_0\partial\rho_0}\Delta\rho, \rho_0]\ . \tag{2.21}$$

This is a more compact form than (2.20) since the right hand side displays a *single term*, which *involves only the second derivative (2.12) of the HF grand potential.*

The two terms in (2.20) can be recovered from (2.21) and from the expression $\Omega(\rho) = E(\rho) - \mu N(\rho) - TS(\rho)$. The term of (2.21) associated with $E(\rho)$ [defined by (2.4)] obviously gives rise to the second term of the r.h.s. of (2.20). The term associated with $-\mu N(\rho)$ vanishes. Hence, we identify the first term of (2.20) with the contribution to (2.21) coming from the entropy. It is interesting to realize that the *two terms of the standard RPA equation* (2.20) can be traced back to the HF grand potential $\Omega(\rho)$, as it is revealed by the form (2.19) of the TDHF equation.

The above interpretation of the first term of (2.20) as an entropy contribution was simple but indirect, relying on (2.11). To show that this correspondence is not trivial, let us check it directly. The contribution of the entropy term to (2.21) is

$$\frac{1}{\mathrm{i}\,\hbar}T\sum_{k\ell}[\rho_0, \frac{\partial}{\partial\rho_{0k\ell}}\,\frac{\partial S}{\partial\rho_0}\Delta\rho_{k\ell}]\ , \tag{2.22}$$

where the matrix $\partial S/\partial\rho$ commutes with ρ, as it is obvious from (2.18). To take advantage of this commutation, we write (2.22) as

$$\frac{1}{\mathrm{i}\,\hbar}T\sum_{k\ell}\Delta\rho_{k\ell}\frac{\partial}{\partial\rho_{0k\ell}}\,[\rho_0, \frac{\partial S}{\partial\rho_0}] - \frac{1}{\mathrm{i}\,\hbar}T\sum_{k\ell}\Delta\rho_{k\ell}[\frac{\partial\rho_0}{\partial\rho_{0k\ell}}, \frac{\partial S}{\partial\rho_0}]\ .$$

The first term vanishes, while the matrix element ij of the second term is

$$\begin{aligned}&\frac{1}{\mathrm{i}\,\hbar}T\sum_{k\ell m}\Delta\rho_{k\ell}(\delta_{ik}\delta_{m\ell}M_{jmj}-M_{0im}\delta_{mk}\delta_{j\ell})\\&=\frac{1}{\mathrm{i}\,\hbar}T\sum_{m}(\Delta\rho_{im}M_{0mj}-M_{0i_{jn}}\Delta\rho_{mj})=\frac{1}{\mathrm{i}\hbar}T[\Delta\rho,M_0]_{ij}\ .\end{aligned}\tag{2.23}$$

We made use of (2.18) to express the matrix $\partial S/\partial\rho_0$ as M_0. The self-consistency condition (2.13) reduces (2.23) to the first term of the r.h.s of (2.20).

The *hidden presence of the entropy* in the RPA equations (2.20) may look surprising since these equations remain unchanged at zero-temperature. Actually, it is already remarkable that the HF equations for the ground state come out alternatively either by accounting for the constraint $\rho^2=\rho$, or by minimizing (2.10) without any constraint on ρ and letting T approach zero. In this limit, the entropy term of (2.10) takes care of the conditions $\rho^2=\rho$. Likewise, when the RPA is written with (2.23), $\partial S/\partial\rho_0$ blows up again in the limit $T\to 0$ but $T\partial S/\partial\rho_0=W(\rho_0)-\mu$ remains finite, producing the first term of (2.20). In both cases, we witness the grinning remnants of the Cheshire Cat Entropy...!

2.3 Liouville representation

The TDHF equations look like *classical* equations of motion. More precisely, it is natural to regard the pair of indices ij denoting the dynamical variables ρ_{ij} as a single index $\alpha=(i,j)$, and to regard ρ_α as a vector. This picture is nothing but a particular instance of the *Liouville representation* of quantum mechanics [19,17]. Rather than focusing on the wave function or on the density operator, the Liouville representation focuses on the expectation values of the observables which are labelled by some index. Here, the index α labels the observable $a_j^\dagger a_i$ according to (2.2) ; the non-linearity of the TDHF motion results from the s.p. approximation, which has eliminated all more complicated observables. When written in terms of the variables ρ_α, the TDHF equations have the structure of a classical dynamical system, and the RPA equations (2.20) or (2.21) appear as their linearized version around a static HF solution. In the Liouville

representation, the RPA equations take the form

$$\frac{d\Delta\rho_{ij}}{dt} = -\mathrm{i} \sum_{k\ell} \mathcal{R}_{ij,k\ell}\, \Delta\rho_{\ell k} \ , \tag{2.24}$$

or, with a more compact notation

$$\frac{d\Delta\rho}{dt} = -\mathrm{i}\, \mathcal{R}\Delta\rho \ , \tag{2.24'}$$

where the matrix $\mathcal{R}$ acts in the Liouville space. The quantity $\mathcal{B}$ defined by (2.12) should also be viewed as a matrix in this space. According to (2.21), $\mathcal{R}$ and $\mathcal{B}$ are related by

$$\mathcal{R}_{ij,k\ell} = \sum_{m,n} \frac{1}{\hbar} \left(\delta_{im}\rho_{0nj} - \rho_{0im}\delta_{nj}\right) \mathcal{B}_{mn,k\ell} \ . \tag{2.25}$$

By introducing in the Liouville space the matrix

$$\mathcal{C}_{0ij,k\ell} \equiv \frac{\mathrm{i}}{\hbar}(\rho_{0i\ell}\delta_{kj} - \delta_{i\ell}\rho_{0kj}) \ , \tag{2.26}$$

one can also write

$$\mathcal{R}_{ij,k\ell} = \mathrm{i}\, \mathcal{C}_{0ij,nm}\mathcal{B}_{mn,k\ell} \ , \tag{2.27}$$

or, more compactly

$$\mathcal{R} = \mathrm{i}\, \mathcal{C}_0\mathcal{B} \ , \tag{2.27'}$$

while (2.21) or (2.24) reads

$$\frac{d\Delta\rho}{dt} = \mathcal{C}_0\mathcal{B}\Delta\rho \ . \tag{2.28}$$

The matrix $\mathcal{C}$ will play an important role in Section 4.

In Sections 3.5 and 3.6, we shall take advantage of the simple form (2.27) of the RPA matrix. In the zero temperature limit, (2.27) expresses that, in a basis where ρ_0 is diagonal ($\rho_{0ii} = 0$ or 1), the matrix elements of $\mathcal{R}$ are equal to the corresponding elements of $\mathcal{B}$ multiplied by 0, $\mathrm{i}/\hbar$ or $-\mathrm{i}/\hbar$.

Note that we have interchanged a pair of indices ij when writing matrix products such as (2.24) or (2.27), in agreement with the definitions (2.2),

(2.12) and with the use of traces in (2.5), (2.9), (2.20), (2.21). Likewise, the definition of hermitean matrices in the Liouville space should include this interchange. Then $\mathcal{B}$ is hermitean and $\mathcal{C}$ is antihermitean since

$$\mathcal{B}^*_{ij,k\ell} = \mathcal{B}_{\ell k,ji} \ , \quad \mathcal{C}^*_{ij,k\ell} = -\mathcal{C}_{\ell k,ji} \ . \tag{2.29}$$

Moreover, $\mathcal{B}$ is symmetric and $\mathcal{C}$ is antisymmetric when the transposition is performed without interchange inside the pair ij (or $k\ell$) :

$$\mathcal{B}_{ij,k\ell} = \mathcal{B}_{k\ell,ij} \ , \quad \mathcal{C}_{ij,k\ell} = -\mathcal{C}_{k\ell,ij} \ . \tag{2.30}$$

The intertwining of some indices can be traced back to the choice of non-hermitean basic operators $a^\dagger_j a_i$ (for $i \neq j$) to define the vector ρ_{ij} in the Liouville representation. Had we chosen a hermitean basis such as

$$a^\dagger_i a_i \ , \quad a^\dagger_j a_i - a^\dagger_i a_j \ , \quad \text{and} \quad \mathrm{i}(a^\dagger_j a_i - a^\dagger_i a_j) \tag{2.31}$$

for the observables labelled by α, their expectation values ρ_α would have been real, the matrix structure would have been the usual one with respect to the indices α, the matrix $\mathcal{B}_{\alpha,\beta}$ would have been symmetric real, and the matrix $\mathcal{C}_{\alpha,\beta}$ antisymmetric real. This choice of a *real Liouville representation* is especially convenient for formal purposes, and it will be helpful in the following Sections.

3 STABILITY OF TDHF AND RPA MOTIONS

We have just recalled that the TDHF equations have the same structure as the equations of motion of a classical dynamical system. The static HF solutions correspond to equilibrium points for this motion. Although their stability against small deviations has been extensively studied, we feel that some questions deserve further investigation.

3.1 Various types of stability and their relations

Before we enter the discussion, let us survey some well-known definitions and interrelations of various types of stability [11,20,21]. We are interested in the trajectories $x(t)$ of a dynamical system evolving around an

equilibrium point. We denote as x the set of dynamical variables governed by the equations $dx/dt = F(x)$, and by x_0 the equilibrium point under consideration, which satisfies $F(x_0) = 0$.

(a) Roughly speaking, the *Lyapunov stability* of an equilibrium point expresses that a trajectory starting near this point stays in its vicinity. We borrow the following definition from Ref. [21] : "the equilibrium point x_0 is said to be (Lyapunov) stable if given any neighborhood U of x_0, there is a sub-neighborhood V of x_0 such that if x lies in V then its orbit remains in U forever". In other words, Lyapunov stability means uniform convergence to x_0 of the trajectories (for $t > 0$) *as their initial point tends to* x_0.

(b) An equilibrium point x_0 is said to be *asymptotically stable* if it is Lyapunov stable and if, in addition, there exists some (fixed) neighborhood W of x_0 such that any trajectory issued from W tends to x_0 *as the time* t *tends to* $+\infty$. Asymptotic stability is the strongest type of stability and it implies all the others.

(c) *Linear stability* means Lyapunov stability for the linearized equations of motion around x_0.

(d) Stability is often studied by looking at the eigenvalues $\lambda_\mu \equiv -i\omega_\mu$ of the matrix relating dx/dt to $x - x_0$ in the linearized regime. We shall use below the term "*eigenfrequency stability*" to express that the eigenfrequencies ω_μ of the linearized motion have non-positive imaginary parts :

$$\mathrm{Im}\,\omega_\mu = \mathrm{Re}\,\lambda_\mu \leq 0\ , \quad \forall \mu\ . \tag{3.1}$$

If all eigenfrequencies ω_μ have negative imaginary parts, asymptotic stability is ensured and $x(t)$ tends to x_0 exponentially with t. If some eigenfrequency has a positive imaginary part, i.e., if the motion is eigenfrequency unstable, the point x_0 is Lyapunov unstable since $x(t)$ diverges from x_0 exponentially.

Lyapunov stability or linear stability imply eigenfrequency stability but the converse is not true. Indeed, in the linear regime, any solution $x(t)$ can

be decomposed into a sum

$$x(t) = \sum_{\omega} P_m^{(\omega)}(t) e^{-\mathrm{i}\,\omega t}$$

of contributions, each associated with an eigenfrequency ω. If this eigenfrequency is of multiplicity n, $P_m^{(\omega)}(t)$ is a polynomial of degree m, with $m \leq n-1$. Thus, if some *real* eigenfrequency ($\mathrm{Im}\,\omega = 0$) is *degenerate* ($n > 1$), eigenfrequency stability does not warrant linear stability, since a time-dependence of $x(t)$ in $t^m e^{-\mathrm{i}\,\omega t}$ ($m \leq n-1$) is not precluded. When a system is eigenfrequency stable, $x(t)$ may diverge from x_0, but at most as a power of t, not exponentially.

Lyapunov stability is not implied by linear stability because non-linear terms in the equations of motion may divert the trajectory. For instance, the two-dimensional motion

$$\dot{x}_1 = -x_2 + x_1(x_1^2 + x_2^2) \ ,$$

$$\dot{x}_2 = x_1 + x_2(x_1^2 + x_2^2) \ ,$$

is linearly stable, since the linearized trajectories are circles around the origin ; but the dynamics is destabilized by the non-linear terms. Conversely, non-linear terms may have a stabilizing effect. Hence, linear stability does not necessarily result from Lyapunov stability. An example is the one-dimensional motion of a particle with Hamiltonian $p^2 + x^4$, which is Lyapunov and eigenfrequency stable but linearly unstable.

3.2 The Lagrange-Dirichlet theorem

In our case, the dynamical variables x are the matrix elements of ρ, the dynamical equations $dx/dt = F(x)$ are the TDHF equations (2.14), the equilibrium point x_0 is the HF solution ρ_0, the linearized equations of motion are the RPA equations (2.20), and the eigenfrequencies ω_μ are the eigenvalues in the Liouville space of the matrix $\mathcal{R}$ of Eq.(2.24). The stability usually discussed in this context [2,5,6] is what we have called the *eigenfrequency stability*. Indeed, it has been shown, both at zero [3] and non-zero temperature [4], that the eigenfrequencies are *all real* if the HF state ρ_0

corresponds to a local minimum of the grand potential $\Omega(\rho)$ [Eq.(2.10)]. In practice, this result is often used the other way around. If the RPA motion about some HF solution is found to be eigenfrequency unstable, then this solution cannot be an acceptable approximation for the ground (or equilibrium) state of the system. This situation discloses the existence of at least one other HF solution with lower energy (or lower grand potential).

However, in view of the above discussion, eigenfrequency stability *warrants neither* the linear stability of the RPA motion, *nor* the Lyapunov stability of TDHF. Indeed, if some eigenfrequency ω happens to be degenerate, though real, the stability of the RPA motion requires the absence of a $t^m e^{-i\omega t}$ behaviour with $m \geq 1$. Moreover, even if the motion is linearly stable, one still has to show that it is also Lyapunov stable, i.e., that the non-linear terms do not create unstabilities in the TDHF motion.

As indicated in the introduction, we shall rely on the Lagrange-Dirichlet theorem, which provides a sufficient condition for the Lyapunov stability of a dynamical system. Suppose there exists a function $G(x)$ of the dynamical variables x which *remains constant* along the trajectories $x(t)$. Suppose also that the point x_0 is a *local minimum* of G. Then *these two conditions ensure that x_0 is Lyapunov stable.*

The proof is rather intuitive. The fact that x_0 is a local minimum of $G(x)$ implies the existence of a neighborhood X in which $G(x) > G(x_0)$. Keeping x inside X, the domain Y_ε defined by $G(x) - G(x_0) < \varepsilon$ and $x \in X$ shrinks to x_0 as $\varepsilon \to 0$. Then, if the initial point of a trajectory lies in Y_ε, the whole trajectory will remain forever in Y_ε since G is conserved. Coming back to the above definition of the Lyapunov stability, let us choose $\varepsilon > 0$ as the lower bound of $G(x) - G(x_0)$ on the border of $U \cap X$. We can take V as Y_ε, and Lyapunov stability follows.

3.3 Lyapunov stability of the TDHF motion

The usual form (2.14) or (2.17) of the TDHF equation exhibits the conservation of the HF energy $E(\rho)$, but it is not directly suitable for the study of stability. Among its many time-independent solutions, nothing in this form singles out the HF equilibrium states (they moreover depend on temperature and chemical potential). The form (2.19) presents an interesting

virtue in this respect. It is expressed in terms of the grand potential $\Omega(\rho)$, which is not only a constant of the motion like $E(\rho)$ or $S(\rho)$, but which is also the very quantity which determines the HF states ρ_0 by minimization.

We are thus in position to apply directly the Lagrange-Dirichlet theorem, with the following result : *the TDHF motion is Lyapunov stable provided the HF solution is a local minimum of the grand potential* $\Omega(\rho)$.

Of course, asymptotic stability cannot be achieved, precisely because the conservation of $\Omega(\rho)$ along the trajectory prevents ρ from approaching ρ_0 as $t \to \infty$.

3.4 Linear stability

Because Lyapunov stability of the TDHF motion does not entail linear stability, we resort again to the Lagrange-Dirichlet theorem to study the stability of the RPA motion. We wish to find a constant of the RPA motion which is also a minimum at the HF state ρ_0.

To this aim, let us consider the truncation of $\Omega(\rho)$ to second order in $\rho - \rho_0$,

$$\Omega^{(2)}(\rho) \equiv \Omega(\rho_0) + \frac{1}{2}\mathrm{tr}\ \mathrm{tr}\ \frac{\partial^2 \Omega}{\partial\rho_0 \partial\rho_0}\Delta\rho\,\Delta\rho\ , \tag{3.2}$$

also written in Liouville space as

$$\Omega^{(2)}(\rho) = \Omega(\rho_0) + \frac{1}{2}\Big(\Delta\rho, \mathcal{B}\,\Delta\rho\Big) \tag{3.2'}$$

in terms of the matrix (2.12).

The RPA equation (2.21) can be rewritten as

$$\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\left[\frac{\partial\Omega^{(2)}}{\partial\rho}, \rho_0\right]\ , \tag{3.3}$$

a form analogous to (2.19), $\Omega(\rho)$ being replaced by $\Omega^{(2)}(\rho)$ and ρ by ρ_0 in the commutator. In spite of these changes, the function $\Omega^{(2)}(\rho)$ is a constant of the RPA motion (3.3), just as $\Omega(\rho)$ was a constant of the TDHF motion (2.19), since (3.3) implies

$$\frac{d}{dt}\Omega^{(2)}(\rho) = \mathrm{tr}\,\frac{\partial\Omega^{(2)}}{\partial\rho}\frac{d\rho}{dt} = \frac{1}{\mathrm{i}\,\hbar}\ \mathrm{tr}\ \frac{\partial\Omega^{(2)}}{\partial\rho}\left[\frac{\partial\Omega^{(2)}}{\partial\rho}, \rho_0\right] = 0\ . \tag{3.4}$$

On the other hand, $\Omega^{(2)}(\rho)$ has a local minimum at $\rho = \rho_0$ when the matrix $\mathcal{B}$ is positive. Thus *the Lyapunov stability of the RPA motion, i.e., the linear stability of TDHF*, is ensured *if all the eigenvalues of* $\mathcal{B}$ *are positive.*

This condition $\mathcal{B} > 0$ for the stability of the RPA motion is slightly more stringent than the stability condition of the TDHF motion, i.e., the existence of a local minimum of $\Omega(\rho)$ at $\rho = \rho_0$. Indeed, the latter condition, which is a consequence of $\mathcal{B} > 0$, may still be satisfied when some eigenvalues of $\mathcal{B}$ vanish. In such a case, the RPA motion may be Lyapunov unstable, while the TDHF motion around ρ_0 is stabilized by the non-linear terms. As an example, consider the TDHF and RPA dynamics generated in a two-state Hilbert space by

$$\Omega \equiv \frac{1}{2}(1-\rho_{11})^2 + \frac{1}{2}\rho_{22}^2 + \frac{1}{2}(\rho_{12}+\rho_{21})^2 + k(\rho_{12}-\rho_{21})^4 \ . \qquad (3.5)$$

(We have chosen a form of Ω which does not keep track of the singularity of the entropy term in (2.10) ; more realistic examples would introduce complications irrelevant to our argument.) For $k > 0$, the HF equilibrium solution is $\rho_{11} = 1$, $\rho_{22} = \rho_{12} = 0$, corresponding to the minimum of Ω. Hence, the TDHF motion is Lyapunov stable. This implies in turn eigenfrequency stability : it is easily checked that the eigenfrequencies of the RPA equations

$$\begin{aligned} &\dot{\rho}_{11} = \dot{\rho}_{22} = 0 \ , \\ &\dot{\rho}_{12} = \tfrac{\mathrm{i}}{\hbar}(\rho_{12}+\rho_{21}) = \dot{\rho}_{21}^* \ , \end{aligned} \qquad (3.6)$$

all vanish. However, the general solution of (3.6),

$$\rho_{12} = \mathrm{i}\,a + b\hbar + 2\mathrm{i}\,bt \ , \qquad (3.7)$$

where a and b are real constants, exhibits a linear unstability coming from the degeneracy of the eigenfrequency $\omega = 0$: in the linear regime the point ρ drifts away from ρ_0 (as t), but it is driven back by the TDHF non-linearity. If in (3.5) the term $(\rho_{12}+\rho_{21})^2$ were replaced by $(\rho_{12}+\rho_{21})^4$, both Lyapunov and linear stability would be satisfied (in spite of the degeneracy of $\omega = 0$). But if in addition k were negative, the motion would be linearly stable and Lyapunov unstable.

3.5 Eigenfrequency stability

We have just given a direct derivation of the stability of the RPA motion when the matrix $\mathcal{B}$ is positive, without relying on the diagonalization of the RPA matrix $\mathcal{R}$. Quite remarkably, this provides us with an alternative proof of the reality of the eigenvalues ω_μ of this matrix. This proof is simpler than the usual one. Indeed, linear stability implies eigenfrequency stability. Hence, if $\mathcal{B} > 0$, Eq.(3.1) is satisfied and the imaginary parts of the eigenfrequencies ω_μ cannot be positive. Moreover, because the RPA motion is reversible, the eigenvalues of $\mathcal{R}$ come in pairs $\pm\omega$. Therefore, *all eigenfrequencies of the RPA are real if* $\mathcal{B} > 0$.

Linear stability has a further implication on the RPA matrix. If an eigenfrequency ω has a multiplicity $n > 1$, the general time-dependence expected is $t^m e^{-\mathrm{i}\,\omega t}$ with $m \leq n-1$. As well-known, there are then $n-m$ linearly independent eigenvectors of $\mathcal{R}$ associated with the eigenvalue ω. However, linear stability implies that $m = 0$ (for any ω), since a trajectory involving a factor $t^m e^{-\mathrm{i}\,\omega t}$ with $m \geq 1$ would move away from the vicinity of ρ_0. Hence, for $\mathcal{B} > 0$, the number of eigenvectors associated with each eigenfrequency ω is equal to its multiplicity, and the overall number of eigenvectors of the matrix $\mathcal{R}$ is equal to its dimension. To summarize, the condition $\mathcal{B} > 0$ *implies that the RPA matrix is diagonalizable*; a similarity $\mathcal{T}^{-1}\mathcal{R}\mathcal{T}$, where $\mathcal{T}$ is some non-singular matrix, brings it into a diagonal *real* form, and any solution of the RPA behaves as a sum of constants or of pure oscillatory terms.

The above derivation of the diagonalizability of $\mathcal{R}$ for $\mathcal{B} > 0$ is perfectly respectable, but somewhat indirect since it goes through the Lagrange-Dirichlet theorem and the Lyapunov stability. In contrast to the standard proof, it does not make use of the particular structure of $\mathcal{R}$ and relies only on the conservation of $\Omega(\rho)$. We present in Appendix A an alternative and more direct derivation, taking advantage of the form (2.27) of $\mathcal{R}$, i.e., $\mathcal{R} = \mathrm{i}\,\mathcal{C}_0\mathcal{B}$. The viewpoint is closer to the current approaches, but the *use of the Liouville representation* simplifies the formalism. We also discuss in Appendix B the case of a stability matrix $\mathcal{B}$ having zero eigenvalues ; this case is relevant when some broken invariance gives rise to Goldstone modes.

4 TDHF AS A LIE-POISSON SYSTEM

The classical structure of the TDHF equations has already drawn much attention in the nuclear context, at least in the zero-temperature limit [12-14]. A natural question is whether these equations can be cast into a hamiltonian form, i.e., whether the dynamical variables ρ_α can be divided into conjugate coordinates and momenta. This is clearly feasible for the RPA around a stable HF equilibrium with $\mathcal{B} > 0$, since the dynamics is then the same as for harmonic oscillators. However, for large amplitude motions described by TDHF, and in particular at finite temperature, no systematic treatment seems available. The forms (2.17) and (2.19) are reminiscent of a classical hamiltonian structure, and they suggest to reexamine the question in the Liouville representation. We shall rely on a formulation of dynamics in terms of Poisson-like brackets which generalizes the usual formulation of Hamiltonian mechanics with canonical Poisson brackets, and which has been found useful in several different contexts [10,11,15,22]. Let us first recall the definition of a Poisson structure.

4.1 Poisson structures

The set x of dynamical variables being represented by a point on a manifold, we consider the functions $f(x)$ defined on this manifold. A Poisson structure is an operation $\{f,g\} = k$ which associates with two functions f and g a third function k, this correspondence having the following properties :

(i) it is bilinear ;

(ii) it is antisymmetric :

$$\{f,g\} = -\{g,f\} ;$$

(iii) it satisfies Jacobi's identity :

$$\{\{f,g\},k\} + \{\{g,k\},f\} + \{\{k,f\},g\} = 0 ; \tag{4.1}$$

(iv) it satisfies Leibniz's derivation rule :

$$\{fg,k\} = f\{g,k\} + \{f,k\}g \ . \tag{4.2}$$

Denoting by x_α a set of coordinates on the manifold, each x_α is a special case of a function f, and a basis for the Poisson structure is defined by the *Poisson tensor*

$$\{x_\alpha, x_\beta\} \equiv C_{\alpha\beta} \ , \tag{4.3}$$

where the $C_{\alpha\beta}$ are functions of x. It is antisymmetric according to property (ii). The property (iv) amounts to the expression

$$\{f,g\} = \sum_{\alpha\beta} \frac{\partial f}{\partial x_\alpha} C_{\alpha\beta} \frac{\partial g}{\partial x_\beta} \tag{4.4}$$

for any pair f,g of functions. Finally, Jacobi's identity (4.1) is equivalent to

$$\sum_\delta \left[\frac{\partial C_{\alpha\beta}}{\partial x_\delta} C_{\delta\gamma} + \frac{\partial C_{\beta\gamma}}{\partial x_\delta} C_{\delta\alpha} + \frac{\partial C_{\gamma\alpha}}{\partial x_\delta} C_{\delta\beta} \right] = 0 \ . \tag{4.5}$$

The standard *canonical Poisson brackets* $\{\ \}_{\rm P}$ of hamiltonian mechanics are a particular example of a Poisson structure. There, the variables x_α denote the set of conjugate pairs q_i, p_i, and the elementary brackets $C_{\alpha\beta}$ which generate the structure have the usual symplectic structure $\{q_i, p_j\}_{\rm P} = \delta_{ij}$, $\{q_i, q_j\}_{\rm P} = \{p_i, p_j\}_{\rm P} = 0$. However, more general Poisson structures exist. An outstanding example is given by *Dirac brackets* [23], defined from the usual Poisson brackets $\{\ \}_{\rm P}$ by

$$\{f,g\}_{\rm D} = \{f,g\}_{\rm P} - \sum_{s,s'} \{f,\theta_s\}_{\rm P} c_{ss'} \{\theta_{s'}, g\}_{\rm P} \ , \tag{4.6}$$

where the functions θ_s account for constraints, and where $c_{ss'}$ is the inverse matrix of $\{\theta_s, \theta_{s'}\}_{\rm P}$.

By introducing Poisson structures one generalizes hamiltonian dynamics to systems in which canonically conjugate variables do not necessarily exist, for instance constrained systems or systems involving overabundant degrees

of freedom. In such cases, the dynamics is generated by a hamiltonian function $h(x)$ providing the equations of motion

$$\frac{df}{dt} = \{f, h\} \tag{4.7}$$

for any function f on the manifold x. This type of dynamics keeps the Poisson structure invariant in time, since according to (4.1), (4.7) we have

$$\{f + \frac{df}{dt}dt, g + \frac{dg}{dt}dt\} = k + \frac{dk}{dt}dt$$

if $\{f, g\} = k$. The dynamical equation (4.7) has the same form as in the usual hamiltonian dynamics, but the extended definition of brackets results in a *non-canonical hamiltonian theory*. Various examples have been worked out [10,16], including classical field theories [15]. For instance, the Vlasov equation was shown to have the form (4.7), where the dynamical variables x_α denote the classical density in phase-space $\rho_{\rm cl}(\mathbf{r}, \mathbf{p})$, the index α standing for the point $(\mathbf{r}, \mathbf{p})$. In this case, the Poisson structure for $\rho_{\rm cl}$ is generated from the underlying canonical structure for the dynamical variables $\mathbf{r}_i, \mathbf{p}_i$ $(1 \leq i \leq N)$ through the definition

$$\rho_{\rm cl}(\mathbf{r}, \mathbf{p}) = < \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i)\delta(\mathbf{p} - \mathbf{p}_i) > \tag{4.8}$$

of $\rho_{\rm cl}$. The non-canonicity of the transformation $\mathbf{r}_i$, $\mathbf{p}_i \rightarrow \rho_{\rm cl}$ gives rise to a non-canonical Poisson structure for $\rho_{\rm cl}$ (see Section 5.3).

Another approach to recognize the existence of a Poisson structure relies on *Lie algebras*. (Actually, the properties (i) (ii) (iii) mean that the Poisson structure is a Lie algebra for the functions f.) Consider a Lie group with generators ξ_α and structure constants $\Gamma^\gamma_{\alpha\beta}$ defined by

$$[\xi_\alpha, \xi_\beta] = \sum_\gamma \Gamma^\gamma_{\alpha\beta}\xi_\gamma \ . \tag{4.9}$$

These constants are antisymmetric and satisfy the Jacobi identity

$$\sum_\delta \left(\Gamma^\delta_{\alpha\beta}\Gamma^\epsilon_{\delta\gamma} + \Gamma^\delta_{\gamma\alpha}\Gamma^\epsilon_{\delta\beta} + \Gamma^\delta_{\beta\gamma}\Gamma^\epsilon_{\delta\alpha}\right) = 0 \ . \tag{4.10}$$

Let us then choose a Poisson tensor (4.3) linear in x and having the form

$$C_{\alpha\beta} \equiv \sum_{\delta} \Gamma^{\delta}_{\alpha\beta} x_{\delta} \ , \tag{4.11}$$

generated from the Lie structure constants. The condition (4.5) is obviously fulfilled, and (4.4) defines a non-canonical structure called *Lie-Poisson structure.*

4.2 The Lie-Poisson structure of TDHF

We wish to apply the above ideas to the TDHF dynamics on the manifold of s.p. densities ρ. Here, the coordinates x_α are the matrix elements ρ_{ij}, considered as vectors ρ_α in the Liouville space. These dynamical variables ρ_{ij} entering the TDHF equations are related by (2.2) to the s.p. operators $a^\dagger_j a_i$. The latter are the generators of the *Lie group of unitary transformations in the s.p. space.* Let us introduce the structure constants Γ :

$$\left[a^\dagger_j a_i, a^\dagger_\ell a_k\right] = \mathrm{i} \sum_{mn} \Gamma^{mn}_{ij,k\ell} a^\dagger_m a_n \ , \tag{4.12}$$

$$\Gamma^{mn}_{ij,k\ell} = \mathrm{i}\left(\delta_{in}\delta_{kj}\delta_{m\ell} - \delta_{i\ell}\delta_{mj}\delta_{kn}\right) . \tag{4.13}$$

[The factor i has been introduced in (4.12) for the following reason. In principle, we should have taken *antihermitean* linear combinations of $a^\dagger_j a_i$ for the generators ξ_α of the Lie group, namely

$$-\mathrm{i}\, a^\dagger_i a_i \ , \quad -\mathrm{i}\left(a^\dagger_i a_j + a^\dagger_j a_i\right) \ , \quad a^\dagger_j a_i - a^\dagger_i a_j \ , \tag{4.14}$$

since this group is unitary. Then the structure constants $\Gamma^\gamma_{\alpha\beta}$ would have been real. The replacement of the generators (4.14) by $-\mathrm{i}\, a^\dagger_j a_i$ gives rise to the factor i of (4.12) and transforms these $\Gamma^\gamma_{\alpha\beta}$ into (4.13).]

The one-to-one correspondence

$$\rho_\alpha = < \mathrm{i}\, \xi_\alpha > \tag{4.15}$$

between our dynamical variables and the generators ξ_α of the Lie group holds of course for any basis of the Liouville space, in particular for the

basis $\xi_{ij} \equiv -\mathrm{i}\, a_j^\dagger a_i$ and for the real basis (2.31), (4.14). It suggests *defining* a *Poisson tensor* $\{\rho_\alpha, \rho_\beta\}$ according to (4.11), (4.13), i.e.,

$$\begin{aligned} \{\rho_{ij}, \rho_{k\ell}\} &= C_{ij,k\ell} = \tfrac{1}{\hbar} \textstyle\sum_{mn} \Gamma^{mn}_{ij,k\ell} \rho_{nm} \\ &= \tfrac{\mathrm{i}}{\hbar} (\rho_{i\ell}\delta_{kj} - \delta_{i\ell}\rho_{kj}) \ . \end{aligned} \tag{4.16}$$

The factor $1/\hbar$ has been introduced in this definition for dimensional reasons implied by the equations of motion (4.7). It will eventually cancel the factor $\hbar$ which enters into the TDHF equation (2.17). We recognize in (4.16) the extension to arbitrary values of ρ of the matrix C_0 which was defined by (2.26) in terms of the static HF value ρ_0. In Appendices A and B, we take advantage of this structure of C_0 to study the RPA. We now consider large amplitude TDHF motions, for which C depends on time through ρ.

Let us denote as $f(\rho)$ functions of the matrix elements ρ_{ij} ; examples are $E(\rho), W_{ij}(\rho), S(\rho)$ defined by (2.4), (2.6), (2.8), respectively. Still regarding the ρ_{ij}'s as coordinates ρ_α in the Liouville space, we infer from (4.4) and (4.16) the Poisson structure

$$\begin{aligned} \{f, g\} &= \sum_{ijk\ell} \frac{\partial f}{\partial \rho_{ij}} C_{ij,k\ell} \frac{\partial g}{\partial \rho_{k\ell}} \\ &= \frac{1}{\mathrm{i}\,\hbar} \sum_{ijk} \rho_{ij} \left(\frac{\partial f}{\partial \rho_{kj}} \frac{\partial g}{\partial \rho_{ik}} - \frac{\partial g}{\partial \rho_{kj}} \frac{\partial f}{\partial \rho_{ik}} \right) \end{aligned} \tag{4.17}$$

on the space of functions $f(\rho)$. Returning to the original s.p. Hilbert space, and defining matrices $\partial f / \partial \rho$ in this space as

$$\left(\frac{\partial f}{\partial \rho} \right)_{jk} \equiv \frac{\partial f}{\partial \rho_{kj}} \ , \tag{4.18}$$

in agreement wi—h the conventions of Section 2, we can rewrite (4.17) as

$$\{f, g\} = \frac{1}{\mathrm{i}\,\hbar} \mathrm{tr}\, \rho \left[\frac{\partial f}{\partial \rho}, \frac{\partial g}{\partial \rho} \right] = \frac{1}{\mathrm{i}\,\hbar} \mathrm{tr}\, \frac{\partial f}{\partial \rho} \left[\frac{\partial g}{\partial \rho}, \rho \right] \ . \tag{4.19}$$

The introduction of the *Poisson structure* (4.19) constitutes the main point of this Section 4. Actually, we could have directly introduced (4.19)

as a definition of the bracket, and checked that it satisfies all the properties listed in Section 4.1. The above derivation *from the Lie algebra* (4.12) makes this verification useless. Alternative forms to (4.19) can be given ; in particular we have for any g

$$\{\rho_{ij}, g\} = \sum_{k\ell} C_{ij,k\ell} \frac{\partial g}{\partial \rho_{k\ell}} = \frac{1}{\mathrm{i}\,\hbar} \left[\frac{\partial g}{\partial \rho}, \rho\right]_{ij} . \tag{4.20}$$

These definitions, together with the form (2.17) of the TDHF equations, make obvious that

$$\frac{d\rho_{ij}}{dt} = \{\rho_{ij}, E(\rho)\} . \tag{4.21}$$

Thus, the TDHF motion can be viewed as *classical* dynamics, *with the HF energy as Hamiltonian*, but with the non-symplectic Lie-Poisson bracket (4.19). This non-canonical hamiltonian structure is alsc called a Lie-Poisson system. Using (4.20), we can express the TDHF equations as

$$\frac{d\rho_{ij}}{dt} = \sum_{k\ell} C_{ij,k\ell} \frac{\partial E}{\partial \rho_{k\ell}} . \tag{4.22}$$

These are a natural generalization of Hamilton's equations, where the symplectic tensor is replaced by C. More generally, any function $f(\rho)$ evolves according to the equation

$$\frac{df}{dt} = \{f(\rho), E(\rho)\} = \sum_{\alpha\beta} \frac{\partial f}{\partial \rho_\alpha} C_{\alpha\beta} \frac{\partial E}{\partial \rho_\beta} . \tag{4.23}$$

The alternative form (2.19) of the TDHF equations also provides

$$\frac{df}{dt} = \{f(\rho), \Omega(\rho)\} . \tag{4.24}$$

Thus, we can also take the s.p. *grand potential* $\Omega(\rho)$ *as a classical Hamiltonian*, to be associated with the Lie-Poisson structure (4.19). We get thus a simple interpretation of the stability properties of the TDHF motion around a HF solution ρ_0, since now $\Omega(\rho)$ appears both as the function which is minimum at ρ_0 and as a classical Hamiltonian.

Here as in Section 2, the use of $\Omega(\rho)$ instead of $E(\rho)$ as a Hamiltonian is helpful for elucidating the formal structure of the RPA. If we rewrite the TDHF equations (4.22) as

$$\frac{d\rho_{ij}}{dt} = \{\rho_{ij}, \Omega(\rho)\} = \sum_{k\ell} C_{ij,k\ell} \frac{\partial \Omega}{\partial \rho_{k\ell}} , \tag{4.25}$$

we note that the right hand side depends on ρ through the Poisson tensor C and through the Hamiltonian Ω. In the expansion of (4.25) to first order in $\Delta\rho = \rho - \rho_0$, where ρ_0 is a static solution, we should in principle get two contributions, one from C and one from Ω. However a HF solution ρ_0 corresponds not only to the vanishing of the right hand side of (4.25), but also of $\partial\Omega/\partial\rho_0$. Hence we can disregard the variations of C around C_0, and expand Ω up to second order as in (3.2). We obtain the RPA equation in the form

$$\frac{d\Delta\rho_{ij}}{dt} = \{\Delta\rho_{ij}, \Omega^{(2)}(\rho)\}_0 = \sum_{k\ell} C_{oij,k\ell} \frac{\partial \Omega^{(2)}}{\partial \Delta\rho_{k\ell}} , \tag{4.26}$$

identified with (2.28). The RPA comes out as a hamiltonian-type of motion with C_0 *as a Poisson tensor and* $\Omega^{(2)}$ *as a Hamilton function.* Its present derivation from (4.25) readily produces the general form $d\Delta\rho/dt = C_0 B \Delta\rho$, which will hold for the various extensions of Sections 5.1 and 5.2.

4.3 Search for canonical variables

The main difference between usual canonical and non-canonical hamiltonian systems of the type (4.23) lies in the possible existence of vanishing eigenvalues of C [11]. At each point of the manifold, the matrix C (which is real and antisymmetric) can be diagonalized, its eigenvalues either coming out in opposite pure imaginary pairs or being zero. By means of a suitable dilatation, one can associate a pair of dynamical variables q_i, p_i (satisfying the usual Poisson algebra) with each pair of eigenvalues of the first type . However, the parametrization of the manifold requires the introduction of additional variables r_k associated with the eigenvalue 0 and satisfying

$$\{r_k, q_i\} = 0 , \quad \{r_k, p_i\} = 0 . \tag{4.27}$$

Moreover, for a general Poisson structure, this canonical choice of variables q, p, r *is only local* and cannot be universal. In particular, the very *number* of variables r_k (i.e., the multiplicity of the eigenvalue 0 of C) *may vary* from point to point.

For the TDHF dynamics, the eigenvalues of the matrix $C_{\alpha\beta}$ defined by (4.16) are equal to the differences $\mathrm{i}\,(\rho_m - \rho_n)$ [for any m and n] between the eigenvalues of ρ considered as a matrix in the s.p. Hilbert space. (In this subsection we take $\hbar = 1$.) The multiplicity of the eigenvalue 0 is equal at least to the dimension of this s.p. space, if the spectrum of ρ presents no degeneracy ; it is much larger for zero temperature dynamics, where all ρ_n are either 0 or 1. This excludes the possibility of finding a *universal* set of canonical variables q, p, r which would replace the parametrization ρ_{ij} of the manifold ρ, since the number of variables r_k depends on the point ρ.

Vanishing eigenvalues for the Poisson tensor C result in the existence of *structural constants of the motion*, irrespective of the Hamiltonian. We have already recalled in Section 2 that any TDHF dynamics conserves the eigenvalues ρ_m of ρ. More generally, we see from (4.20), (4.23) that the functions g of the matrix elements of ρ which satisfy

$$\left[\frac{\partial g}{\partial \rho}, \rho\right] = 0 \tag{4.28}$$

also satisfy $\{g, E\} = 0$ for any Hamiltonian $E(\rho)$ and are thus constants of the motion. Such quantities depend in general on the initial conditions : if the degeneracy of the eigenvalues of ρ increases, more functions g are conserved in any TDHF motion. In particular, functions g of the form $\mathrm{tr}\,\varphi(\rho)$, where φ is some function of a single variable, are conserved along the hamiltonian flow for arbitrary initial conditions, and for an arbitrary Hamiltonian, since

$$\{f(\rho), \mathrm{tr}\,\varphi(\rho)\} = 0\ , \quad \forall f\ . \tag{4.29}$$

Examples are $S(\rho)$ and $N(\rho)$, and (4.29) explains why $E(\rho)$ can be replaced by $\Omega(\rho) = E(\rho) - TS(\rho) - \mu N(\rho)$ in the equations of motion (4.21-4.25).

The conservation of the eigenvalues of ρ implies that the *eigenvalues of the Poisson tensor are conserved* along the hamiltonian flow. Thus, the manifold ρ can be split into sheets, each one characterized by given eigenvalues ρ_m of ρ, inside which the TDHF motion takes place. *For each*

sheet, the multiplicity of the zero-eigenvalue of $\mathcal{C}$ is fixed, and we can expect therein to find *canonical parametrizations* q, p, r. The variables r satisfying (4.27) will remain fixed along any TDHF trajectory, while the conjugate pairs q, p will obey ordinary Hamilton's equations.

The simplest example of a canonical parametrization of ρ is provided by the RPA. Since the Poisson tensor $\mathcal{C}_0$ is *fixed* once and for all in (4.26), its diagonalization is sufficient for constructing the canonical set q, p, r which can replace the non-canonical dynamical variables ρ_{ij}. Let us take a basis in which ρ_0 and hence $\mathcal{C}_0$ are diagonal matrices in the s.p. space and in the Liouville space respectively. The Poisson structure is given in this diagonal representation by

$$\{\rho_{ij}, \rho_{k\ell}\} = \mathrm{i}\, \delta_{i\ell}\delta_{kj}(\rho_{oi} - \rho_{oj}) \ , \tag{4.30}$$

where $\rho_{oij} \equiv \rho_{oi}\delta_{ij}$. The variables r satisfying (4.27) include the diagonal matrix elements of ρ, and more generally the off-diagonal elements ρ_{ij} such that (4.30) vanishes, i.e.,

$$r_{ij} = \rho_{ij} \quad \text{for} \quad \rho_{oi} - \rho_{oj} = 0 \ . \tag{4.31}$$

The remaining parameters can be taken as the conjugate pairs

$$q_{ij} = \frac{\rho_{ij} + \rho_{ji}}{\sqrt{2(\rho_{oi} - \rho_{oj})}} \ , \quad p_{ij} = \frac{\mathrm{i}\,(\rho_{ij} - \rho_{ji})}{\sqrt{2(\rho_{oi} - \rho_{oj})}} \qquad \text{for} \quad \rho_{oi} - \rho_{oj} > 0 \ . \tag{4.32}$$

Indeed, the inversion of these equations into

$$\rho_{ij} = \sqrt{\frac{\rho_{oi} - \rho_{oj}}{2}}(q_{ij} - \mathrm{i}\, p_{ij}) = \rho^*_{ji} \quad \text{for } \rho_{oi} - \rho_{oj} > 0 \ , \tag{4.33}$$

and (4.31) exhibit (4.30) as a direct consequence of the canonical structure of the set q, p, r. If we express the Hamiltonian $\Omega^{(2)}(\rho)$ entering (4.26) in terms of the variables q, p, r by (4.31) and (4.33), the RPA equations take the form of *Hamilton's equations*

$$\frac{dq_{ij}}{dt} = \frac{\partial \Omega^{(2)}}{\partial p_{ij}} \ , \quad \frac{dp_{ij}}{dt} = -\frac{\partial \Omega^{(2)}}{\partial q_{ij}} \ , \tag{4.34}$$

supplemented by the conservation equations $dr_{ij}/dt = 0$. This hamiltonian structure was recognized long ago for the zero-temperature RPA, where $\rho_{oi} - \rho_{oj}$ is just 1 in (4.32) and $\{\rho_{ij}, \rho_{ji}\} = \mathrm{i}$ for hole-particle matrix elements. Writing the RPA dynamics as (4.34) reduces the study of its stability to a problem of linearized classical *hamiltonian* dynamics. We recover thus the results of Section 3 as consequences of the general theory, as it is explained for instance in [11]. In particular, the fact that $\Omega^{(2)}$ is a minimum in terms of the variables ρ implies that the Hamiltonian $\Omega^{(2)}(q,p)$ is also a minimum in terms of q and p (its dependence on r is irrelevant since the variables r remain fixed), and this ensures linear stability.

The extension of this scheme to large-amplitude TDHF motions is non-trivial, since the Poisson tensor C which is to be diagonalized depends on the point ρ. Local canonical coordinates can be constructed as above around each point, but matching them into a unique global set is not obvious, even if we stay on submanifolds in which the number of variables r is constant.

Let us illustrate these difficulties by looking for canonical variables q, p, r in the case when all the eigenvalues ρ_m of ρ (conserved in the TDHF motion) are different from one another and from zero. These eigenvalues ρ_m are the variables r which satisfy (4.27). To analyze the remaining degrees of freedom, we write ρ as

$$\rho_{ij} = \sum_m \varphi_{mi} \varphi^*_{mj} \tag{4.35}$$

in terms of its eigenvectors normalized according to

$$\sum_i |\varphi_{mi}|^2 = \rho_m \ . \tag{4.36}$$

We then parametrize φ_{mi} as

$$\begin{gathered} \varphi_{mi} = \tfrac{1}{\sqrt{2}}(q_{mi} + \mathrm{i}\, p_{mi}) \ , \\ q_{mi} = \tfrac{1}{\sqrt{2}}(\varphi_{mi} + \varphi^*_{mi}) \ , \quad p_{mi} = \tfrac{\mathrm{i}}{\sqrt{2}}(\varphi^*_{mi} - \varphi_{mi}) \ . \end{gathered} \tag{4.37}$$

Canonical Poisson brackets between the variables q, p provide $\{\varphi^*_{mi}, \varphi_{nj}\} = \mathrm{i}\, \delta_{mn}\delta_{ij}$ and thus generate for ρ_{ij} the Poisson tensor (4.16). However, this canonical parametrization of ρ is overabundant, since a change in the phase of each eigenvector φ_m does not modify ρ. Moreover, the variables q, p, r

are constrained by the normalization conditions (4.36), and by the orthogonality of any two eigenvectors φ_m. This is the price paid for obtaining a *global* parametrization of ρ, valid on the whole manifold.

The parametrization (4.35) in terms of canonically conjugate variables (4.37) has been introduced long ago in zero temperature TDHF dynamics [12], when all eigenvalues ρ_m of ρ are either 0 or 1. In that case, the number of variables r is larger since i $(\rho_m - \rho_n)$ vanishes for any pair of holes or particles. The arbitrariness of the variables q, p is also larger since it corresponds to all unitary transformations in the hole space, instead of the phase change of the eigenvectors φ_m. These difficulties were carefully studied in the case of large amplitude adiabatic motions [14]. Dirac brackets were introduced so as to deal with the corresponding constraints. Their occurrence can be interpreted in the present framework as a specialization of the general Poisson structure exhibited in Section 4.2.

The equations of motion generated by the Hamiltonian $E(\rho)$ [or $\Omega(\rho)$] for the variables q, p, r with the canonical Poisson brackets [supplemented by (4.27)] preserve the norm (4.36) of the eigenvectors φ_m and their orthogonality, if these properties are imposed at the initial time. However, the dynamics generated on q, p includes a time-dependence of the phase of the eigenvectors φ_m of ρ which is irrelevant. This phase is unphysical, and its dynamics does not affect the motion of ρ [the only physical quantity]. The situation is reminiscent of a gauge invariance associated with changes of the redundant variables q, p which leave ρ invariant. Once the gauge (here the phases of φ_m) is fixed at the initial time, its choice is set forward in time by the evolution associated with $E(\rho)$. We can, however, modify the Hamiltonian by adding terms such as

$$\frac{1}{2} \sum_{mi} \alpha_m (p_{mi}^2 + q_{mi}^2) \tag{4.38}$$

which only modify the time-dependence of the gauge without any consequence on the motion of ρ. This change in the spurious dynamics is of interest in the framework of adiabatic TDHF theory, where ρ evolves slowly. In spite of this adiabaticity, the phases of φ_m may present fictitious rapid oscillations, and hence nothing warrants that the dummy variables q, p vary slowly. The freedom in the choice of the overabundant variables

has been used (at zero temperature) to keep the motion of all variables slow by means of an adequate parametrization of ρ [13,14].

We can find the roots of the decomposition (4.35) in terms of canonical variables in a Lie group argument. In order to build the Lie-Poisson structure (4.19), we started from the algebra (4.12) associated with unitary transformations in the s.p. space. This algebra resulted from the anticommutation relations of the fermion operators $a_i, a_j^\dagger$. However, the same algebra (4.12) can also be represented in terms of *boson* operators $b_i, b_j^\dagger$ since the s.p. space is the same for fermions and for bosons. As well-known, the algebra of boson operators is equivalent to the symplectic algebra of canonical pairs of position and momentum operators, and the Lie-Poisson construction then leads to standard Poisson brackets for the variables q, p. When we parametrize ρ_{ij} as (4.35), the variables φ_{mi} , φ^*_{mi} correspond to the boson operators $b_i, b_i^\dagger$ generating the boson Lie algebra. Thus, the canonical variables (4.37) reflect the underlying representation $-\mathrm{i}\, b_j^\dagger b_i$ of the generators of the unitary group in terms of boson operators, and the non-canonical Poisson structure (4.19) for the physical variables ρ_{ij} is induced from the Poisson bracket $\{q, p\}$ by the same mechanism from which the Lie-algebra (4.12) is induced from the boson commutation relations. The superabundance of the variables (4.37) comes from the need for representing ρ_{ij} as a sum (4.35), whereas the corresponding generator $-\mathrm{i}\, b_j^\dagger b_i$ is just a product of two operators.

We have discussed at length the canonical (but redundant) parametrization (4.35) of ρ. The general method based on the analysis of the Poisson tensor and on changes of variables by standard methods of classical dynamics would easily lead to alternative parametrizations suited to one purpose or another, for instance in dealing with TDHF equations in the hydroynamic limit or in contracting further the description to a few collective variables.

5 POSSIBLE EXTENSIONS

5.1 Pairing

As well-known, both the static and dynamic Hartree-Fock theories are extended to account for pairing (either for nuclei or for superconductors) by the inclusion, besides the s.p. operators $c_i^\dagger c_j$, of the pairs $c_i c_j$ and $c_i^\dagger c_j^\dagger$. Let us denote by

$$\xi_\alpha = c_i^\dagger c_j \ , \quad c_i c_j \ , \quad c_i^\dagger c_j^\dagger \ , \quad 1 \tag{5.1}$$

all these operators, including the unit operator, and by $\rho_\alpha =< \xi_\alpha >$ their expectation values ; here, the index α denotes not only a pair i, j but also the nature of the operators ξ_α. If the density operator D of the trial state is the exponential of a linear combination of the ξ_α's as in (2.1), the entropy $S(\rho)$ is easy to express and the energy $E(\rho)$ can be evaluated by means of Wick's theorem. Then, the minimization of the grand potential $\Omega(\rho)$ provides the self-consistent Hartree-Fock-Bogoliubov (HFB) equations. The stability matrix $\mathcal{B}$ involves, instead of (2.12), the second derivative of $\Omega(\rho)$ with respect to all components of ρ, normal and abnormal. The time-dependent HFB equations, which generalize the TDHF equations, conserve $\Omega(\rho)$.

Thus the entire analysis of stability made in Section 3 can easily be transposed to the TDHFB motion of the variable ρ_α around a minimum of $\Omega(\rho)$, and to its linearized version. However, the invariance under the transformation $e^{i\lambda N}$ is broken since the operator N does not commute with the effective Bogoliubov Hamiltonian. The TDHFB dynamics around a minimum of Ω is thus Lyapunov stable, except for motions associated with this broken invariance for which the discussion of the end of Appendix B is relevant.

In the Liouville space generated from the operators ξ_α, the structure of the RPA equations with pairing is a straightforward extension of the structure written in Section 2.3 and studied in the Appendices A and B. Indeed, the basic equation (2.28) retains its factorized form, $\mathcal{C}_0$ and $\mathcal{B}$ being matrices in the larger Liouville space in which we now work.Here again, we can use alternatively the HFB energy or the grand potential to generate the TDHFB equations of motion. The construction of the Poisson structure

proceeds as in Section 4.2 from the remark that the operators (5.1) are the generators of a Lie group, the Bogoliubov group [24]. Thus, in spite of the occurence of pairing, TDHFB is a Lie-Poisson system. A classical (but non-canonical) structure underlies its dynamics, with the HFB energy or grand potential as Hamiltonian, in the manifold of the normal and abnormal variables ρ_α.

5.2 Bosons

The same considerations apply to Bose systems, including the possibility of condensation. Here, the operators ξ_α are the set

$$\xi_\alpha = b_i^\dagger b_j \ , \quad b_i b_j \ , \quad b_i^\dagger b_j^\dagger \ , \quad b_i \quad , \quad b_i^\dagger \ , \ 1 \tag{5.2}$$

which again generate a Lie group [24]. Within the above theory one could study the stability of the Gross-Pitaevskii equation [25] and exhibit its Poisson structure.

5.3 Wigner representation

In the Liouville space, the Wigner representation $\rho_{\rm W}\,(\mathbf{r},\mathbf{p})$ of the s.p. density is just a reparametrization of the dynamical variables ρ_{ij} generated by a change of basis in the set (2.31) ; see for instance [17,26]. More precisely, for spinless particles, if we denote by $\psi^\dagger(\mathbf{r})$ the creation operator at the point $\mathbf{r}$, we have

$$\rho_{\rm W}\,(\mathbf{r},\mathbf{p}) = \int \frac{d\mathbf{s}}{(2\pi\hbar)^3} e^{i\,\mathbf{p}.\mathbf{s}/\hbar} \rho(\mathbf{r}-\frac{\mathbf{s}}{2},\mathbf{r}+\frac{\mathbf{s}}{2}) \ , \tag{5.3}$$

$$\rho(\mathbf{r}',\mathbf{r}'') \equiv < \psi^\dagger(\mathbf{r}'')\psi(\mathbf{r}') > = \int d\mathbf{p}\ e^{i\,\mathbf{p}.(\mathbf{r}'-\mathbf{r}'')/\hbar}\ \rho_{\rm W}\left(\frac{\mathbf{r}'+\mathbf{r}''}{2},\mathbf{p}\right) \ . \tag{5.4}$$

(This definition corresponds to the normalization $\int \mathbf{drdp}\ \rho_{\rm W}\,(\mathbf{r},\mathbf{p}) = N$, but $\rho_{\rm W}$ is also currently defined with respect to the measure $\mathbf{drdp}/(2\pi\hbar)^3$ in phase space.) From (5.3), (5.4) and from the bracket (4.16) between the

variables $\rho(\mathbf{r}', \mathbf{r}'')$ we get the expression of the Poisson tensor

$$\{\rho_W(\mathbf{r},\mathbf{p}), \rho_W(\mathbf{r}',\mathbf{p}')\} = \int \frac{du dv}{(2\pi^2\hbar)^3} \sin[\mathbf{u}.(\mathbf{p}-\mathbf{p}') - \mathbf{v}.(\mathbf{r}-\mathbf{r}')]\ \rho_W\left(\frac{\mathbf{r}+\mathbf{r}'+\hbar\mathbf{u}}{2}, \frac{\mathbf{p}+\mathbf{p}'+\hbar\mathbf{v}}{2}\right) \tag{5.5}$$

in the Wigner representation. The TDHF evolution of ρ_W is therefore governed by a classical hamiltonian dynamics generated by the bracket (5.5) from a Hamiltonian equal to the HF energy or grand potential (expressed in terms of ρ_W).

The *classical limit* of the Poisson structure is obtained by expanding the right hand side of (5.5) in powers of $\hbar$, which allows integration over $\mathbf{u}$ and $\mathbf{v}$. This yields

$$\{\rho_W(\mathbf{r},\mathbf{p}), \rho_W(\mathbf{r}',\mathbf{p}')\} \underset{\hbar\to 0}{\longrightarrow} \delta(\mathbf{p}-\mathbf{p}')\nabla\delta(\mathbf{r}-\mathbf{r}').\nabla_p\rho_W(\mathbf{r},\mathbf{p}) - \delta(\mathbf{r}-\mathbf{r}')\nabla\delta(\mathbf{p}-\mathbf{p}').\nabla_r\rho_W(\mathbf{r},\mathbf{p})\ . \tag{5.6}$$

We recognize the Poisson structure which was directly written in classical statistical mechanics for the s.p. density in phase space $\rho_{cl}(\mathbf{r},\mathbf{p})$ [16]. This structure was simply induced on $\rho_{cl}(\mathbf{r},\mathbf{p})$ by the standard Poisson brackets between the coordinates $\mathbf{r}_i$ and $\mathbf{p}_i$ of the N particles and by the definition (4.8) which relates the dynamical variables ρ_{cl} to the canonical variables $\mathbf{r}_i, \mathbf{p}_i$. The resulting form of the Vlasov equation is hamiltonian [with the Poisson structure (5.6)] for the variables ρ_{cl}, the Hamiltonian being equal to the s.p. classical energy $E_{cl}(\rho_{cl})$ [or $\Omega_{cl}(\rho_{cl})$], a functional of $\rho_{cl}(\mathbf{r},\mathbf{p})$.

For $\hbar$ finite, the Hartree energy $E_H(\rho_W)$, when expressed in terms of the Wigner density ρ_W, has exactly the same form as the classical s.p. energy $E_{cl}(\rho_{cl})$ in terms of ρ_{cl}. Thus, the time-dependent *Hartree* equation has the *same Hamiltonian* as the *Vlasov* equation but the Poisson structures (5.5) and (5.6), which define the dynamical law $d\rho/dt = \{\rho, H\}$, are not the same. In the present formalism, quantum mechanics enters the mean-field equation simply through a *modification of the Poisson structure* (and through inclusion of the exchange term in the energy). The quantum corrections to the Vlasov equation are given by expanding the Poisson tensor (5.5) in powers of $\hbar$ beyond the leading term (5.6).

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We dedicate this paper to Herman Feshbach for his 71st birthday.

APPENDIX A :

DIAGONALIZATION OF THE RPA MATRIX FOR $\mathcal{B} > 0$

We start from the form (2.27) of $\mathcal{R}$, and assume that $\mathcal{B}$ is a positive matrix. We have noted in Section 2.3 that, in a Liouville representation, $\mathcal{B}$ is hermitean while $\mathcal{C}_0$ is antihermitean. The condition $\mathcal{B} > 0$ allows us to define the matrix $\mathcal{B}^{1/2}$, which (like $\mathcal{B}$ itself) is hermitean, positive and invertible. Thus, we can rewrite (2.27) as

$$\mathcal{R} = \mathrm{i}\,\mathcal{C}_0\mathcal{B} = \mathrm{i}\,\mathcal{B}^{-1/2}(\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2})\mathcal{B}^{1/2}\ , \qquad (A.1)$$

which expresses that the matrices $\mathcal{R}$ and $\mathrm{i}\,\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ are related by a similarity. The latter matrix is hermitean. Therefore $\mathcal{R}$ can be diagonalized, and all its eigenvalues ω are real. Among them, some are zero (even though $\mathcal{B}$ is strictly positive). Indeed, the vanishing eigenvalues of $\mathcal{R} = \mathrm{i}\,\mathcal{C}_0\mathcal{B}$ are in a one-to-one correspondence with those of $\mathcal{C}_0$ (with the same left eigenvectors). From (2.26) the matrix $\mathcal{C}_0$ is diagonal in the Liouville space if ρ_0 is diagonal in the original Hilbert space, and its eigenvalues are all the differences $\mathrm{i}\,(\rho_{om} - \rho_{on})$ between eigenvalues of ρ_0. This form of $\mathcal{C}_0$ generates eigenvalues $\omega = 0$ for $\mathcal{R}$ if $\rho_{om} = \rho_{on}$. The non-zero eigenvalues are those of $\mathrm{i}\,\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$, which is an antisymmetric hermitean matrix in a real Liouville representation (as we have seen at the end of Section 2, $\mathcal{B}$ is then real symmetric and $\mathcal{C}_0$ real antisymmetric). Hence, the non-zero eigenvalues of $\mathcal{R}$ *come out in pairs* $\pm\omega$.

This proof also provides a construction of the right and left eigenvectors of $\mathcal{R}$. Let us denote as $\mathcal{U}$ the unitary matrix which diagonalizes $\mathrm{i}\,\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ into

$$\mathcal{R}_{\mathrm{d}} = \mathrm{i}\,\mathcal{U}^{\dagger}\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}\,\mathcal{U}\ , \qquad (A.2)$$

where $\mathcal{R}_{\mathrm{d}}$ is a diagonal matrix whose elements ω_λ are the eigenvalues of $\mathcal{R}$. We get from $(A.1)$

$$\mathcal{R} = \mathcal{T}\,\mathcal{R}_{\mathrm{d}}\,\mathcal{T}^{-1}\ , \qquad (A.3)$$

with

$$\mathcal{T} = \mathcal{B}^{-1/2}\mathcal{U}\ . \qquad (A.4)$$

In the Liouville space, the right eigenvectors $\varphi_\alpha^{(\mu)}$ of $\mathcal{R}$ are the columns of the matrix $\mathcal{T}$,

$$\varphi_\alpha^{(\mu)} = \mathcal{T}_{\alpha\mu} = (\mathcal{B}^{-1/2}\mathcal{U})_{\alpha\mu} \ , \qquad (A.5)$$

the corresponding eigenvalue ω_μ being $\mathcal{R}_{d\,\mu\mu}$. Its left eigenvectors $\chi_\alpha^{(\mu)}$ are the lines of the matrix $\mathcal{T}^{-1}$,

$$\chi_\alpha^{(\mu)} = (\mathcal{T}^{-1})_{\mu\alpha} = (\mathcal{B}^{1/2}\mathcal{U})_{\alpha\mu}^* \ . \qquad (A.6)$$

An explicit diagonalization of $\mathcal{R}$ thus involves the following steps : diagonalization of $\mathcal{B}$ (a real symmetric matrix in a real Liouville space), which makes the construction of $\mathcal{B}^{1/2}$ trivial ; then diagonalization of $\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ (a real antisymmetric matrix) which provides the ω's, the matrix $\mathcal{U}$ and hence the φ's.

The relations between the right eigenvectors of $\mathcal{R}$, which are interpreted as elementary excitations of the system around the HF equilibrium, take especially simple forms in the Liouville representation. We first get from $(A.5), (A.6)$

$$\chi_\alpha^{(\mu)*} = \sum_\beta \mathcal{B}_{\alpha\beta}\varphi_\beta^{(\mu)} \ . \qquad (A.7)$$

Hence, the biorthonormality of the right and left eigenbasis φ, χ of $\mathcal{R}$ provides

$$\sum_{\alpha\beta} \varphi_\alpha^{(\mu)*}\, \mathcal{B}_{\alpha\beta}\, \varphi_\beta^{(\nu)} = \delta_{\mu\nu} \ , \qquad (A.8)$$

which expresses that the eigenmodes of $\mathcal{R}$ are *orthogonal with respect to the stability matrix* $\mathcal{B}$. The closure relation $\sum_\mu \varphi_\alpha^{(\mu)}\chi_\beta^{(\mu)} = \delta_{\alpha\beta}$ also yields

$$\sum_\mu \varphi_\alpha^{(\mu)}\varphi_\beta^{(\mu)*} = (\mathcal{B}^{-1})_{\alpha\beta} \ . \qquad (A.9)$$

The relations arising from the symmetry $\pm\omega$ are best expressed in a real Liouville representation. Because $\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ is then antisymmetric and real, the matrix $\mathcal{U}$ which diagonalizes it can be chosen in such a way that its columns corresponding to the eigenvalue 0 are real, and that all other columns can be associated in pairs $(\mu, -\mu)$ corresponding to opposite eigenvalues, $\pm i\,\omega_\mu$, with complex conjugate eigenvectors :

$$\varphi_\alpha^{(\mu)*} = \varphi_\alpha^{(-\mu)} \ . \qquad (A.10)$$

This property reflects the reality of the solutions $\Delta\rho_\alpha(t)$ of the RPA equation in any real Liouville representation (in the Liouville representation (2.31), $\Delta\rho_\alpha$ denotes either $\Delta\rho_{ij} + \Delta\rho_{ji}$ or $\mathrm{i}\,\Delta\rho_{ij} - \mathrm{i}\,\Delta\rho_{ji}$, for $i \neq j$).

APPENDIX B :

EIGENFREQUENCIES AND EIGENMODES OF THE RPA FOR $\mathcal{B} \geq 0$

We study below the case $\mathcal{B} \geq 0$ along the lines of Appendix A. For continuity reasons, all eigenvalues of $\mathcal{R}$ are still real as for $\mathcal{B} > 0$. However, as we noted in Section 3, the RPA or TDHF motions may now be Lyapunov unstable, although eigenfrequency stability still holds. At the end of Section 3.4 we gave an example in which $\mathcal{B}$ had a vanishing eigenvalue responsible for linear unstability. To explore linear stability, we need to study the diagonalizability of $\mathcal{R}$. If its right eigenvectors span the whole space as they do when $\mathcal{B} > 0$, linear stability follows. But we may find a time-behaviour in $t^m e^{-i\omega t}$ if some eigenvectors are lost, as in (3.7).

We first note that several steps of Appendix A remain valid if some eigenvalues of $\mathcal{B}$ approach zero : the diagonalization of $\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ still provides a unitary matrix $\mathcal{U}$; the left eigenvectors (A.6) would remain well-defined but now they may fail to span the whole Liouville space, and the right eigenvectors (A.5) may diverge. We thus need to reconsider the approach.

Let us denote by ℓ the dimension of the Liouville space, and choose a basis in such a way that the *stability matrix* $\mathcal{B}$ *is diagonal*, its first q eigenvalues b_α being equal to 0. We denote as $\mathcal{P}$ the projector on the subspace $\alpha \leq q$. The first q columns of $\mathcal{R} = i\mathcal{C}_0\mathcal{B}$ vanish, while its diagonal block $\alpha > q$, $\beta > q$ has exactly the same form as for a strictly positive matrix $\mathcal{B}$. In the subspace $\alpha > q$, this block $i\mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$ can be diagonalized into $\hat{\mathcal{R}}_{\rm d}$ by means of a unitary transformation $\hat{\mathcal{U}}$ (we use a hat to denote a matrix which vanishes outside the subspace $\alpha > q$, i.e., such that $\hat{\mathcal{U}}\mathcal{P} = \mathcal{P}\hat{\mathcal{U}} = 0$). Denoting by $\hat{\mathcal{B}}^{-1/2}$ the inverse of $\mathcal{B}^{1/2}$ in the subspace $\alpha > q$, and introducing the invertible matrix

$$\mathcal{T} = \mathcal{P} + \hat{\mathcal{B}}^{-1/2}\hat{\mathcal{U}} \quad , \quad \mathcal{T}^{-1} = \mathcal{P} + \hat{\mathcal{U}}^\dagger\mathcal{B}^{1/2} \, , \tag{B.1}$$

we get

$$\mathcal{T}^{-1}\mathcal{R}\mathcal{T} = \hat{\mathcal{R}}_{\rm d} + i\,\mathcal{P}\mathcal{C}_0\mathcal{B}^{1/2}\hat{\mathcal{U}} \, . \tag{B.2}$$

This form shows that $\mathcal{R}$ is similar to a diagonal matrix in the subspace $\mathcal{B} \neq 0$, plus an off-diagonal block astride the subspaces $\mathcal{B} = 0$ and $\mathcal{B} \neq 0$.

For all the non-zero eigenvalues of $\mathcal{R}$ (which are the non-zero values of $\hat{\mathcal{R}}_{\rm d}$), the analysis proceeds as for $\mathcal{B} > 0$. If we denote as $q < \mu \leq q+s$ the indices μ such that $\hat{\mathcal{R}}_{{\rm d}\,\mu} = 0$, the right eigenvectors associated with non-zero eigenvalues are given by

$$\begin{aligned} \varphi_\alpha^{(\mu)} &= {\rm i}\,(\mathcal{C}_0 \mathcal{B}^{1/2}\hat{\mathcal{U}})_{\alpha\mu}\hat{\mathcal{R}}_{{\rm d}\,\mu}^{-1} \\ &= (\hat{\mathcal{B}}^{-1/2}\hat{\mathcal{U}})_{\alpha\mu} + {\rm i}\,(\mathcal{P}\mathcal{C}_0\mathcal{B}^{1/2}\hat{\mathcal{U}})_{\alpha\mu}\mathcal{R}_{{\rm d}\,\mu}^{-1}\,, \quad \mu > q+s\,, \end{aligned} \tag{B.3}$$

which is more complicated than the formula $(A.5)$ for a strictly positive matrix $\mathcal{B}$. The corresponding left eigenvectors are

$$\chi_\alpha^{(\mu)} = (\mathcal{B}^{1/2}\hat{\mathcal{U}})_{\alpha\mu}^{*}\,. \tag{B.4}$$

The number of linearly independent right (or left) eigenvectors associated with eigenfrequencies $\omega \neq 0$ is thus equal to their multiplicity. Hence , if $\mathcal{B} \geq 0$, RPA solutions *cannot behave as* $t^m e^{-{\rm i}\,\omega t}$ *with* $m \geq 1$ for *eigenfrequencies* $\omega \neq 0$.

It remains to discuss the eigenfrequency $\omega = 0$. The $(\ell - q) \times (\ell - q)$ matrix $\hat{\mathcal{C}}_0 \equiv \mathcal{B}^{1/2}\mathcal{C}_0\mathcal{B}^{1/2}$, or equivalently the truncated matrix $\mathcal{C}_{0\alpha\beta}$ with $\alpha > q$, $\beta > q$, has s vanishing eigenvalues. Thus, the multiplicity of the eigenvalue 0 of $\mathcal{R} = {\rm i}\,\mathcal{C}_0\mathcal{B}$ is equal to $q+s$ and has two origins : (i) the multiplicity s arises from $\hat{\mathcal{C}}_0$ (and was also present for $\mathcal{B} > 0$) ; (ii) the multiplicity q arises from $\mathcal{B}$. From $(B.2)$, we find s linearly independent left eigenvectors, still given by $(B.4)$. A remaining set of q left eigenvectors is also readily constructed if the conditions

$$(\mathcal{C}_0\mathcal{B}^{1/2}\hat{\mathcal{U}})_{\alpha\beta} = 0\,, \quad \forall \alpha \leq q\,, \quad \forall q < b \leq q+s \tag{B.5}$$

are fulfilled. Under the same conditions, $q+s$ linearly independent right eigenvectors (eigenmodes of $\mathcal{R}$) are given by

$$\varphi_\alpha^{(\mu)} = \mathcal{T}_{\alpha\mu}\,, \qquad \mu \leq q+s\,. \tag{B.6}$$

However, if $(B.5)$ is not satisfied, a number $1 \leq m \leq q$ of left (or right) eigenvectors is missing. To evaluate m, we note that the right and left eigenvectors associated with $\omega = 0$ are obtained by solving

$$\sum_{\beta > q} \mathcal{C}_{o\alpha\beta}\mathcal{B}_\beta\varphi_\beta = 0\,, \quad \forall \alpha\,, \tag{B.7}$$

$$\sum_{\alpha} \chi_\alpha C_{o\alpha\beta} = 0 \ , \quad \forall \beta > q \ . \tag{B.8}$$

Let us denote by r the rank of the rectangular matrix $C_{o\alpha\beta}$, with α arbitrary and $\beta > q$, which is also the rank of $\mathcal{R}$. The number of linearly independent solutions of $(B.7)$ or $(B.8)$ is $\ell - r$. On the other hand the number of non-vanishing eigenvalues of $\mathcal{R}$ is the rank $\hat{r}$ of the truncated matrix $\mathcal{B}^{1/2} C_0 \mathcal{B}^{1/2}$, also equal to $\ell - q - s$. Hence, the number m of missing eigenvectors is

$$m = (q + s) - (\ell - r) = r - \hat{r} \leq q \ . \tag{B.9}$$

Altogether, *if the stability matrix $\mathcal{B}$ of* HF *satisfies $\mathcal{B} \geq 0$, the RPA motion is stable only if (B.5) is satisfied* ; otherwise, there exist solutions $\rho(t)$ *deviating from* ρ_0 *as* t^m, with $m = r - \hat{r}$, where r is the rank of $\mathcal{R}$ and $\hat{r}$ the rank of $\mathcal{B}\mathcal{R}$.

These considerations are not academic. In particular, when some *continuous invariance is spontaneously broken* by the HF *approximation*, the minima of $\Omega(\rho)$ lie on a q-dimensional manifold, and we have $\mathcal{B} \geq 0$. Then, a HF state may be Lyapunov unstable with respect to RPA or TDHF motions, with a time-dependence in t^m. This behaviour is associated with *Goldstone modes*, or with the "*spurious states*" of the RPA, which arise for $\omega = 0$. As an example, the breaking of the translational invariance for a nucleus gives rise to solutions of the TDHF equations which describe static HF states boosted at some constant velocity. The associated RPA solutions then behave as t, and the index m given by $(B.9)$ is one.

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